Quantum Mechanics in Pennsylvania-Undergraduate Course Updated 2022-08-31
Chapter 9, Angular Momentum, 2- and 3- Dimensions. Problem 9.7.1 Position representation wave function

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Remarks, Questions and Exercises.
Based on the *Course Quantum Mechanics, Mathematical Structure and Physical Structure Part 1, 2014.*
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## Inhoudsopgave

# 1 Motivation, Page 1

"*Understanding the universe of quantum mechanics is much like an understanding of a new culture where appropriate language is mathematics and the experiences we are tempting to put in context are experiments*".
Feynman is cited. By the way, Feynman admired Dirac.
Furthermore. Boccio paid attention to the work of Dirac and denoted it the Dirac Language.
I denoted it the Dirac Algebra.

## 1.1 Basic Principles and Concepts of Quantum Theory, page 4

Two equivalent formulation of Quantum Mechanics are presented:
- Schrödinger wave mechanics
- Heisenberg matrix mechanics

Dirac developed a general formulation for quantum theory.

### 1.1.1 Mathematical Methods, page 4

Boccio presented in this section a list of techniques to be used.

### 1.1.2 Classical Concept, page 5

Boccio summarized the various classical theories which quantum theory relies on.

### 1.1.3 The Fundamental Principle of Quantum Mechanics, page 6

On page 9, Boccio presents the Basic Principle of Quantum Mechanics.

## 1.2 Simple Ideas about Probability, page 10

The principles of probability are presented.

### 1.2.1 Discrete Distribution, page 10

### 1.2.2 Continuous distribution

Remark: Bottom of page 13
The expression for $\Delta u$ should read:
$(\Delta u)^2 = \langle u^2\rangle - 2\langle (u\langle u\rangle\rangle + \langle\langle u\rangle^2\rangle = \langle u^2\rangle - 2\langle u\rangle\langle u\rangle + \langle\langle u\rangle^2\rangle =$
$= \langle u^2\rangle - 2\langle u\rangle\langle u\rangle + \langle u\rangle^2 = \langle u^2\rangle - \langle u\rangle^2$, a typo.
Bottom page 14:
"*Another trick*" to evaluate $\int_{-\infty}^{\infty} w^2\, e^{-w^2} dw$ , Eq.(1.18),is integration by parts.
So,
$\int_{-\infty}^{\infty} w^2\, e^{-w^2} dw = -\frac{1}{2} we^{-w^2}|_{-\infty}^{\infty} + \frac{1}{2}\int_{-\infty}^{\infty} e^{-w^2}\, dw = \frac{\sqrt{\pi}}{2}$ .

### 1.2.3 Review of waves and diffraction of waves, page 15

In this section the equation of plane- and spherical waves are recapitulated.

At the bottom of page 16 Boccio presented the correct and proper definition of a wave.

Note: $F' = \frac{\partial F}{\partial(\bar{x}\cdot\bar{n}-vt)}$ .

### 1.2.4 Diffraction of Waves, page 24

This section is about diffraction at an opaque screen, Fig. 1.9, page 24.

On page 26 an application of diffraction is presented, Fig. 1.10.

The interference pattern is shown in Fig. 1.12.

## 1.3 Review of Particle Dynamics, page 28

In this chapter the analysis is relativistic

### 1.3.1 Relativistic Dynamics, page 28

The kinetic energy is dealt with.

I suppose in the analysis: $m = m_0$.

Deriving Eq.1.82, use has been made of the substitution: $u = \frac{v^2}{c^2}$ .

Furthermore, the integral $\int \gamma du \frac{du}{\sqrt{1-u}}$ , should be $\int \frac{du}{\sqrt{1-u}}$ .

With Eqs.(1.77) and (1.85)→Eq.(1.86).

Eq.(1.77):

$$\gamma = \frac{1}{\sqrt{1-(\frac{v}{c})^2}} \rightarrow \gamma^2(c^2 - v^2) = c^2 \rightarrow m_0^2\gamma^2(c^2 - v^2) = m_0^2c^2,$$

and

$(\frac{E}{c})^2 - p^2 = m_0^2\gamma^2c^2 - m_0^2\gamma^2v^2 = m_0^2c^2$, Eq.(1.87).

## 1.4 Wave-Particle Duality of Light, page 30

- Wave nature→diffraction pattern.
- Particle nature→photoelectric effect.

On page 30, Fig. 1.13, an experiment representing the photoelectric effect is shown. Photoelectrons are mentioned (as Fitzpatrick did). Well, I know of photons and electrons. Photoelectrons?

### 1.4.1 Einstein's Photon Hypothesis, page 32

In Eq. (1.91), the linear relation between the maximum kinetic energy and the frequency is presented. This relation is shown in Fig. (1.15).

The double slit experiment is discussed and presented in the Figs. (1.16) and (1.17).

### 1.4.2 Wave-Particle Duality of Electrons, page 35

The particle-like properties are illustrated with the trajectory of an electron in a bubble chamber.

The wave like properties are demonstrated with the diffraction of electrons by a crystal.

The Broglie wavelength Eq.(1.97) is introduced.

Then Boccio formulated the question: *Why isn't the diffraction of macroscopic objects observed*? The answer to this question is illustrated by the experiment shown in Fig. (1.19).

# 2. Formulation of Wave Mechanics -Part I, page 39

## 2.1 Basic Theory, page 39

### 2.1.1 Postulate 1a, page 39

The wave function $\psi(\vec{x}, t)$ or probability amplitude is defined by the Eqs (2.1) and (2.2). The wave function is normalizable and continuous.
The plane wave function is not normalizable.
On page 42, the third integral in the proof is obtained by representing the complex numbers and functions in a real and an imaginary part.

### 2.1.2 Postulate 1b, page 43

Just above the definition on page 43, use has been made of the results in the foregoing section: $|u_1^* u_2| \leq \frac{1}{2}[|u_1^2| + |u_2^2|$.
On page 43 Boccio introduced the Properties of the Inner Product and the properties to be obvious by inspection.
Well, Dirac: page 21 "*We assume that these two numbers are always equal*".
Now by inspection the first property.
$\langle\phi_1|\phi_2\rangle^* = \langle\phi_2|\phi_1\rangle$?
*Proof*
Assume $\langle\phi_1|\phi_2\rangle^* = \langle\phi_2|\phi_1\rangle$, to be correct. The complex conjugate of this expression is:
$\langle\phi_1|\phi_2\rangle^{**} = \langle\phi_2|\phi_1\rangle^* \rightarrow \langle\phi_1|\phi_2\rangle = \langle\phi_2|\phi_1\rangle^* \rightarrow \langle\phi_1|\phi_2\rangle^* = \langle\phi_1|\phi_2\rangle^{**} \rightarrow$
$\rightarrow \langle\phi_1|\phi_2\rangle^* = \langle\phi_2|\phi_1\rangle$.
*End of Proof*
The second property:
$\langle\phi_1|(\lambda_2\phi_2 + \lambda_3\phi_3)\rangle = \langle\phi_1|\lambda_2\phi_2\rangle + \langle\phi_1|\lambda_3\phi_3\rangle$ .
I assume $\lambda_2$ and $\lambda_3$ to be complex numbers.
Susskind mentioned this to be the axiom of linearity. Obvious by inspection? I do not know.
Furthermore for the second property, denoted by me property 2a:
$\langle\phi_1|(\lambda_2\phi_2 + \lambda_3\phi_3)\rangle = \langle\phi_1|\lambda_2\phi_2\rangle + \langle\phi_1|\lambda_3\phi_3\rangle = \lambda_2\langle\phi_1|\phi_2\rangle + \lambda_3\langle\phi_1|\phi_3\rangle$.
In Eq. (2.8) it is shown by the integral representation of the inner product that the complex numbers $\lambda_2$ and $\lambda_3$ can be written of $\langle\phi_1|\phi_2\rangle$ and $\langle\phi_1|\phi_3\rangle$.
For the second property there is another one denoted 2b. Take the complex conjugate and use property 1 and property 2a(linearity):
$\langle(\lambda_2\phi_2 + \lambda_3\phi_3)|\phi_1\rangle^* = \langle\phi_1|\lambda_2\phi_2\rangle + \langle\phi_1|\lambda_3\phi_3\rangle = \lambda_2\langle\phi_1|\phi_2\rangle + \lambda_3\langle\phi_1|\phi_3\rangle$.
Take the complex conjugate of the latter expression and use property 1:
$\langle(\lambda_2\phi_2 + \lambda_3\phi_3)|\phi_1\rangle = {\lambda_2}^*\langle\phi_2|\phi_1\rangle + {\lambda_3}^*\langle\phi_3|\phi_1\rangle$.
The third property:
$\langle\phi|\phi\rangle$ is real, with $\langle\phi|\phi\rangle \geq 0$.
With the first property: $\langle\phi|\phi\rangle = \langle\phi|\phi\rangle^*$. Suppose $\langle\phi|\phi\rangle$ is a complex number. $\langle\phi|\phi\rangle^*$ is the complex conjugate. When a complex number equals its complex conjugate, the imaginary part of that complex number must be zero. So, $\langle\phi|\phi\rangle$ is a real number.
*Proof*:
Represent $\langle\phi|\phi\rangle$ by $a + ib$, where $\{a, b \in \mathbb{R}\}$.
Then,

$a + ib = (a + ib)^* = a - ib \rightarrow b = 0.$

*End of Proof.*

***Note****: Dirac page 21.*

On page 44 Boccio proved Schwarz In equality.

### 2.1.3 Fourier Series and Transforms and Dirac Delta Function, page 47

Fourier Series.

The theory of Fourier transforms is presented. An example of a Gaussian function is given on page 50.

The Dirac delta function, a generalized function.

The properties of the Dirac delta function are presented. The integral representation of the delta function is given.

In section 15 of his book, pages 58-61, Dirac presented the $\delta$ function.

Chisholm and Morris analysed the Dirac $\delta$-function, Fourier Series, and Integrals in Chapter 18.

### 2.1.4 Postulate 2, page 59

Motivation.

Postulate 2.

In postulate 2, Boccio writes: "*…the position and momentum distribution are related!!!".*

Eq.(2.96), the momentum operator is defined.

Then, the operator for the non-relativistic kinetic energy is derived.

Boccio: "*Operators will play a fundamental role in our development of quantum theory."*

### 2.1.5 Operator Formalism, page 64

Keep in mind: an operator always operate on something. This is not trivial as illustrated in the example Eq. (2.105). This is also illustrated with the commutator of the position and the momentum operator, Eq.(2.107).

In this section, Boccio presented a couple of examples of commutators:

$[x_j, x_i] = 0$ ,→ position operators are independent. Consequently $x_j = x_i$.

Furthermore, the definition of linear operators to be Hermitian is given.

### 2.1.6 Heisenberg's Uncertainty Principle, page 66

To derive Heisenberg's Uncertainty Principal, Fourier transforms are used.

First Boccio started with an Heuristic argument.

On page 67, Boccio explained the difference between the classical and the quantum mechanical case with the Heisenberg Uncertainty principal.

Deriving (2.125), with for example the operator $\hat{D}$ to be Hermitian:

$\langle\psi|\hat{D}\hat{D}\psi\rangle = \langle\hat{D}^{\dagger}\psi|\hat{D}\psi\rangle = \langle\hat{D}\psi|\hat{D}\psi\rangle.$

**Remark.**

I do not understand Boccio did not introduce the dagger, † .

The Hermitian conjugate of a matrix $A = (A^T)^* = A^{\dagger}$.

A square matrix $A$ is Hermitian if it is its own Hermitian conjugate $(A^T)^*$ , (Chisholm and Morris, page 456, and Susskind, page 61).

### 2.1.7 Postulate 3a, page 78

For every physical quantity there exist a linear operator.
The comments on the postulate are interesting insofar operators are used which do not commute. So, e.g., position and momentum cannot be measured simultaneously.
Boccio explained how to construct a Hermitian operator out of two non-commuting operators: Eq. (2.182).

### 2.1.8 Postulate 3b, page 80

Boccio presented a physical quantity to be a function of position and momentum. The operator depends on the ordering of position and momentum. This ambiguity is partially removed by requiring the operator to be Hermitian.
Boccio: "*Only experiment can determine which ordering of non-commuting factors yield the Hermitian operator that corresponds to a physical quantity, depending on position and momentum, measured in a specific way.*"
Two examples are presented:
- Energy of a particle in a conservative force field→no ambiguity in ordering of factors.
- Angular momentum of a particle→no ambiguity in ordering of factors.

Some general rules for commutators are given.

### 2.1.9 Important Questions, page 82

The first question is about the eigenvalue of an operator.
At the top of page 84 Boccio introduced the theorem: The eigenvalue of a Hermitian operator is real.
Proving this theorem, Boccio used eigenvalues $\lambda$ and $a$. I do not see why.
Let's look at the proof in a slightly different way, with operator $A$, wave function $\psi_0$ and eigenvalue $\lambda$:

$$A|\psi_0\rangle = \lambda|\psi_0\rangle. \qquad \text{(C.2.1.9.1)}$$

The Hermitian conjugate:

$$\langle\psi_0|A^\dagger = \langle\psi_0|\lambda^*. \qquad \text{(C.2.1.9.2)}$$

Since $A$ is Hermitian, (C.1.2.9.2) can be written as

$$\langle\psi_0|A = \langle\psi_0|\lambda^*. \qquad \text{(C.1.2.9.3)}$$

Multiply (C.2.1.9.1) with $\langle\psi_0|$, and (C.1.2.9.3) with $|\psi_0\rangle$. The result is:

$$\langle\psi_0|A|\psi_0\rangle = \lambda\langle\psi_0|\psi_0\rangle,$$

and

$$\langle\psi_0|A|\psi_0\rangle = \lambda^*\langle\psi_0|\psi_0\rangle.$$

For both expression to be true: $\lambda^* = \lambda$.

### 2.1.10 The Time-Independent Schrödinger Equation, page 84

As an operator we have the Hamiltonian.
Boccio postponed the solution of Eq. (2.204) and considered first the eigenvalue equations for linear momentum, position, and angular momentum.

### 2.1.11 Some Operator Eigenvalue/Eigenfunction Equations, page 84

**Linear Momentum**

The eigenvalue equation, a first order differential equation and the solution are given, Eqs. (2.207) and (2.208).

Conclusion: there are no physical solutions to the eigenvalue equations for $p_x$.
Measurements of linear momentum performed on identical prepared particles will always yield a spread result.

**Position**

The eigenvalue equation, Eq.(2.211) and the solution, a $\delta$-function are given (see also Susskind, Lecture 8.2.1).
There are no physical solutions to the eigenvalue equations for position.
Measurements of position performed on identical prepared particles will always yield a spread result.

Angular Momentum

The eigenvalue equation in Cartesian coordinates: Eq.(2.215).
Boccio switched to spherical polar coordinates.
The eigenvalue equation and solution are given in Eqs.(2.219) and (2.220).
In Eq.(2.219): $a$ is the complex eigenvalue.

**Important Observations**

From the singlevaluedness assumption follows the eigenvalue: $a = l\hbar$ , with $l = 0, \pm 1, \pm 2, ..$
There are physical solutions for the wave function for a measurement of $L_z$, the angular momentum operator. The measurement results in the eigenvalue $a = l\hbar$, with certainty.
**Notes** On angular momentum, page 89. (See also Fitzpatrick, *Undergraduate Course*, Chapter 8).
Boccio made observations on the probability of finding a particle in a certain region of space, using the eigenfunction of $L_z$.
Given $\langle L_z \rangle = l\hbar$ , $\langle L_x \rangle = \langle L_y \rangle = 0$ is derived.
Next the case is analysed where the wavefunction is not an eigenfunction of the operator $A$ with eigenvalue $a$. The results of this analysis are a couple of difficulties which will be ignored.
**Notes** On linear operators.
At the top of page 91, Boccio introduced the dagger †.
Boccio writes: *"Thus: if $A$ is a linear operator, their exists an operator $A^\dagger$called the adjoint operator of $A$ such that*
$\langle \phi_1 | A\phi_2 \rangle = \langle A^+ \phi_1 | \phi_2 \rangle, Eq. (2.231)."$

*The adjoint operator is presented by Dirac on page 26 and 27, Section 8 Conjugate relations. On page 27 Dirac concludes: Thus the adjoint of the adjoint of a linear operator is the original linear operator.*

In the notes, Boccio explained the relation between $A^\dagger$and $A^+$?
In note 1, $A$ is treated to be Hermitian. The proof of note 4 can be found on page 27 of Dirac.
May we also conclude $A^\dagger = A^+$?
On page 96, degeneracy is defined.

## 2.2 Energy Measurements, page 102

The eigenvalue equation for energy is the time-independent Schrödinger equation.
Normalizable solution of the Schrödinger equation are called bound states.

As an example, Boccio analysed a particle in a rigid box, with the potential → ∞, at the boundaries of the box.

**General discussion on boundary conditions.**

Boccio analysed the examples of

- the potential $V(x)$ to be continuous,
- $V(x)$ an infinite jump(square well and $\delta$-function potentials).

**One-dimensional Infinite Square Well.**

The one-dimensional Schrödinger equation is solved for the given boundary conditions.
The energy eigenvalues are derived, Eq.(2.308).
Each eigenvalue is non-degenerate. The energy levels are quantized. The ground state $\neq 0$ .
The energy levels for a macroscopic object, an electron confined to an atomic distance and a proton confined to a nuclear distance are given: Eqs. (2.313) -(2.315).
Then, the orthogonality of the eigenfunctions is checked.
On page 113, Eq.(2.328) for $x \in [0, l]$ should read $x \in [0, L]$, I suppose.
On page 115, another example is analysed: A positive potential barrier of height $\frac{1}{\sqrt{L}}$ and width $L$. The wave function $\psi_0(x) \neq 0$ within the barrier.
Question: Is it a barrier?
On the next pages, Boccio discussed the spectra, discrete and continuous, of all eigenvalues of an operator $A$.
At the bottom of page 120 a Basic Problem is introduced. It is about what values can be obtained from the measurement and with what probability.

## 2.3 Collapse

*The question: How to prepare a particle so that the wave function at $t_0$ is completely determined?*
Based on experimental result, Boccio explained how to make subsequent measurements to replicate a measurement.

### 2.3.1 Postulate 4: Collapse of the Wave Function

The postulate is based upon a set of discrete and continues eigenfunctions.
The first part of the postulate: the measurement of the observable $A$ yields the value $a_n$,then the wave function collapses to the discrete part of the wave function. The second part of the postulate is about the continuous part of the wave function.
*The collapse of the wave function has a simple geometric interpretation*, Illustrated on page 126. Two cases are presented: 1) All non-degenerate eigenvalues and 2) Some degenerate eigenvalues. The same geometrical approach cannot be used for the continuum eigenfunctions.
Next, Boccio elaborate on measurements using a discrete spectrum and explained *to be careful in choosing which subsequent measurements to make,* bottom of page 127.
Then, on page 128, Boccio explained that for subsequent measurements where the observables to be compatible, operators-commute, there will be no problem.

# 3 Formulation of Wave Mechanics – Part 2

## 3.1 Complete Orthonormal Sets

In this section, Boccio starts with the proof: $[A, B] = 0$, implies $A$ and $B$ are compatible.
At the bottom of page 139, summarizes the result about compatible observables:
*compatibility is equivalent to commutativity.*
This section is concluded with an example of a free particle in Three Dimensions. The Hamiltonian is presented in Eq.(3.26), where to methods are used to find the eigenvalues and eigenfunctions.

## 3.2 Time development

To find the probability distribution at a particular time, the time-development of the wave function between measurements must be specified.

### 3.2.1 Mathematical Preliminaries

Some proofs about operators are discussed.
Next the time development of the wave function is considered.
In Eq. (3.83), the time dependent Schrödinger equation is presented and the Hamiltonian operator, Eq. (3.88).

### 3.2.2 Postulate 5: Time Development of the Wave Function

Here, the time dependent Schrödinger equation is presented without the function $c(t)$.
*"From this equation, one can determine the wave function $\psi(\vec{x}, t)$ at time $t$ by knowing $\psi(\vec{x}, t_0)$, the wave function at some initial time $t_0$."*

## 3.3 Structure of Quantum Theory

### 3.3.1 Initial preparation of the Wave Function at $t_0$

Here, Boccio presented the steps to be taken to measure a complete set of compatible observables at $t_0$ to determine $\psi(\vec{x}, t_0)$.
The conceptual difference between the time-dependent Schrödinger equation,
$H\psi = i\hbar \frac{\partial\psi}{\partial t}$,
and the time-independent Schrödinger equation,
$H\psi = E\psi$,
is presented.

### 3.3.2 Basic Problem of Quantum Mechanics

By plugging a general expression of the wave function into the time dependent Schrödinger equation, a solution is presented for the wave function: *it represents the general result for* ***expansion of an arbitrary wave function in terms of energy eigenfunctions.***
The general solution is presented in Eq.(3.106).
Important conclusion: The particle therefore remains in the same eigenfunction of energy for all $t$ if it is initially in an eigenfunction of energy.
This section is concluded with an example of a Non-Stationary State.

## 3.4 Free Particle in One Dimension (motion along the x-axis).

The Hamiltonian is presented in Eq. (3.123). Momentum is used to denote the eigenvalues.
The wave function is presented in Eq. (3.135) and is denoted a wave packet.
The difference between group velocity and phase velocity is explained.

### 3.4.1 The Method of Stationary Phase.

The wave function is presented in Eq. (3.143).
The maximum value of the wave function is found where the integrand's phase is stationary.
The next estimate of time and position where the wave function is appreciable is estimated.

### 3.4.2 Application to a Free-Particle Wave Packet

The velocity of the peak of the wave packet is determined: Eq. (3.152).

## 3.5 Constants of the Motion

Boccio started with the time dependent Schrödinger equation: Eq. (3.154).
The Hermitian operator $A$ is assumed to be time independent. This is defined in Eq. (3.158):
$\frac{d}{dt}\langle A\rangle = 0$ .
Boccio showed a couple of examples.

## 3.6 Harmonic Oscillator in One Dimension

The Hamiltonian is given by Eq. (3.168).

The classical result is presented.
Boccio showed the quantum mechanical of $\langle x\rangle$ follows the classical trajectory.
Then Boccio looked for the eigenfunctions and eigenvalues.
Two methods are used:
- Differential equation method
- Operator algebra method.

### 3.6.1 Differential Equation Method

The time independent Schrödinger equation: Eq. (3.176).
The result of this analyses is presented by the Eqs. (3.206) - (3.210).
A similar analyses is given by Fitzpatrick and Mahan.

### 3.6.2 Algebraic Method

The Hamiltonian is given in Eq. (3.221).
The concept of raising and lowering operators are presented by Eqs. (3.225) and (3.226), bottom of page 177. See also Dirac and Susskind.

### 3.6.3 Use of Raising and Lowering Operators

The position operator and the momentum operator are expressed in the raising and lowering operator: Eq. (3.272).
Expectation values can be obtained by using the operators without evaluating integrals. See, e.g., Eq.(3.276), the harmonic oscillator:
$\langle x^2\rangle = \frac{\hbar}{m\omega}(N+\frac{1}{2})$.
Furthermore,

$E_N = \hbar\omega(N + \frac{1}{2})$, Eq.(3.277).

With this expression for $E_N$ the time-dependent part of the wave function in Eq.(3.2.82) is obtained.

## 3.7 General Potential Functions

The Hamiltonian is presented in Eq. (3.300).

The time dependent wave function is presented in Eq. (3.302).

A general potential function is presented in Fig.3.11.

### 3.7.1 Methods for Solving this Eigenvalue Equation

Boccio discussed the solution for this general potential and referred to Chapter 2.

Furthermore, several general potential functions are analysed.

The step function potential Fig.3.18, is used to illustrate a piecewise constant potential energy.

### 3.7.2 Symmetrical Potential Well Finite depth)

The case is illustrated in Fig. (3.21). with the Hamiltonian the parity operator $\Pi$ is used: $\Pi f(x) = f(-x)$. This parity operator commutes with the Hamiltonian. Boccio proved the commutation on page 203.

## 3.8 General One-Dimensional Motion

The potential is given in Fig. (3.24).

Incident, reflected, and transmitted waves, eigenfunctions, are analysed.

### 3.8.1 Physical Significance of form of $\psi(x,t)$

It is about wave packet evolution: incident, reflected and transmitted.

On page 218, the results for incident, reflected and transmitted waves are summarized.

### 3.8.2 General Comments

As the title indicates, comments are summarized comparing the classical case and the quantum mechanical case.

## 3.9 The Symmetrical Finite Potential Well

The potential energy function is presented in Fig.3.33.

The various coefficients of the reflected and transmitted wave functions are expressed in the amplitude of the incoming wave $A$.

In Fig.3.34, the transmission coefficient is shown.

## 3.10 The Complex Energy Plane.

The potential energy is presented in Eq. (3.453).

## 3.11. Problems Boccio(1)

### 3.11.1 Free Particle in One-Dimension-Wave Functions

Consider a free particle in one-dimension. Let

$\psi(x,0) = Ne^{-\frac{(x-x_0)^2}{4\sigma^2}} e^{i\frac{p_0 x}{\hbar}}$ ,

where $x, p_0$ and $\sigma$ are real constants and $N$ is a normalisation constant.

a) Find $\tilde{\psi}(p,0)$.

Looking at the solutions, it appears to me Boccio used:

$\psi(x,0) = Ne^{-\frac{(x-x_0)^2}{4\sigma^2}} e^{-i\frac{p_0 x}{\hbar}}$ .

Does it matter?

So, the Fourier Transform from the position into the momentum representation is:

$\tilde{\psi}(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{i\frac{px}{\hbar}} \psi(x,0)dx.$

Plug $\psi(x,0)$ in this expression$\Longrightarrow \tilde{\psi}(p,0) = \frac{N}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{i\frac{(p-p_0)x}{\hbar}} e^{-\frac{(x-x_0)^2}{4\sigma^2}} dx.$

I do not present the evaluation of the integral in detail. Basically, it is about using:

$\int_{-\infty}^{\infty} e^{-y^2} dy$. So, the integrand $e^{i\frac{(p-p_0)x}{\hbar}} e^{-\frac{(x-x_0)^2}{4\sigma^2}}$ has to be rewritten:

$-\frac{(x-x_0)^2}{4\sigma^2} - i\frac{(p-p_0)x}{\hbar} = -\left[\frac{x^2}{4\sigma^2} - \left(\frac{x_0}{2\sigma^2} - i\frac{(p-p_0)}{\hbar}\right)x + \frac{{x_0}^2}{4\sigma^2}\right]$.

This finally results into

$\tilde{\psi}(p,0) = \frac{N\sigma\sqrt{2}}{\sqrt{\hbar}} e^{-\left(\frac{p-p_0}{\hbar}\sigma\right)^2} e^{-i\frac{(p-p_0)x_0}{\hbar}}.$

b) Find $\tilde{\psi}(p,t)$.

So, it is about the time dependent Schrödinger equation in momentum representation.

$i\hbar\frac{\partial\tilde{\psi}(p,t)}{\partial t} = H\tilde{\psi}(p,t) = E_p\tilde{\psi}(p,t) = \frac{p^2}{2m}\tilde{\psi}(p,t).$

Then, this differential equation can be solved with the initial condition at $t = 0$:

$\tilde{\psi}(p,t) = \tilde{\psi}(p,0)e^{-\frac{iE_p t}{\hbar}} = \tilde{\psi}(p,0)e^{-\frac{ip^2 t}{2m\hbar}}$, with $\tilde{\psi}(p,0)$ derived in a).

c) Find $\psi(x,t)$.

Again, Fourier Transformation is used.

Now, look under a). There Boccio used Fourier Transformation with $e^{i\frac{px}{\hbar}}$ in the integrand. Again, in this part of the exercise, Boccio used $e^{i\frac{px}{\hbar}}$ in the integrand instead of $e^{-i\frac{px}{\hbar}}$ here or in a). Looking into the details of the answers produced by Boccio, it appears to me that $e^{-i\frac{px}{\hbar}}$ is used.

I do not present the evaluation of the integral in detail. Basically, it is again about using:

$\int_{-\infty}^{\infty} e^{-y^2} dy.$

Then, $\psi(x,t)$ is obtained:

$$\psi(x,t) = N\sigma e^{\frac{ip_0 x_0}{\hbar}} e^{\left(\frac{p_0\sigma}{\hbar}\right)^2} \frac{1}{\sqrt{\sigma^2 + i\frac{t\hbar}{2m}}} e^{-\frac{\left(x - x_0 - \frac{2ip_0\sigma^2}{\hbar}\right)^2}{4\left(\sigma^2 + i\frac{t\hbar}{2m}\right)}}.$$

Keep in mind:

$\frac{1}{\sqrt{\sigma^2 + i\frac{t\hbar}{2m}}} = \frac{e^{-i\alpha/2}}{\left[\sigma^4 + \left(\frac{t\hbar}{2m}\right)^2\right]^{\frac{1}{4}}}$ , where $\alpha = \tan^{-1}\left(\frac{t\hbar}{2m\sigma^2}\right)$ represents a phase shift being of no importance for the probability density.

Similarly, the exponent, $\frac{(x - x_0 - 2ip_0\sigma^2/\hbar)^2}{4(\sigma^2 + i\frac{t\hbar}{2m})}$, can be rewritten as a real and imaginary part. Only the real part contributes to the probability density.

d) Show that the spread in the spatial probability distribution increases with time.

We need to analyse $|\psi(x,t)|^2$. I will present the time dependent components of the probability distribution.

In the factor in front of the exponential, time dependency is found in:

$\frac{1}{[\sigma^4 + \left(\frac{t\hbar}{2m}\right)^2]^{1/2}} \Rightarrow$ the amplitude decreases with time.

In the exponent of the wave function, $e^{-\frac{\left(x-x_0-\frac{2ip_0\sigma^2}{\hbar}\right)^2}{4\left(\sigma^2+i\frac{t\hbar}{2m}\right)}}$, for the time dependent factor in the probability distribution, I left out constant real factors in the exponent, the factor $\frac{p_0\sigma^2(x-x_0)t/m}{\sigma^4+\left(\frac{t\hbar}{2m}\right)^2}$, shows the spreading of the probability.

### 3.11.2 Free Particle in One-Dimension - Expectation Values and Commutators

For a free particle in one-dimension with Hamiltonian: $H=\frac{p^2}{2m}$,

a) Show $\langle p_x\rangle=\langle p_x\rangle_{t=0}$.

Well, suppose the assumption to be correct $\langle p_x\rangle=\langle p_x\rangle_{t=0}$, then:

$\frac{d}{dt}\langle p_x\rangle=0$, a free particle.

With Eqs.(3.74) and (3.88):

$\frac{d}{dt}\langle p_x\rangle=\frac{1}{i\hbar}\langle|[p_x,H]|\rangle=0\Rightarrow\langle p_x\rangle_t$ is a constant$\Rightarrow\langle p_x\rangle=\langle p_x\rangle_{t=0}$.

This is also denominated Ehrenfest's Theorem (actually Heisenberg), in general (the proof is textbook material):

$\frac{d}{dt}\langle A\rangle=\frac{1}{i\hbar}\langle|[A,H]|\rangle+\langle\frac{\partial A}{\partial t}\rangle$.

So,

$\frac{d}{dt}\langle p_x\rangle=\frac{1}{i\hbar}\langle|[p_x,H]|\rangle$, since $\langle\frac{\partial p_x}{\partial t}\rangle=0$.

Furthermore, $[p_x^2,H]=0\Rightarrow[p_x,H]=0$.

b) Show $\langle x\rangle=\left[\frac{\langle p_x\rangle_{t=0}}{m}\right]\cdot x+\langle x\rangle_{t=0}$.

$\frac{d}{dt}\langle x\rangle=\frac{1}{i\hbar}\langle|[x,H]|\rangle=\frac{1}{2i\hbar m}\langle|[x,p_x^2]|\rangle=\frac{1}{2i\hbar m}\langle|xp_x^2-p_xxp_x+p_xxp_x-p_x^2x|\rangle=$

$=\frac{1}{2i\hbar m}\langle|[x,p_x]p_x+p_x[x,p_x]|\rangle=\frac{1}{m}\langle|p_x|\rangle$.

Then with a):

$\frac{d}{dt}\langle x\rangle=\frac{1}{m}\langle p_x\rangle_{t=0}$.

Integrating this expression:

$\langle x\rangle_t=\frac{1}{m}\langle p_x\rangle_{t=0}\cdot t+\langle x\rangle_{t=0}$.

c) Show $(\Delta p_x)^2=(\Delta p_x)^2_{t=0}$.

Using Ehrenfest's theorem:

$\frac{d}{dt}\langle p_x^2\rangle=\frac{1}{i\hbar}\langle|[p_x^2,H]|\rangle=0$. $H$ commutes with itself.

Then, by definition:

$(\Delta p_x)_t^2=\langle(p_x-\langle p_x\rangle)_t^2\rangle=\langle {p_x}^2\rangle_t-2\langle p_x\langle p_x\rangle\rangle_t+\langle p_x\rangle_t^2=\langle {p_x}^2\rangle_t-\langle p_x\rangle_t^2$.

We know already: $\langle {p_x}^2\rangle_t-\langle p_x\rangle_t^2=\langle {p_x}^2\rangle_0-\langle p_x\rangle_0^2$.

So,

$(\Delta p_x)^2=(\Delta p_x)^2_{t=0}$.

d) Find $(\Delta x)^2$ as a function of time and initial conditions.

Here Boccio gave some hints: Find $\frac{d}{dt}\langle x^2\rangle$. Furthermore, to solve the resulting differential equation, one needs to know the time dependence of $\langle xp_x+p_xx\rangle$. Why? To get rid of Quadratic expressions? This operator is shows us something: $[xp_x+(xp_x)^\dagger]=$

$[xp_x + (p_x)^\dagger (x)^\dagger] = [xp_x + p_x x]$ ⇒the operator is Hermitian. $x$ and $p_x$ are Hermitian.
Definition:
$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2$ (Note: in the answers you will find a + sign, a typo).
To find out about the time dependency, we start with $\frac{d}{dt}\langle x^2\rangle - \frac{d}{dt}\langle x\rangle^2 = \frac{d}{dt}(\Delta x)^2$.
With Ehrenfest's theorem:
$\frac{d}{dt}\langle x^2\rangle = \frac{1}{i\hbar}\langle [x^2, H]\rangle = \frac{1}{2im\hbar}\langle [x^2, p_x^2]\rangle$.
Now, use $[x, p_x] = i\hbar$, in $\langle [x^2, p_x^2]\rangle$. Furthermore, b), $[x, p_x^2] = [x, p_x]p_x + p_x[x, p_x] = 2i\hbar p_x$.
Then,
$[x^2, p_x] = x[x, p_x] + [x, p_x]x = 2i\hbar x$.
In this way, I obtain for $[x^2, p_x^2]$:
$[x^2, p_x^2] = [x^2, p_x]p_x + p_x[x^2, p_x] = x[x, p_x]p_x + [x, p_x]xp_x + p_x x[x, p_x] + p_x[x, p_x]x =$
$= 2i\hbar(xp_x + p_x x)$.
So, Ehrenfest's Theorem,
$\frac{d}{dt}\langle x^2\rangle = \frac{1}{2im\hbar}\langle [x^2, p_x^2]\rangle = \frac{1}{m}\langle xp_x + p_x x\rangle$.
A bit shorter than presented by Boccio. More elegant?
Now we have to consider:
$\frac{d}{dt}\langle xp_x + p_x x\rangle = \frac{1}{i\hbar}\langle [(xp_x + p_x x), H]\rangle = \frac{1}{2im\hbar}\langle [p_x x, p_x^2] + [xp_x, p_x^2]\rangle =$
$= \frac{1}{2im\hbar}\langle xp_x^3 - p_x xp_x^2 + p_x xp_x^2 - p_x^3 x + p_x xp_x^2 - p_x^2 xp_x\rangle =$
$= \frac{1}{2im\hbar}\langle (xp_x - p_x x)p_x^2 + p_x(xp_x^2 - p_x^2 x) + p_x(xp_x - p_x x)p_x\rangle =$
$\frac{1}{2im\hbar}\langle i\hbar p_x^2 + p_x 2i\hbar p_x + + p_x i\hbar p_x\rangle = \frac{2}{m}\langle p_x^2\rangle$,
where use has been made of $[x, p_x^2] = [x, p_x]p_x + p_x[x, p_x]$, see above.
Hence,
$\frac{d}{dt}\langle xp_x + p_x x\rangle = \frac{2}{m}\langle p_x^2\rangle$ .
Then,
$\langle xp_x + p_x x\rangle_t = \frac{2}{m}\langle p_x^2\rangle \cdot t + \langle xp_x + p_x x\rangle_{t=0}$
In c) we obtained:
$\langle p_x^2\rangle_t = \langle p_x^2\rangle_0$ .
The ingredients are available.
$\frac{d}{dt}(\Delta x)^2 = \frac{d}{dt}\langle x^2\rangle - \frac{d}{dt}\langle x\rangle^2 = \frac{2}{m^2}\langle p_x^2\rangle_0 \cdot t + \frac{1}{m}\langle xp_x + p_x x\rangle_0 - \frac{d}{dt}\left(\frac{1}{m}\langle p_x\rangle_0 \cdot t + \langle x\rangle_0\right)^2 =$
$= \frac{2}{m^2}\langle p_x^2\rangle_0 \cdot t + \frac{1}{m}\langle xp_x + p_x x\rangle_0 - 2\left(\frac{1}{m^2}\langle p_x\rangle_0{}^2 \cdot t + \frac{1}{m}\langle p_x\rangle_0\langle x\rangle_0\right) =$
$= \frac{2}{m^2}(\Delta p_x)_0^2 + \frac{1}{m}\langle xp_x + p_x x\rangle_0 - \frac{2}{m}\langle p_x\rangle_0\langle x\rangle_0$.
Note: Boccio left out $\frac{2}{m^2}(\Delta p_x)_0^2$. I do not see why.
**Remark**: $\frac{d}{dt}\langle xp_x + p_x x\rangle$ can be dealt with in a slightly different way., using the commutator.
Then, $\frac{d}{dt}\langle xp_x + p_x x\rangle = \frac{d}{dt}\langle [x, p_x]\rangle + 2\frac{d}{dt}\langle p_x x\rangle = 2\frac{d}{dt}\langle p_x x\rangle = \frac{1}{im\hbar}\langle [p_x x, p_x^2]\rangle =$
$= \frac{1}{im\hbar}\langle [p_x x, p_x]p_x + p_x[p_x x, p_x]\rangle = \frac{1}{im\hbar}\langle p_x xp_x^2 - p_x^3 x\rangle = \frac{1}{im\hbar}\langle p_x(xp_x^2 - p_x^2 x)\rangle =$
$= \frac{1}{im\hbar}\langle 2i\hbar p_x^2\rangle = \frac{2}{m}\langle p_x^2\rangle$,

where use has been made of the result derived above: $[x, p_x^2] = [x, p_x]p_x + p_x[x, p_x] = 2i\hbar p_x$. This approach is a bit more efficient.

### 3.11.3 Time Dependence

Given

$H\psi = i\hbar\frac{\partial\psi}{\partial t}$,

with

$H = \frac{\vec{p}\cdot\vec{p}}{2m} + V(\vec{x})$.

a) Show that $\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle = 0$.

Using the continuous representation:

$\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle = \frac{d}{dt}\int\psi(t)^*\ \psi(t)dx = \int\frac{d\psi(t)^*}{dt}\psi(t)dx + \int\psi(t)^*\frac{d\psi(t)}{dt}dx.$

Use the time dependent Schrödinger equation and the Hamiltonian to be Hermitian:

$\int\frac{d\psi(t)^*}{dt}\psi(t)dx + \int\psi(t)^*\frac{d\psi(t)}{dt}dx = -\frac{1}{i\hbar}[\int(H\psi)^*\psi dx - \int\psi^*H\psi dx] =$

$= -\frac{1}{i\hbar}[\int\psi^*H\psi dx - \int\psi^*H\psi dx] = 0.$

Note: when $|\psi\rangle$ is normalizable $\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle$ is always zero?!

b) Show $\frac{d}{dt}\langle x\rangle = \langle\frac{p_x}{m}\rangle$.

This problem has already be dealt with in 3.11.2:

With Ehrenfest's theorem and $[x, p_x^2] = [x, p_x]p_x + p_x[x, p_x] = 2i\hbar p_x \Longrightarrow \frac{d}{dt}\langle x\rangle = \langle\frac{p_x}{m}\rangle$.

c) Show $\frac{d}{dt}\langle p_x\rangle = \langle-\frac{\partial V}{\partial x}\rangle$.

With Ehrenfest's Theorem:

$\frac{d}{dt}\langle p_x\rangle = \frac{1}{i\hbar}\langle[p_x, H]\rangle = \frac{1}{i\hbar}\langle[p_x, V(x)]\rangle$ ,

since $[p_x, p_x^2] = 0$.

Furthermore, we may suppose $V(x)$ can be written as a polynomial:

$V(x) = \sum_n V_n x^n$.

So, $\frac{1}{i\hbar}\langle[p_x, V(x)]\rangle = \frac{1}{i\hbar}\sum_n V_n\langle[p_x, x^n]\rangle$ .

Now use $[p_x, x^n] = p_x x^n - x^n p_x = -i\hbar\frac{d}{dx}x^n - x^n\left(-i\hbar\frac{d}{dx}\right) = -i\hbar x^{n-1} - x^n\left(i\hbar\frac{d}{dx}\right) +$
$+x^n\left(i\hbar\frac{d}{dx}\right) = -i\hbar x^{n-1}$.

Then,

$\frac{1}{i\hbar}\sum_n V_n\langle[p_x, x^n]\rangle = -\langle\sum_n V_n n x^{n-1}\rangle = \langle-\frac{\partial V}{\partial x}\rangle \Rightarrow \frac{d}{dt}\langle p_x\rangle = \langle-\frac{\partial V}{\partial x}\rangle$.

d) Find $\frac{d}{dt}\langle H\rangle$.

With the theorem: $\frac{d}{dt}\langle H\rangle = \frac{1}{i\hbar}\langle[H, H]\rangle = 0$,

The Hamiltonian commute with itself.

e) Find $\frac{d}{dt}\langle L_z\rangle$ .

The time derivative of the $z$-componet of the orbital angular momentum operator $L_z$:

$L_z = xp_y - yp_x$.

With the Ehrenfest's Theorem:

$\frac{d}{dt}\langle L_z\rangle = \frac{1}{i\hbar}\langle[xp_y - yp_x, H]\rangle = \frac{1}{i\hbar}\langle[xp_y - yp_x, (\frac{p^2}{2m} + V(\vec{x}))]\rangle =$
$\frac{1}{i\hbar}\{\langle\left[xp_y, \frac{p^2}{2m}\right]\rangle - \langle\left[yp_x, \frac{p^2}{2m}\right]\rangle + \langle\left[xp_y, V(\vec{x})\right]\rangle - \langle[yp_x, V(\vec{x})]\rangle\}.$
With $p^2 = p_x^2 + p_y^2 + p_z^2$, we find for $\langle\left[xp_y, \frac{p^2}{2m}\right]\rangle - \langle\left[yp_x, \frac{p^2}{2m}\right]\rangle = \langle\left[xp_y, \frac{p_x^2}{2m}\right]\rangle - \langle\left[yp_x, \frac{p_y^2}{2m}\right]\rangle.$
Then,
$\langle[xp_y, V(\vec{x})]\rangle = \langle xp_y V(\vec{x}) - V(\vec{x})xp_y\rangle = \langle xp_y V(\vec{x}) - xV(\vec{x})p_y\rangle = \langle x[p_y, V(\vec{x})]\rangle$ .
Simarlily,
$\langle[yp_x, V(\vec{x})]\rangle = \langle yp_x V(\vec{x}) - V(\vec{x})yp_x\rangle = \langle yp_x V(\vec{x}) - yV(\vec{x})p_x\rangle = \langle y[p_x, V(\vec{x})]\rangle.$
Putting the ingredients together:
$\frac{d}{dt}\langle L_z\rangle = \frac{1}{2i\hbar m}\{\langle\left[xp_y, p_x^2\right]\rangle - \langle\left[yp_x, p_y^2\right]\rangle\} + \frac{1}{i\hbar}\{\langle x\left[p_y, V(\vec{x})\right]\rangle - \langle y[p_x, V(\vec{x})]\rangle\}.$
Next,
$\langle\left[xp_y, p_x^2\right]\rangle = \langle xp_y p_x^2 - p_x^2 xp_y\rangle = \langle[x, p_x^2]\rangle p_y = \langle 2i\hbar p_x p_y\rangle,$
where use has been made of $[x, p_x^2] = [x, p_x]p_x + p_x[x, p_x]$.
Simarlily,
$\langle\left[yp_x, p_y^2\right]\rangle = \langle 2i\hbar p_y p_x\rangle.$
Hence,
$\frac{d}{dt}\langle L_z\rangle = \frac{2i\hbar}{2i\hbar m}\langle p_x p_y\rangle - \frac{2i\hbar}{2i\hbar m}\langle p_x p_y\rangle - \frac{i\hbar}{i\hbar}\langle x\frac{\partial V}{\partial y}\rangle + \frac{i\hbar}{i\hbar}\langle y\frac{\partial V}{\partial x}\rangle.$
Finally,
$\frac{d}{dt}\langle L_z\rangle = \langle yF_x\rangle - \langle xF_y\rangle.$
This expression corresponds with the classical equivalent.

### 3.11.4 Continuous Probability

If $p(x) = xe^{-x/\lambda}$, is the probability density function over the interval $0 < x < \infty$, find the mean, standard deviation and most probable value ( where the probability density is maximum) of $x$ .
The mean value is defined as:
$\bar{x} = \langle x\rangle.$
We could work on this problem in various ways. Boccio used straightforward approach. Let's look into it in a slightly different way.
Given the probability for the interval $0 < x < \infty$, to be 1, we have:
$\int_0^\infty xe^{-x/\lambda}\,dx = 1.$
After integration by parts we obtain $\lambda^2 = 1 \Longrightarrow \lambda = 1$.
In quantum mechanical terms, normalized wave function becomes:
$\psi = \sqrt{x}e^{-x/2}.$
Obviously I could have included in the wave function a factor $e^{i\alpha}$. However, this factor does not contribute in solving this problem.
Then, using integration by parts,
$\bar{x} = \langle x\rangle = \int_0^\infty \sqrt{x}e^{-x/2}x\sqrt{x}e^{-x/2}dx = 2,$
or without the quantum mechanical approach and integration by parts,
$\bar{x} = \frac{\int_0^\infty xp(x)dx}{\int_0^\infty p(x)dx} = \frac{2\lambda^3}{\lambda^2} = 2\lambda.$

Next the standard deviation $\sigma$, with integration by parts and $\langle x \rangle = 2$

$$\sigma^2 = \int_0^\infty (x - \langle x \rangle)^2 |\psi|^2 dx = \int_0^\infty x^3 \, e^{-x} dx - \langle x \rangle^2 \int_0^\infty |\psi|^2 dx = 6 - 4 = 2,$$

and

$$\sigma = \sqrt{2} \, .$$

The most probably value of $x$ . This value of $x$ is obtained for the maximum value of the probability density $p$.

$$\frac{dp}{dx} = e^{-x} - xe^{-x} = 0 \Longrightarrow x = 1.$$

$$\frac{d^2p}{dx^2} = -2e^{-x} + \; xe^{-x}.$$

Then, for $x = 1$,

$$\frac{d^2p}{dx^2} < 0 \Longrightarrow \text{a maximum.}$$

### 3.11.5 Square Wave Packet.

Consider a free particle, initially with a well-defined momentum $p_0$, whose wave equation is well approximated by a plane wave. At $t = 0$, the particle is localized in a region $-a/2 \leq x \leq a/2$ , so that its wave function is :

$$\psi(x) = \{ Ae^{ip_0 x/\hbar} \, , -a/2 \leq x \leq a/2 \, ,$$

and

$$\psi(x) = 0 \text{ , otherwise.}$$

a) Find the normalization constant $A$, a complex number.

We are dealing with a wave packet of a width $a$, at time $t = 0$.

Normalisation:

$$\int_{-a/2}^{a/2} Ae^{ip_0 x/\hbar} Ae^{-ip_0 x/\hbar} \, dx = \int_{-a/2}^{a/2} |A|^2 \, dx = a|A|^2 = 1.$$

Since $A$ can be a complex number:

$$a|A|^2 = 1 \Longrightarrow A = \frac{1}{\sqrt{a}} e^{i\phi}.$$ Boccio set $\phi = 0$.

Then,

$$\psi(x) = \left\{ \frac{1}{\sqrt{a}} e^{ip_0 x/\hbar} \, , -a/2 \leq x \leq a/2 \, , \right.$$

and

$$\psi(x) = 0 \text{ , otherwise.}$$

The real part of the wave function is a cosine function on the interval $-a/2 \leq x \leq a/2$ , the imaginary part a sine function on the interval $-a/2 \leq x \leq a/2$ . The probability density $|\psi(x)|^2$ , is a hat function of width $a$ and of height $\frac{1}{a}$ .

b) Find the momentum space function $\tilde{\psi}(p)$ and show it too is normalized.

The momentum wave function is obtained by the Fourier transform of $\psi(x)$ :

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} \, dx = \frac{1}{\sqrt{2\pi\hbar a}} \int_{-a/2}^{a/2} e^{-i(p-p_0)x/\hbar} \, dx =$$

$$= \frac{1}{\sqrt{2\pi\hbar a}} \frac{\hbar}{-i(p-p_0)} e^{-i(p-p_0)x/\hbar} \Big|_{-a/2}^{a/2} = \sqrt{\frac{a}{2\pi\hbar}} \frac{\sin[\frac{(p-p_0)a}{2\hbar}]}{\frac{(p-p_0)a}{2\hbar}} = \sqrt{\frac{a}{2\pi\hbar}} \, \text{sinc}[\frac{(p-p_0)a}{2\hbar}] \, .$$

A sketch of the sinc function shows a concentration around $p_0 a/\hbar$ .

The normalization of the wave function in momentum representation.

$$\int_{-\infty}^{\infty} |\tilde{\psi}(p)|^2 dp = \frac{a}{2\pi\hbar} \int_{-\infty}^{\infty} \text{sinc}^2 \left[ \frac{(p-p_0)a}{2\hbar} \right] dp = \frac{1}{\pi} \int_{-\infty}^{\infty} \text{sinc}^2 y dy = 1,$$

since, with WolframAlpha or a textbook, $\int_{-\infty}^{\infty} \text{sinc}^2 y dy = \pi$.

c) Find the uncertainties $\Delta x$ and $\Delta p$ at $t = 0$ . How close is this to the minimum uncertainty wave function?

At $t = 0$, the probability density in the coordinate representation is a hat function of width $a$. So, it is reasonable to assume uncertainty in position $\Delta x$ to be approximately equal to $a$. For the probability density in momentum representation we can estimate the uncertainty in momentum $\Delta p$ with the width of the spike in $|\tilde{\psi}(p)|^2 = \frac{a}{2\pi\hbar} \text{sinc}^2[\frac{(p-p_0)a}{2\hbar}]$ to be $4\pi\hbar/a$.

It is always helpful to look into the dimensions.

Hence, with these estimates:

$\Delta x \Delta p \approx 4\pi\hbar$ .

An estimate , since the relation is: $\Delta x \Delta p \geq \hbar/2$. A difference of $8\pi$. Not close.

Then, Boccio calculated $\Delta x$ and $\Delta p$ with help of the wave function in position and momentum representation. Boccio showed the problem: $\Delta p = \infty$ .

### 3.11.6 Uncertainty Dart

A dart of mass 1 kg is dropped from a height of 1 m, with the intention to hit a certain point on the ground. Estimate the limitation set by the uncertainty principle of the accuracy that can be achieved.

I suppose a 2-dimensional approach will suffice. For the we choose the $x - y$ plane ($y$ vertical). Furthermore, $y(t = 0) = h = 1\ m$ and $v_y(t = 0) = 0$, and neglect the uncertainty in the vertical direction.

We need to deal with $\Delta x \Delta p \geq \hbar/2$ .

Boccio assumed $x(t = 0) = \Delta x$, and $v_x(t = 0) = \frac{p_x(t=0)}{m} = p_x(t = 0) = \Delta p$.

Note: Initially, $\Delta x \neq 0$ . If not. There is no $\Delta x$ at all. Boccio mentioned: "*Uncertainty principle effects will be negligible in the vertical direction*". I suppose in comparison with the free fall. Otherwise, $\Delta y$ is of the order $\Delta x$.

At time is $t \neq 0$, there are two equations:

$y(t) = y(t = 0) + v_y(t = 0)t - \frac{1}{2}gt^2 = h - \frac{1}{2}gt^2$,

And

$x(t) = x(t = 0) + v_x(t = 0)t = \Delta x + \Delta p \cdot t \therefore t = \frac{x-\Delta x}{\Delta p}$ .

Then,

$y = h - \frac{1}{2}g(\frac{x-\Delta x}{\Delta p})^2$.

This equation gives an expression for $x$ at $y = 0$, with $\Delta x \Delta p = \hbar$:

$x = \Delta x + \frac{0.45\hbar}{\Delta x}$ .

This expression leads to the minimum value of $\Delta x$, obtained from

$\frac{\partial x}{\partial \Delta x} = 0 \Longrightarrow x_{min} = 2\sqrt{0.45\hbar}$ .

A minimum, since $\frac{\partial^2 x}{\partial \Delta x^2} > 0$.

### 3.11.7 Find the Potential and the Energy for a given wave function

Suppose the wave function of a(spinless particle) of mass $m$ to be:

$\psi(r,\theta,\phi) = A\frac{e^{-\alpha r}-e^{-\beta r}}{r}$,

where $A, \alpha$, and $\beta$ are constants with $0 < \alpha < \beta$.

Find the potential $V(r,\theta,\phi)$ and the energy $E$ of the particle.

The wave function depends only on $r$ . There is no angular dependency. Consequently, the quantum numbers $l, m$ are zero. So, $\psi(r,\theta,\phi) = \psi(r)$ and $V(r,\theta,\phi) = V(r)$.

In spherical coordinates, the Schrödinger equation is separable. We only consider the radial part. The Schrödinger equation is:

$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) - \frac{2m}{\hbar^2}[V(r) - E)]\,\psi = 0.$

Now,

$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) = \frac{1}{r}\frac{d^2(r\psi)}{dr^2}.$

This suggest to define the radial function

$u(r) = r\,\psi(r)$ .

Then,

$u(r) = A\left(e^{-\alpha r} - e^{-\beta r}\right).$

The Schrödinger equation becomes:

$\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} - (V - E)u = 0 \Longrightarrow (V - E) = \frac{\hbar^2}{2mu}\frac{d^2u}{dr^2}.$

With the expression for $u(r)$:

$(V - E) = \frac{\hbar^2}{2m}\frac{\alpha^2 e^{-\alpha r}-\beta^2 e^{-\beta r}}{e^{-\alpha r}-e^{-\beta r}}.$

For $r \longrightarrow \infty \Longrightarrow V(r) \to 0.$

Using $0 < \alpha < \beta$:

$E = -\frac{\hbar^2}{2m}\lim_{n\to\infty}\frac{\alpha^2-\beta^2 e^{-(\beta-\alpha)r}}{1-e^{-(\beta-\alpha)r}} = -\frac{\hbar^2}{2m}\alpha^2.$

Hence,

$V = \frac{\hbar^2}{2m}\frac{\alpha^2 e^{-\alpha r}-\beta^2 e^{-\beta r}}{e^{-\alpha r}-e^{-\beta r}} + E = \frac{\hbar^2}{2m}\left(\frac{\alpha^2 e^{-\alpha r}-\beta^2 e^{-\beta r}}{e^{-\alpha r}-e^{-\beta r}} - \alpha^2\right).$

In the answers, Boccio presented the potential for small $r$ and indicated, by adding $\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$, the angular dependency is included. The same procedure can be followed for obtaining $V$ and $E$.

### 3.11.8 Harmonic Oscillator Wave Function

In a harmonic oscillator a particle of mass $m$ and frequency $\omega$ is subject to a parabolic potential $V(x) = m\omega^2x^2/2$. One of the energy eigenstates is $u_n(x) = Axe^{(-\frac{x^2}{x_0^2})}$, as sketched by Boccio in the answers.

a) Is this the ground state, the first exited state, second exited state, or third?

The plot shows one node. Well, http://en.wikipedia.org/ , *quantum harmonic oscillato*r, a movie and wave function representations are shown. There you see, Fig. 3.5 , Boccio, the first exited state is shown.

So, $u_n(x) = Axe^{(-\frac{x^2}{x_0^2})} \Longrightarrow u_1(x)$ is a solution of the one-dimensional Schrödinger equation.

Plug this solution into the Schrödinger equation. For $x \longrightarrow \infty$, the wave equation vanishes. This creates an additional expression for $x_0 \Longrightarrow \frac{4\hbar^2}{2mx_0^4} = \frac{m\omega^2}{2} \therefore x_0^2 = \frac{2\hbar}{m\omega}$.

Consequently, $E = -\frac{\hbar^2}{2m}\left(-\frac{6}{x_0^2}\right) = \frac{3}{2}\hbar\omega$ , the energy of the first exited state.
In addition we find out about the ground state. To this end I will use the lowering operator, $\left(-i\hbar\frac{\partial}{\partial x} - im\omega\right)$. Apply this operator on the first exited state: $\left(-i\hbar\frac{\partial}{\partial x} - im\omega\right)u_1(x) \Longrightarrow$
$\Longrightarrow \left(-i\hbar\frac{\partial}{\partial x} - im\omega\right)Axe^{\left(-\frac{m\omega x^2}{2\hbar}\right)} \Longrightarrow -i\hbar Ae^{\left(-\frac{m\omega x^2}{2\hbar}\right)}$.
Hence, the ground state $u_0(x) \propto e^{\left(-\frac{m\omega x^2}{2\hbar}\right)}$. The usual suspect of the harmonic oscillator.
b) Is $u_1(x)$ an eigenstate of parity?
Well, $u_1(x) = Axe^{(-\frac{x^2}{x_0^2})}$ is an odd function. So, $u_1(x)$ is suspected to be an eigenfunction of the parity operator.
$\hat{P}u_1(x) = \hat{P}\ Axe^{(-\frac{x^2}{x_0^2})}$.
With $x \to -x$ : $\hat{P}u_1(x) = -u_1(x)$.$\Longrightarrow u_1(x)$ is an eigenstate of parity with eigenvalue $-1$.
c) Find the constant $A$.
With normalization of $u_1(x)$:
$\int_{-\infty}^{\infty} |u_1(x)|^2\, dx$ and using $\int_{-\infty}^{\infty} y^2 e^{-y^2} dy$, $A = 2[\sqrt{\frac{2}{\pi}\frac{1}{x_0^3}}]^{1/2}$.

### 3.11.9 Spreading of a Wave Packet

A localized wave packet in free space will spread due to its initial distribution of momenta. This wave phenomenon is known as dispersion, arising because the relation between frequency $\omega$ and wavenumber $k$ is not linear.
Let us look at this in detail.
The wave function of a particle which is somewhere localized in $x$ can be constructed by linear combinations of plane waves of different wave numbers.
So, we start at $t = 0$ and wave function $\psi(x, 0)$.
This is extensively analysed by Boccio(1) on pages 13- 15. I will not repeat the analyses here. Fitzpatrick the subject matter in The *Undergraduate Course*, Chapter 3. The process of spreading is illustrated with a Gaussian wave function as Fitzpatrick did. Boccio used the propagator to show the wave packet probability density remains Gaussian. The same result is obtained with Fitzpatrick.

### 3.11.10 The Uncertainty Principle says …

Show that, for the one- dimensional wave function:
$\psi(x,) = \frac{1}{\sqrt{2a}}$ for $|x| < a$ ,
and
$\psi(x,) = 0$ for $|x| > a$ ,
the rms uncertainty in momentum is infinite( HINT: you need to Fourier transform $\psi$).
Comment on the relation of this result to the uncertainty principle.
See also problem 3.11.5: The Square Wave Packet.

The Fourier transform:

$\tilde{\phi}(p) = \frac{1}{\sqrt{4\pi\hbar a}}\int_{-a}^{a} e^{-ipx/\hbar}dx = \sqrt{\frac{a}{\pi\hbar}}\,\mathrm{sinc}(\frac{pa}{\hbar})$.

Then, calculate $\langle p\rangle$:

$\langle p\rangle = \frac{a}{\pi\hbar}\int_{-\infty}^{\infty} p\,\mathrm{sinc}^2\left(\frac{pa}{\hbar}\right)dp = 0 \Longrightarrow$The integration of an odd function.

Or,

$\langle p\rangle = \int_{-a}^{a}\frac{1}{\sqrt{2a}}(-i\hbar\frac{d}{dx})\frac{1}{\sqrt{2a}}dx = 0$, for obvious reason.

The root mean square uncertainty, exercise 3.11.5:

$\Delta x = \sqrt{\langle p^2\rangle - \langle p\rangle^2}$.

So, we need $\langle p^2\rangle$:

$\langle p^2\rangle = \frac{a}{\pi\hbar}\int_{-\infty}^{\infty} p^2\,\mathrm{sinc}^2\left(\frac{pa}{\hbar}\right)dp = \infty$ .

Consequently,

$\Delta x = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \infty$ .

### 3.11.11 Free Particle Schrödinger Equation

The time-independent Schrödinger Equation for a free particle is:

$\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial\vec{x}}\right)^2\psi(\vec{x}) = E\psi(\vec{x})$.

With the energy for the free particle, $E$, expressed in a wave number $k$, we have:

$E = \frac{\hbar^2 k^2}{2m}$ .

The equation in terms of $k$ becomes:

$(\nabla^2 + k^2)\psi(\vec{x}) = 0$.

Show that a plane wave and a spherical wave satisfy $(\nabla^2 + k^2)\psi(\vec{x}) = 0$.

a) The plane wave $\psi(\vec{x}) = e^{ikz}$.

So, the operator $\nabla^2 = \frac{d^2}{dz^2}$ ,

and

$\frac{d^2}{dz^2}e^{ikz} = -k^2 e^{ikz}$.

Hence, the plane wave satisfies the time-independent Schrödinger Equation

$(\nabla^2 + k^2)\psi(\vec{x}) = 0$.

b) The spherical wave $\psi(\vec{x}) = \frac{e^{ikr}}{r}$ ,

and $r = \sqrt{x^2 + y^2 + z^2}$.

The operator $\nabla^2 = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)\frac{e^{ikr}}{r} = \frac{1}{r^2}\left(-ike^{ikr} + ike^{ikr} - k^2 re^{ikr}\right) = -k^2\frac{e^{ikr}}{r}$ .

Hence, the spherical wave satisfies the time-independent Schrödinger Equation

$(\nabla^2 + k^2)\psi(\vec{x}) = 0$.

### 3.11.12 Double Pinhole Experiment as a variant of the double slit experiment.

The double pinhole is used for reasons of simplicity.

There are two spherical waves leaving the pinholes separated by the distance $d$. A second screen is positioned at a distance $z = L$ of the first screen. $L \gg d$ and also much larger than the wave length $\lambda$ of the two spherical waves.

For the two distances, $r_{\pm}$, from the pinholes to the second screen we have the expression:

$r_\pm = \sqrt{x^2 + (y \mp \frac{d}{2})^2 + L^2}$.

The setup is shown in Fig.3.7, Boccio (1). In this figure the $z$-axis is not indicated.

The spherical wave at the second screen is the sum of the spherical wave functions from each pinhole:

$\psi(x, y) = \frac{e^{ikr_+}}{r_+} + \frac{e^{ikr_-}}{r_-}$,

where $k = 2\pi/\lambda$ .

a) Considering the exponential factors, show that constructive interference appears approximately at: $\frac{y}{r} = n\frac{\lambda}{d}$, with $\{n \in \mathbb{Z}\}$ .

To find out, I approximate, $r_\pm = \sqrt{x^2 + (y \mp \frac{d}{2})^2 + L^2}$, to $O(d^2)$ .

$r_\pm = \sqrt{x^2 + (y \mp \frac{d}{2})^2 + L^2} = \sqrt{x^2 + y^2 + L^2 \mp yd + (\frac{d}{2})^2} =$

$= \sqrt{x^2 + y^2 + L^2}\sqrt{1 \mp \frac{yd}{x^2+y^2+L^2}} + O(d^2)$.

Neglect $O(d^2)$. Then,

$r_\pm = \sqrt{x^2 + y^2 + L^2} \mp \frac{yd}{2\sqrt{x^2+y^2+L^2}}$ .

Plug this result into the wave equation:

$$\psi(x, y) = \frac{e^{ikr_+}}{r_+} + \frac{e^{ikr_-}}{r_-} = \frac{e^{ik\sqrt{x^2+y^2+L^2}}}{r}\left[e^{\frac{-ikyd}{2\sqrt{x^2+y^2+L^2}}} + e^{\frac{ikyd}{2\sqrt{x^2+y^2+L^2}}}\right] =$$

$$= 2\frac{e^{ik\sqrt{x^2+y^2+L^2}}}{r}\cos[k\frac{yd}{2\sqrt{x^2+y^2+L^2}}] .$$

$\cos[k\frac{yd}{2\sqrt{x^2+y^2+L^2}}] = \pm 1$, for $k\frac{yd}{2\sqrt{x^2+y^2+L^2}} = n\pi$,

with $\{n \in \mathbb{Z}\}$.

Hence,

$\frac{yd}{\sqrt{x^2+y^2+L^2}} = \frac{2\pi n}{dk} \Longrightarrow \frac{y}{r} = n\frac{\lambda}{d}$ .

Then , the next part of the problem, b) and c) is to plot the intensity $|\psi(0, y)|^2$ and a contour plot of the intensity $|\psi(x, y)|^2$ with help of the Mathematica Plot function and Mathematica ContourPlot function. Boccio(1) presented nice plots on pages 21 and 22.

d) place a counter at both of the pinholes to find out about the existence of an electron. From the double slit experiment it is well known the wave function collapses.

The electron passes through the upper pinhole ⟹the wave function is: $\psi_+(x, y) = \frac{e^{ikr_+}}{r_+}$ .

When through the lower pinhole⟹the wave function is: $\psi_-(x, y) = \frac{e^{ikr_-}}{r_-}$ .

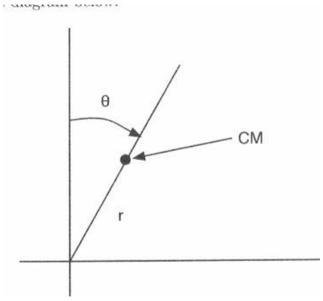
Repeat this experiment many times and the expected probabilities for each pinhole to be : $|\psi_+(x, y)|^2$ and $|\psi_-(x, y)|^2$, respectively. From the double slit experiment we know the interference pattern on the screen to disappear.

The total probability is: $|\psi_+(x, y)|^2 + |\psi_-(x, y)|^2$.

With the Plot function and the ContourPlot the disappearance of interference on the screen is nicely illustrated. See the plots Boccio(1) page 23.

### 3.11.13 A Falling Pencil

Using the uncertainty principle estimate how long a time a pencil can be balanced on its point. In the diagram, given by Boccio, a pencil making an $\theta$ with the vertical axis is shown.




The centre of mass CM, is at a distance r from the point of the pencil.
Then the equation of motion for the CM is:

$I\ddot{\theta} = mgr\sin\theta,$

where $I$ is the moment of inertia.

Use $\ddot{\theta} = \dot{\theta}\frac{d\dot{\theta}}{d\theta} = \dot{\theta}\frac{d\dot{\theta}}{dt}\frac{dt}{d\theta}$,

then

$I\ddot{\theta} = mgr\sin\theta \Longrightarrow \dot{\theta}\frac{d\dot{\theta}}{d\theta} = \frac{mgr}{I}\sin\theta.$

Boccio integrated the preceding equation, with respect to $\theta$:

$\int_{\dot{\theta}_0}^{\dot{\theta}}\dot{\theta}\,d\dot{\theta} = \frac{mgr}{I}\int_{\theta_0}^{\theta}\sin\theta\,d\theta \Longrightarrow \frac{\dot{\theta}^2-\dot{\theta}_0^2}{2} = -\frac{mgr}{I}(\cos\theta - \cos\theta_0)$ ⟹the energy conservation equation.

Then, $\frac{d\theta}{dt} = \sqrt{\dot{\theta}_0^2 - \frac{2mgr}{I}(\cos\theta - \cos\theta_0)} = \sqrt{\frac{2mgr}{I}}\sqrt{\frac{I}{2mgr}\dot{\theta}_0^2 - (\cos\theta - \cos\theta_0)}$ .

This results into an expression for the time:

$$t = \sqrt{\frac{I}{2mgr}}\int_{\theta_0}^{\theta_f}\frac{d\theta}{\sqrt{\frac{I}{2mgr}\dot{\theta}_0^2-(\cos\theta-\cos\theta_0)}},$$

with subscript $f$ ⟹ pencil down.

Now, Boccio presented the best estimate of the initial conditions based on the uncertainties of $\theta_0 \approx (\Delta\theta)_0$ and $\dot{\theta}_0 \approx (\Delta\dot{\theta})_0$. An additional assumption is, trying to balance the pencil as long as possible, then $\theta_0$ and $\dot{\theta}_0$ must be as small as possible.

$\frac{I}{2mgr}\dot{\theta}_0^2 - (\cos\theta - \cos\theta_0) = \frac{I\dot{\theta}_0^2+2mgr\cos\theta_0}{2mgr} - \cos\theta$, and $\frac{I\dot{\theta}_0^2+2mgr\cos\theta_0}{2mgr}$ be approximated by:

$1+\epsilon$ , with $\epsilon \ll 1$ .

As explained by Boccio, the pencil spends most of its time at small $\theta$. Leading to the estimate $\cos\theta \approx 1 - \frac{\theta^2}{2}$.

The integral for the time can be written as:

$$t = \sqrt{\frac{I}{2mgr}}\int_{\theta_0}^{\theta_f}\frac{d\theta}{\sqrt{\frac{I}{2mgr}\dot{\theta}_0^2-(\cos\theta-\cos\theta_0)}} = \sqrt{\frac{I}{2mgr}}\int_{\theta_0}^{\theta_f}\frac{d\theta}{\sqrt{1+\epsilon-\cos\theta}} = \sqrt{\frac{I}{2mgr}}\int_{\theta_0}^{\theta_f}\frac{d\theta}{\sqrt{\epsilon+\frac{\theta^2}{2}}}.$$

Then, Boccio evaluated the preceding integral, leading to an expression for the time:

$$t = \sqrt{\frac{I}{mgr}} \ln \frac{\sec\phi_f + \tan\phi_f}{\sec\phi_0 + \tan\phi_0},$$

with $\phi_0 = \tan^{-1}\frac{\theta_0}{\sqrt{2\epsilon}}$, and $\phi_f = \tan^{-1}\frac{\theta_f}{\sqrt{2\epsilon}}$.

Next, Boccio comes back to the uncertainty principle, initially,

$$(\Delta x)_0(\Delta p_x)_0 = \hbar \Longrightarrow (r\Delta\theta)_0\left(mr\Delta\dot{\theta}\right)_0 = \hbar .$$

So, using the expressions above for $\Delta\theta(=\theta_0)$, and $\Delta\dot{\theta}(=\dot{\theta}_0)$ for initial conditions:

$$mr^2\theta_0\dot{\theta}_0 = \hbar \Longrightarrow \dot{\theta}_0 = \frac{\hbar}{mr^2\theta_0}$$

In this way an estimate for $\dot{\theta}_0$ is obtained.

Then,

$$\frac{I\dot{\theta}_0^2 + 2mgr\cos\theta_0}{2mgr} = \cos\theta_0 + \frac{I\dot{\theta}_0^2}{2mgr} = 1 + \frac{\theta_0^2}{2} + \frac{I}{2mgr}\frac{\hbar^2}{m^2r^4{\theta_0}^2} = 1 + \epsilon.$$

Now Boccio estimated $\theta_0 \approx \sqrt{2\epsilon} \Longrightarrow \tan\phi_0 \approx 1 \approx \sec\phi_0$

With $\theta_f = \frac{\pi}{2} \Longrightarrow \frac{\theta_f}{\sqrt{2\epsilon}} \gg 1$:

and, $\phi_f = \tan^{-1}\frac{\theta_f}{\sqrt{2\epsilon}} \Longrightarrow \tan\phi_f = \frac{\theta_f}{\sqrt{2\epsilon}} = \frac{\pi}{2\sqrt{2\epsilon}} \approx \sec\phi_f$.

Now, we have for the time $t$:

$$t \approx \sqrt{\frac{I}{mgr}} \ln \frac{\pi}{2\sqrt{2\epsilon}}.$$

We were looking for the maximum time in upright position:

$$\frac{dt}{d\theta_0} = 0 = \sqrt{\frac{I}{mgr}} \frac{2\sqrt{2\epsilon}}{\pi} \frac{d}{d\theta_0}\left(\frac{\pi}{2\sqrt{2\epsilon}}\right) \Longrightarrow \frac{d\epsilon}{d\theta_0} = 0.$$

In this way, with some numerical estimates, Boccio obtained an estimate for $t$.

# 4 The mathematics of quantum Physics: Dirac Language.

It is about linear vector spaces. The algebra of linear operators on Hilbert space are used.

## 4.1 Mappings

In this section Boccio presented 4 classes of mappings.

- $T$ is a mapping of $A$ *into* $B$.
- $T$ is a mapping of $A$ *onto* $B$.
- A *one-to-one* mapping.
- A *one-to-one* mapping from $A$ *onto* $B$.

## 4.2 Linear Vector Spaces

Boccio explained how to deal with finite spaces and infinite spaces.

*"The results pertaining to finite-dimensional spaces, necessary for the understanding of the structure of quantum mechanics, are presented with thoroughness. The generalisation to infinite-dimensional spaces, which is a difficult task, is discussed in less detail".*

## 4.3 Linear Spaces and Linear Functionals

The field $C$ of complex numbers is considered.

**Ket Vectors**

Ket vectors, $|\ldots\rangle$, are used to describe physical states. All of the important features of quantum mechanics are represented by these kets. Different vector states will be labelled and this will be inserted in the ket like: $|a, b, \ldots\rangle$.

Next, Boccio stated a couple of basic properties of the ket vector:

- kets can be multiplied by complex numbers and can be added to get another ket vector, Eq.(4.2).
- each state of a physical system can be described by a ket vector.
- superposition is defined, an example is given of the double slit experiment, Eq.(4.3).

**Definition:**

A linear vector space is spanned by a set of ket vectors.

On page 243, 7 properties have been summarized, such as the multiplication is: distributive and associative. Furthermore, addition is commutative and associative.

The null vector presented and additive inverse vector.

In Eq.(4.5), a ket vector is represented as a column vector in finite dimensional space: 3-D,

$$|i\rangle = \begin{pmatrix} a_i \\ b_i \\ c_i \end{pmatrix}.$$

Then addition is defined as the sum of two column vectors. Also multiplication by a scalar and the null vector in column representation are given, Eqs.(4.6)-(4.8).

**Isomorphism**

Isomorphism is defined.

**Definition**

In Eq.(4.9), linear independence is defined and examples are presented.

The maximum number of linearly independent vectors in a space $V$ is called the dimension of the space: $dim(V)$.

On pages 246-248 definitions and examples are presented.

## 4.4 Inner Products

Boccio first discussed the inner product using standard mathematical notation.

The inner product for a set of vectors $f, g \Longrightarrow (f, g)$, a complex number.

The two definitions:

$$(f, g) = (g, f)^*,$$

and

$$(f, c_1 g_1 + c_2 g_2) = c_1 (f, g_1) + c_2 (f, g_2),$$

imply:

$$(f, c_1 g_1 + c_2 g_2) = (c_1 g_1 + c_2 g_2, f)^* = c_1{}^* (g_1, f)^* + c_2{}^* (g_2, f)^* = c_1{}^* (f, g_1) + c_2{}^* (f, g_2).$$

Furthermore , the norm of a vector, the orthogonality of two vectors, the orthonormality, the Schwarz's Inequality and the Triangle Inequality are presented.

## 4.5 Linear Functionals

Linear complex-valued functions of vectors are called linear functionals on the vector space $V$ .
In Eq.(4.35), the Riesz Theorem is presented.
With the definitions(1-4) of the inner product on page 248, the definitions of addition and scalar multiplication, Eqs. (4.33) and (4.34), Eqs. (4.36)-(4.39) can be demonstrated.

## 4.6 The Dirac Language of Kets and Bras

In this section Boccio rewrite functionals, inner product, orthonormality, expansion of an arbitrary state and the expansion coefficients in Dirac language.
For example, the relation is presented between linear functionals and bras, $\langle b|$ .
Correspondence between kets and bras is written as:
$|a\rangle \leftrightarrow \langle a|$ , Eq.(4.46), etc, up to Eq. (4.54).

## 4.7 Gram-Schmidt Orthogonalization Process

The key issue here is: An orthonormal basis can always be constructed given any set of $n$ linearly independent vectors.
The Gram-Schmidt Orthogonalization Process is explained. An example illustrates the process, page 254.

## 4.8 Linear Operators

In general: *"an operator on a vector space maps vectors into vectors."*
An operator satisfies the linearity relation, Eq. (4.58).
*Quantum mechanics works exclusively with linear operators.*
The sum and product of operators are defined, Eqs (4.59)-(4.62).
with Eqs. (4.63)-(4.64), the non-commutativity of two operators is defined and the commutator is presented by Eq. (4.65).

## 4.9 An Aside: The Connection to Matrices

With Eqs. (4.71) and (4.72) it is demonstrated the operator to be represented by a matrix. In Eq. (4.71), the matrix elements are given.
The construction of matrix elements are presented, Eqs. (4.73) and (4.72).

## 4.10 More about Vectors, Linear Functionals, Operators

Here Boccio starts with the operator acting on the bra vector.
The adjoint operator is defined in Eq. (4.78).
The goal here is to have the operator on bra vectors to create new bra vectors similar to ket vectors. With the Eqs. (4.82)-(4.85) this is clearly demonstrated.
In addition to the inner product of a bra and ket vector, the outer product is presented in Dirac(See page 25) notation, Eq. (4.92).

Note:
Dirac , page 27 , proofs the conjugate complex of the outer product, $|A\rangle\langle B|$, to be:
$|A\rangle\langle B| \Longrightarrow \overline{|A\rangle\langle B|} = |B\rangle\langle A|$.
I do not see how this relates with Eq.(4.96).

Then, Boccio presented an example the matrix representation of two projection operators given in Eq.(4.99).
I will look into this example in a slightly different way.
Two kets spanning a 2-dimensional vector space, in column representation:
$|1\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, and $|2\rangle = \begin{pmatrix}0\\1\end{pmatrix}$, Eq.(4.98).
Two projections operators:
$\hat{P}_1 = |1\rangle\langle 1|$ , and $\hat{P}_2 = |2\rangle\langle 2|$ , Eq.(4.99).
I obtain the matrix representation of these projection operators by representing the bras as row vectors, then:
$\hat{P}_1 = |1\rangle\langle 1| = \begin{pmatrix}1\\0\end{pmatrix}(1{,}0) = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$ , Eq. (4.100),
and
$\hat{P}_2 = |2\rangle\langle 2| = \begin{pmatrix}0\\1\end{pmatrix}(0{,}1) = \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}$ , Eq. (4.101).
Next, with the arbitrary vector $|a\rangle$ given in Eq.(4.102), Boccio operates first the projection operator in Dirac notation on $|a\rangle$, using normalization and orthogonality, resulting into Eq.(4.103).
In addition, Boccio used the matrix representation for the projection operator, operating on $|a\rangle$, leading to the same result as shown in Eq.(4.104).
To me, Eq. (4.106) is not completely clear. It should read:
$(\hat{P}_1 + \hat{P}_2)|a\rangle = |1\rangle\langle 1|a\rangle + |2\rangle\langle 2|a\rangle = \sum_{j=1}^{2} |j\rangle\langle j|\, a\rangle$.
We further know:
$\hat{P}_1 + \hat{P}_2 = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} + \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix} = \hat{I}$ , the identity operator, Eq. (4.105).
Hence,
$(\hat{P}_1 + \hat{P}_2)|a\rangle = \sum_{j=1}^{2} |j\rangle\langle j|\, a\rangle = \hat{I}|a\rangle$.
In this way, we obtained the elegant expression: $\sum_{j=1}^{2} |j\rangle\langle j| = \hat{I}$.
**Return to Gram-Schmidt**
With the projection operator an orthogonal set of vectors can be constructed.
Suppose two non-orthogonal vectors:
$|\alpha_1\rangle = |1\rangle$ , and $|\alpha_3\rangle = |3\rangle$ .
Assume non-orthogonality for these two vectors: $\langle \alpha_1|\alpha_3\rangle \neq 0$ .
With the projection operator $|\alpha_1\rangle\langle\alpha_1|$ , construct a new vector:
$|\alpha_2\rangle = |3\rangle - |\alpha_1\rangle\langle\alpha_1|3\rangle = |2\rangle$.
Then,
$\langle\alpha_1|\alpha_2\rangle = \langle\alpha_1|3\rangle - \langle|\alpha_1||\alpha_1\rangle\langle|\alpha_1|3\rangle = \langle\alpha_1|3\rangle - \langle\alpha_1|3\rangle = 0$.
**Important Point**
Here Boccio mentioned, something I already used, "*kets can always be treated as column*

*vectors and bras as row vectors."*
Furthermore, the trace operator is introduced, Eq. (4.116).

## 4.11 Self-Adjoint Operators

The Hermitian or self-adjoint operator is introduced.
In Eq. (4.123) the properties of Hermitian operators are summarized.
The antihermitian operator is introduced.

## 4.12 Eigenvalues and eigenvectors.

With Eq. (4.127) the eigenvector and eigenvalue are defined.
An important property of Hermitian operators: the eigenvalues of a Hermitian operator are real.
Another one is: the eigenvectors corresponding to distinct eigenvalues are orthogonal.

## 4.13 Completeness

The completeness of an orthonormal set vectors $|\alpha_i\rangle$ is expressed by Eq. (4.145).
Boccio: "*The most important result to be derived is, for a complete set of vectors* $\{|q_k\rangle\,, k \in \mathbb{P}\}$*, the sum over all of the projection operators* $|q_k\rangle\langle q_k|$ *is the identity operator."*

## 4.14 Expand Our Knowledge – Selected Topics

### 4.14.1 Hilbert Space

*In infinite dimensional space, we must determine whether the sums involved in many of our definitions converge.*
What is a Hilbert space? *"If a linear space with an inner product defined is complete, then it is called a Hilbert space."*
Some examples are presented.

### 4.14.2 Bounded Operators

Here continuous and bounded operators are defined.

### 4.14.3 Inverses

The inverse is defined by Eq. (4.161).
A necessary and sufficient condition for the existence of an inverse is presented.

### 4.14.4 Unitary Operators

The unitary operator is defined.
Important: The evolution of quantum systems in time will be given by a unitary operator.

### 4.14.5 More on Matrix Representations

If for a given representation of the matrix $\hat{A}$ , $\hat{A}$ is Hermitian then, $A_{ij} = A_{ji}^*$ .
**Change of Representation**

Eq. (4.174) is obtained with:
$\langle \bar{b}_i| = \sum_j \langle b_j|\bar{b}_i\rangle\langle b_j|$ .
Eq. (4.175) can be written as:
$\sum_k S_{ik}S_{jk}^* = \sum_k \langle b_k|\bar{b}_i\rangle \langle b_k|\bar{b}_j\rangle^* = \sum_k \langle b_k|\bar{b}_i\rangle \langle \bar{b}_j|b_k\rangle = \delta_{ij}$.

### 4.14.6 Projection Operators

Given a vector $|\alpha\rangle$ . The associated projection operator $\hat{P}_\alpha = |\alpha\rangle\langle\alpha|$ . Then, with an arbitrary vector $|\beta\rangle$ , we obtain with the projection operator:
$\hat{P}_\alpha|\beta\rangle = |\alpha\rangle\langle\alpha|\beta\rangle = a|\alpha\rangle$, (Eq.(4.178),
where $a = \langle\alpha|\beta\rangle$ . (See also Eqs. (4.185 and (4.186).
Boccio writes: "…*by definition, $\hat{P}_\alpha|\alpha\rangle = |\alpha\rangle$*, …".
Well, $\hat{P}_\alpha|\alpha\rangle = |\alpha\rangle\langle\alpha|\alpha\rangle = |\alpha\rangle$.
Furthermore, Boccio introduced orthogonality of projection operators, e.g., $\hat{P}_{\alpha 1}$ and $\hat{P}_{\alpha 2}$,
$|\eta\rangle = \hat{P}_{\alpha 1}|\beta\rangle = a_1|\alpha\rangle$,
and
$|\sigma\rangle = \hat{P}_{\alpha 2}|\beta\rangle = a_2|\alpha\rangle$.
Then, $\langle\eta|\sigma\rangle = a_1 a_2\langle\alpha|\alpha\rangle = a_1 a_2$ .
Orthogonality means $a_1 a_2 = 0$ .
With Eqs. (4.181)-(4.182), Boccio proved the eigenvalues of any projection operator to be 0,1.
On page 273 Boccio presented some examples of the usefulness of projection operators.

### 4.14.7 Unbounded operators

Unbounded operators are Hermitian provided the integrals involved do converge.

## 4.15 Eigenvalues and Eigenvectors of Unitary Operators

The properties of eigenvectors and eigenvalues of unitary operators are presented.

## 4.16 Eigenvalue Decomposition.

The decomposition is given by Eq. (4.197)

## 4.17 Extension to Infinite-Dimensional Spaces

The properties discussed in the foregoing sections is extended to infinite-dimensional spaces.
The definition of a projection operator is extended onto larger subspaces. Larger than the one-dimensional subspace.
*"The more general projection operators $\hat{E}_M$, satisfy all the same properties listed earlier for the single-state projection operators $\hat{P}_\alpha$."*
An example is given for a 2-dimensional space $C$, page 275.
Then, the properties of projections are discussed in more detail.
**Functions of a Hermitian Operator**

With the spectral resolution of a Hermitian operator, the definition of a function of a Hermitian operator is presented, Eq. (4.212).
Next, the discrete infinite sample space is discussed.
Then, page 283, Unitary operators can be dealt with in the same manner as projection operators.

## 4.18 Spectral Decomposition – More Details

*"…..for infinite-dimensional vector spaces there exist Hermitian and unitary operators that have no eigenvectors and eigenvalues."*
With Eq. (4.260), for the continuous case and the operator $\widehat{D} = -i\frac{d}{dx}$ ,there is the possibility $\widehat{D}$ not to be Hermitian. This is illustrated by four cases.
*"So, a Hermitian operator on an infinite space may or may not possess a complete set of eigenfunctions, depending on the precise nature of the operator and the vector space."*
**The Eigenvalue Problem and the Spectrum**
Then Boccio presented an example of projection operators and continuous spectra. It is about position measurement and a calibrated ruler. This can be tested in an experimental set up for a quantum test.

## 4.19 Functions of Operators (general case); Stone's Theorem

"*The ability to deal with functions of operators will be very important in quantum mechanics,….*".
In Eq. (4.318), the function of an operator is defined.
Then, Boccio investigated the reasonability of the definition by looking at some properties and some examples.
In my copy of Boccio, Eq. (4.320) was not quite clear. However on the left hand side of this equation I read:
$\langle\alpha|\hat{I}|\beta\rangle$ , where $\hat{I}$ is the identity operator.
Furthermore, in the Eqs. (4.321)-(4.324) Boccio shows that sums and multiples of functions of operators are defined in a standard way.
In Eq. (4.330) the "-" should be read as "=", I suppose?
Eq. (4.348) leads to the Schrödinger equation (See also Susskind, the time dependent Schrödinger equation page 102).
**Examples – Functions of Operators**
On page 302 Boccio presented a numerical example with the operator
$\hat{A} = \begin{pmatrix} 4 & 3 \\ 3 & 4 \end{pmatrix}$ .
The eigenvalues $\lambda$ of this matrix follows from the determinant:
$\begin{vmatrix} 4-\lambda & 3 \\ 3 & 4-\lambda \end{vmatrix} = 0 \Longrightarrow \lambda^2 - 8\lambda + 7 = 0$ .
So the eigenvalues are 1 an 7.
The eigen vectors $\begin{pmatrix} a \\ b \end{pmatrix}$ are obtained, with eigenvalue 1, from
$\begin{pmatrix} 4 & 3 \\ 3 & 4 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix} \Longrightarrow a = -b$, and with $a^2 + b^2 = 1$, the eigen vector denoted by $|1\rangle$ , is

$|1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$.

For the eigenvalue 7:

$\begin{pmatrix}4 & 3\\3 & 4\end{pmatrix}\begin{pmatrix}a\\b\end{pmatrix} = 7\begin{pmatrix}a\\b\end{pmatrix} \Rightarrow a = b$, and with $a^2 + b^2 = 1$, the eigen vector denoted by $|7\rangle$, is

$|7\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$.

Then, Boccio presented the projection operator matrices:

$\hat{P}_7 = |7\rangle\langle 7| = \frac{1}{2}\begin{pmatrix}1\\1\end{pmatrix}(1\,,\ 1) = \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}$.

Simarlily,

$\hat{P}_1 = |1\rangle\langle 1| = \frac{1}{2}\begin{pmatrix}1\\-1\end{pmatrix}(1\,,-1) = \frac{1}{2}\begin{pmatrix}1 & -1\\-1 & 1\end{pmatrix}$.

With this example it is illustrated, the $\hat{A}$ operator is the sum of the product of the eigenvalues times the respective projection operators.

With (4.358) the logarithmic function of an operator is given:

$f(\hat{A}) = \sum_{k=1}^{N} f(a_k)\hat{P}_k \Rightarrow \log\hat{A} = \sum_{k=1}^{N}(\log a_k)\,\hat{P}_k$.

Consequently,

$\log\hat{A} = (\log 7)\,\hat{P}_7 + (\log 1)\,\hat{P}_1 = (\log 7)\,\hat{P}_7 = (\log 7)\,\frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}$.

Other examples of functions of the operator are presented like the square and the square root of the operator $\hat{A}$.

Then, Boccio showed the straight forward result of

$\log\hat{A}|7\rangle$ and $\log\hat{A}|1\rangle$.

## 4.20 Commuting operators

To summarize it briefly: "*If two operators commute and are self-adjoint, these operators possess a common set of eigenvectors".*

Then Boccio discussed operators with pure point spectra and operators possessing point and continuous spectra.

**Study of continuous spectra.**

To obtain Eq. (4.380), use is made of Eq. (4.378).

Eq. (4.392) demonstrates the usefulness of the Dirac $\delta$-function(See also Susskind pages 252-253 about the position operator).

## 4.21 Another Continuous Spectrum Operator

In Eq. (4.411) the integral representation of the Dirac $\delta$-function is presented. An integration over the momentum $p$. See, a.o., Chisholm and Morris, page 604 and 605 for the derivation of this standard representation. There the wave $k$ is used in the integration $\Rightarrow p = \hbar k$. (See also Eq. 4.446).

**More about Fourier Transforms ( in general).**

Some of the mathematical concepts connected with Fourier transforms are reviewed by Boccio.

## 4.22 Problems Boccio-1

### 4.22.1. Simple Basis Vectors.

There are two vectors

$\vec{A} = 7\hat{e}_1 + 6\hat{e}_2$ , $\vec{B} = -2\hat{e}_1 + 16\hat{e}_2$ ,

written in the $\{\hat{e}_1, \hat{e}_2\}$ basis set and given another basis set

$\hat{e}_q = \frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2$ , $\hat{e}_p = -\frac{\sqrt{3}}{2}\hat{e}_1 + \frac{1}{2}\hat{e}_2$, $\Rightarrow |\hat{e}_q| = 1$, and $|\hat{e}_p| = 1$.

a) Show that $\hat{e}_q$ and $\hat{e}_p$ are orthonormal.

$\{\hat{e}_1, \hat{e}_2\}$ the basis set, meaning:

$|\hat{e}_1| = 1,\ |\hat{e}_2| = 1$ , and $\hat{e}_1 \cdot \hat{e}_2 = 0$.

Then the inner product $\hat{e}_q \cdot \hat{e}_p$, can be evaluated.

As demonstrated by Boccio: $\hat{e}_q \cdot \hat{e}_p = 0$ .

As mentioned above $\{\hat{e}_q, \hat{e}_p\}$, is another basis set.

b) Determine the new components of $\vec{A}, \vec{B}$ in the basis set $\{\hat{e}_q, \hat{e}_p\}$.

We write $\vec{A}$:

$\vec{A} = A_q\hat{e}_q + A_p\hat{e}_p = 7\hat{e}_1 + 6\hat{e}_2$ .

Take the inner product of $A_q\hat{e}_q + A_p\hat{e}_p = 7\hat{e}_1 + 6\hat{e}_2$, with $\hat{e}_q$:

$A_q\hat{e}_q \cdot \hat{e}_q + A_p\hat{e}_q \cdot \hat{e}_p = \hat{e}_q \cdot (7\hat{e}_1 + 6\hat{e}_2)$.

So,

$A_q = \hat{e}_q \cdot (7\hat{e}_1 + 6\hat{e}_2)$.

With $\hat{e}_q = \frac{1}{2}\hat{e}_1 + \frac{\sqrt{3}}{2}\hat{e}_2$, and the preceding expression:

$A_q = \frac{7}{2} + 3\sqrt{3}$,

as given by Boccio.

Similarly, $A_p, B_q$ and $B_p$ are obtained.

### 4.22.2 Eigenvalues and Eigenvectors.

Find the eigenvalues and normalized eigenvectors of the matrix

$$A = \begin{pmatrix} 1 & 2 & 4 \\ 2 & 3 & 0 \\ 5 & 0 & 3 \end{pmatrix}.$$

The determinant to be analysed is:

$$\begin{vmatrix} 1-\lambda & 2 & 4 \\ 2 & 3-\lambda & 0 \\ 5 & 0 & 3-\lambda \end{vmatrix} = 0.$$

In general:

$$\begin{vmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{vmatrix} = 0 \Rightarrow$$

$$\Rightarrow b_{11}b_{22}b_{33} + b_{12}b_{23}b_{31} + b_{13}b_{21}b_{32} - b_{11}b_{23}b_{32} - b_{12}b_{21}b_{32} - b_{13}b_{22}b_{31}.$$

The resulting polynomial in $\lambda$ is: $(3-\lambda)(\lambda^2 - 4\lambda - 21) = 0$ .

The solutions, $\lambda_i$ , given by Boccio are: $\lambda_1 = 3, \lambda_2 = -3$, and $\lambda_3 = 7$.

The general eigenvector is: $\begin{pmatrix} a \\ b \\ c \end{pmatrix}$.

The equations to be solved are:

$$A\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \lambda_i \begin{pmatrix} a \\ b \\ c \end{pmatrix}.$$

Using normalisation, the three vectors $|\lambda_i\rangle$, are obtained.

By calculating the three inner products of these vectors, these vectors appears not to be orthogonal. That comes with no surprise, since $A$ is not Hermitian.

### 4.22.3 Orthogonal Basis Vectors

Determine the eigenvalues and eigenstates of the following matrix

$$A = \begin{pmatrix} 2 & 2 & 0 \\ 1 & 2 & 1 \\ 1 & 2 & 1 \end{pmatrix}.$$

Using Gram-Schmidt, construct an orthonormal basis set from the eigenvectors of the operator.

The eigenvectors:

The determinant to be analysed is:

$$\begin{vmatrix} 2-\lambda & 2 & 0 \\ 1 & 2-\lambda & 1 \\ 1 & 2 & 1-\lambda \end{vmatrix} = 0.$$

Then

$$(2-\lambda)^2(1-\lambda) + 2 - (2-\lambda)2 - 2(1-\lambda) = -\lambda(\lambda-4)(\lambda-1) = 0 \Longrightarrow \lambda_i = 0{,}1{,}4.$$

The eigenvectors are obtained from

$$A\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \lambda_i \begin{pmatrix} a \\ b \\ c \end{pmatrix}.$$

Boccio presented the three eigenvectors:

$|0\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$, $|1\rangle = \frac{1}{\sqrt{6}}\begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix}$, and $|4\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$, all normalized.

Now Gram-Schmidt:

One of the eigenvectors is chosen as a basis vector$\Longrightarrow |0\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$.

Then, with the projection operator $|0\rangle\langle 0|$, the second basis vector is:

$$|1'\rangle = |1\rangle - |0\rangle\langle 0|1\rangle = |1\rangle - \langle 0|1\rangle|0\rangle.$$

***Intermezzo***

$|1'\rangle$ has to be normalized.

In general:

Let us introduce a number $a$:

$$a|1'\rangle = a|1\rangle - a\langle 0|1\rangle|0\rangle,$$

and

$$|a|^2\langle 1'|1'\rangle = 1 \Longrightarrow (a^*\langle 1| - a^*\langle 0|\langle 0|1\rangle^*)(a|1\rangle - a\langle 0|1\rangle|0\rangle) = 1 \Longrightarrow$$
$$\Longrightarrow |a|^2\langle 1|1\rangle - |a|^2\langle 1|0\rangle\langle 0|1\rangle - |a|^2|\langle 0|1\rangle|^2 + |a|^2|\langle 0|1\rangle|^2 = 1 \Longrightarrow$$
$$\Longrightarrow |a|^2(1 - |\langle 0|1\rangle|^2) = 1.$$

Neglecting phase ambiguity:
$a = \frac{1}{(1-|\langle 0|1\rangle|^2)^{1/2}}$ ,
So, we finally obtain the normalized version of
$|1'\rangle = \frac{|1\rangle - \langle 0|1\rangle|0\rangle}{(1-|\langle 0|1\rangle|^2)^{1/2}}$.
*End of Intermezzo*

Plugging into the preceding expression the above eigenvectors and normalize, we arrive at the result presented by Boccio: $|1'\rangle = \frac{1}{\sqrt{42}}\begin{pmatrix} 4 \\ -1 \\ -5) \end{pmatrix}$.
Similarly, $|4'\rangle$ is obtained:
$|4'\rangle = \frac{1}{\sqrt{14}}\begin{pmatrix} 2 \\ 3 \\ 1) \end{pmatrix}$.
Note: with the projection operator
$|1'\rangle = |1\rangle - |0\rangle\langle 0|1\rangle$ ,
we have
$\langle 0|1'\rangle = \langle 0|1\rangle - \langle 0|0\rangle\langle 0|1\rangle = 0,$
since $|0\rangle$ is normalized.

### 4.22.4 Operator Matrix Representation

If the states $\{|1\rangle, |2\rangle, 3\rangle\}$, form an orthonormal basis and if the operator $\hat{G}$ has the properties
$\hat{G}|1\rangle = 2|1\rangle - 4|2\rangle - 7|3\rangle,$
$\hat{G}|2\rangle = -2|1\rangle + 3|3\rangle,$
and
$\hat{G}|3\rangle = 11|1\rangle + 2 - 6|3\rangle,$
what is the matrix representation of $\hat{G}$ in the $\{|1\rangle, |2\rangle, 3\rangle\}$ basis? Use is made of section 4.9 on An Aside: The Connection to Matrix.
There you find the expression for the matrix element, Eqs. (4.66)-(4.75).
In general for the matrix element:
$\langle k|\hat{G}|i\rangle = \sum_{i=1}^{3} c_i\langle k|i\rangle,$
where $k = 1{,}2{,}3$, and the expansion $\hat{G}|i\rangle = \sum_{i=1}^{3} c_i|i\rangle$ is given above.
Consequently, the inner product $\langle k|k\rangle$ is projected out in $\sum_{i=1}^{3} c_i\langle k|i\rangle$.
So in the preceding expression $c_k$represents the matrix elements $\langle k|\hat{G}|i\rangle$.
The result of this is presented by Boccio, an exercise with blanks for filling in.

### 4.22.5 Matrix Representation and Expectation Value

If the states $\{|1\rangle, |2\rangle, 3\rangle\}$, form an orthonormal basis and if the operator $\hat{K}$ has the properties
$\hat{K}|1\rangle = 2|1\rangle,$

$\hat{K}|2\rangle = 3|2\rangle$,
and
$\hat{K}|3\rangle = -6|3\rangle$ .
a) Write an expression for $\hat{K}$ in terms of its eigenvalues and eigen vectors and eigenvectors ( projection operators[1]). Use this expression to derive the matrix representing $\hat{K}$ in the $|1\rangle, 2\rangle, |3\rangle$ basis. In problem 4.22.4 we used $\langle k|\hat{K}|i\rangle = \sum_{i=1}^{3} c_i \langle k|i\rangle$ to find the matrix elements. Using this approach, the resulting matrix elements are:
$\langle 1|\hat{K}\,|1\rangle = 2\langle 1|1\rangle = 2 = K_{11}$,
$\langle 2|\hat{K}\,|1\rangle = 2\langle 2|1\rangle = 0 = K_{21}$,
$\langle 3|\hat{K}\,|1\rangle = 2\langle 3|1\rangle = 0 = K_{31,}$
$\langle 1|\hat{K}\,|2\rangle = 3\langle 1|2\rangle = 0 = K_{12}$,
$\langle 2|\hat{K}\,|2\rangle = 3\langle 2|2\rangle = 3 = K_{22}$,
$\langle 3|\hat{K}\,|2\rangle = 3\langle 3|2\rangle = 0 = K_{32}$,
$\langle 1|\hat{K}\,|3\rangle = -6\langle 1|3\rangle = 0 = K_{13}$,
$\langle 2|\hat{K}\,|3\rangle = -6\langle 2|3\rangle = 0 = K_{23}$,
$\langle 3|\hat{K}\,|3\rangle = -6\langle 3|3\rangle = -6 = K_{33}$.
Then, the matrix
$$\hat{K} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -6 \end{pmatrix}.$$
Boccio showed another representation based on the basis and projection operators.
$\hat{K}|1\rangle\langle 1| = 2|1\rangle\langle 1|$,
$\hat{K}|2\rangle\langle 2| = 3|2\rangle\langle 2|$,
$\hat{K}|3\rangle\langle 3| = -6|3\rangle\langle 3|$.
Now,
$\sum_{i=1}^{3} \hat{K}\,|i\rangle\langle i| = \hat{K}\sum_{i=1}^{3}|i\rangle\langle i| = \hat{K} = 2|1\rangle\langle 1| + 3|2\rangle\langle 2| - 6|3\rangle\langle 3|$.
Represent the projection operators in their respective matrices:
$$|1\rangle\langle 1| = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, |2\rangle\langle 2| = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \text{ and } |3\rangle\langle 3| = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$
So, again the matrix representation of
$$\hat{K} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -6 \end{pmatrix}, \text{ is obtained.}$$
b) What is the expectation value or average value of $\hat{K}$, defined as $\langle \alpha|\hat{K}|\alpha\rangle$ in the state $|\alpha\rangle = \frac{1}{\sqrt{83}}(-3|1\rangle + 5|2\rangle + 7|3\rangle)$.
Boccio presented three ways to evaluate the expectation value.
- Matrix Multiplication.
All the ingredients are there:
$\langle \hat{K}\rangle = \langle \alpha|\hat{K}|\alpha\rangle$.
The column representation of $|\alpha\rangle$ is:

[1] Projection operator a matrix or a vector?

$|\alpha\rangle = \frac{1}{\sqrt{83}}[-3\begin{pmatrix}1\\0\\0\end{pmatrix} + 5\begin{pmatrix}0\\1\\0\end{pmatrix} + 7\begin{pmatrix}0\\0\\1\end{pmatrix} = \begin{pmatrix}-3\\5\\7\end{pmatrix}]$.

Then, with $\widehat{K} = \begin{pmatrix}2 & 0 & 0\\0 & 3 & 0\\0 & 0 & -6\end{pmatrix}$, we have the ingredients to evaluate:

$\langle\widehat{K}\rangle = \langle\alpha|\widehat{K}|\alpha\rangle = -\frac{201}{83}$.

- Bra-Kets

With

$|\alpha\rangle = \frac{1}{\sqrt{83}}(-3|1\rangle + 5|2\rangle + 7|3\rangle)$,

$\langle\alpha| = \frac{1}{\sqrt{83}}(-3\langle 1| + 5\langle 2 + 7\langle 3|)$

and

$\widehat{K} = 2|1\rangle\langle 1| + 3|2\rangle\langle 2| - 6|3\rangle\langle 3|$,

$\langle\widehat{K}\rangle = \langle\alpha|\widehat{K}|\alpha\rangle = -\frac{201}{83}$.

- Probabilities

$\langle\widehat{K}\rangle = \langle\alpha|\widehat{K}|\alpha\rangle = \sum_{n=1}^{3} k_n P(k_n) = -\frac{201}{83}$.

### 4.22.6 Projection Operator Representation

Let the states $\{|1\rangle, |2\rangle, |3\rangle\}$, form an orthonormal basis. We consider the operator given by $\hat{P}_2 = |2\rangle\langle 2|$.

a) What is the matrix representation of this operator $\hat{P}_2 = |2\rangle\langle 2|$?

A 3-D space of states is considered with an orthonormal basis.

Then,

$\hat{P}_2 = |2\rangle\langle 2| = \begin{pmatrix}0\\1\\0\end{pmatrix}(0\,,1\,,0) = \begin{pmatrix}0 & 0 & 0\\0 & 1 & 0\\0 & 0 & 0\end{pmatrix}$.

b)The eigenvalues:

$\begin{vmatrix}0-\lambda & 0 & 0\\0 & 1-\lambda & 0\\0 & 0 & 0-\lambda\end{vmatrix} = 0 \Longrightarrow \lambda_i = 0, 1, 0$.

The eigenvectors: the orthonormal basis $\{|1\rangle, |2\rangle, |3\rangle\}$.

In column vector representation:

$|1\rangle = \begin{pmatrix}0\\0\\0\end{pmatrix}, |2\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}$ and $|3\rangle = \begin{pmatrix}0\\0\\0\end{pmatrix}$.

c) $\hat{P}_2|A\rangle$, where $|A\rangle = \frac{1}{\sqrt{83}}(-3|1\rangle + 5|2\rangle + 7|3\rangle)$,:

$\hat{P}_2|A\rangle = |2\rangle\langle 2|A\rangle = \frac{1}{\sqrt{83}}(-3|2\rangle\langle 2|1\rangle + 5|2\rangle\langle 2|2\rangle + 7|2\rangle\langle 2|3\rangle) = \frac{5}{\sqrt{83}}|2\rangle$.

d) Boccio also paid analysed the quadratic operator $\hat{P}_2^2$:

- $\hat{P}_2^2 = (|2\rangle\langle 2|)(|2\rangle\langle 2|) = |2\rangle\langle 2| = \hat{P}_2$.

- $\hat{P}_2^2|\lambda\rangle = \hat{P}_2|\lambda\rangle = \lambda|\lambda\rangle$,

and

$\hat{P}_2^2|\lambda\rangle = \hat{P}_2\hat{P}_2|\lambda\rangle = \hat{P}_2\,\lambda|\lambda\rangle = \lambda\hat{P}_2|\lambda\rangle = \lambda^2|\lambda\rangle$.

Consequently,
$\lambda^2|\lambda\rangle = \lambda|\lambda\rangle \Longrightarrow (\lambda^2 - \lambda)|\lambda\rangle = 0.$
So,
$|\lambda\rangle = 0$, or $(\lambda^2 - \lambda) = 0 \Longrightarrow \lambda = 0{,}1.$

### 4.22. 7 Operator Algebra

An operator for a two-state system is given by
$\hat{H} = a\{|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|\},$
where $a$ is a number.
I assume the orthonormal basis to be $\{|1\rangle, |2\rangle\}$. Then, with matrix representations of the projector operators, matrix representation of $\hat{H}$:
$\hat{H} = \begin{pmatrix} a & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 0 & a \end{pmatrix} + \begin{pmatrix} 0 & a \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ a & 0 \end{pmatrix} = \begin{pmatrix} a & a \\ a & -a \end{pmatrix}.$
The eigenvalues are obtained with:
$\begin{vmatrix} a-\lambda & a \\ a & -a-\lambda \end{vmatrix} = 0 \Longrightarrow -a^2 + \lambda^2 - a^2 = 0$
Resulting into two eigenvalues:
$\lambda_+ = a\sqrt{2}$, and $\lambda_- = -a\sqrt{2}$ .
With these eigenvalues two eigenkets are obtained.
In column representation:
$\hat{H}|+\rangle = \lambda_+\hat{H}|+\rangle \Longrightarrow \begin{pmatrix} a & a \\ a & -a \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = a\sqrt{2}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$
This gives two equation for $\alpha$ and $\beta$, resulting into a ratio:
$\frac{\beta}{\alpha} = (\sqrt{2} - 1).$

Note: Boccio obtained $\beta = (\sqrt{2} - 1)a$.
You do not obtain this from the two aforementioned equations. Since $a$ cancels out.

With $\frac{\beta}{\alpha} = (\sqrt{2} - 1)$, normalization gives a quadratic equation:
$\alpha^2(4 - 2\sqrt{2}) = 1.$
Two values for $\alpha$:
$\alpha = \pm\frac{1}{\sqrt{4-2\sqrt{2}}}$ . I choose the $+$ sign.
So,
$\beta = \frac{\sqrt{2}-1}{\sqrt{4-2\sqrt{2}}}.$
Or,
choose $\alpha = a, \Longrightarrow \beta = (\sqrt{2} - 1)a$ .
$|+\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = a\begin{pmatrix} 1 \\ \sqrt{2} - 1 \end{pmatrix}.$
Normalization gives for $a$:
$a = \pm\frac{1}{\sqrt{4-2\sqrt{2}}}$. I choose the $+$ sign. Leading to the same result as above.
Now,

$|+\rangle = \frac{1}{\sqrt{4-2\sqrt{2}}}\begin{pmatrix} 1 \\ \sqrt{2}-1 \end{pmatrix} = \frac{1}{\sqrt{4-2\sqrt{2}}}[|1\rangle + (\sqrt{2}-1)|2\rangle].$

The other eigenket:

$\hat{H}|-\rangle = \lambda_{-}\hat{H}|-\rangle \Longrightarrow \begin{pmatrix} a & a \\ a & -a \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = -a\sqrt{2}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$

This gives two equation for $\alpha$ and $\beta$, resulting into a ratio:

$\frac{\beta}{\alpha} = -(\sqrt{2}+1).$

With $\frac{\beta}{\alpha} = -(\sqrt{2}+1)$, normalization gives a quadratic equation:

$\alpha^2(4+2\sqrt{2}) = 1.$

Two values for $\alpha$:

$\alpha = \pm\frac{1}{\sqrt{4+2\sqrt{2}}}$ . I choose the + sign.

So,

$\beta = -\frac{\sqrt{2}+1}{\sqrt{4+2\sqrt{2}}}.$

$|-\rangle = \frac{1}{\sqrt{4+2\sqrt{2}}}\begin{pmatrix} 1 \\ -[\sqrt{2}+1] \end{pmatrix} = \frac{1}{\sqrt{4+2\sqrt{2}}}[|1\rangle - (\sqrt{2}+1)|2\rangle.$

Similarly, with the choice $\alpha = a \Longrightarrow \beta = -(\sqrt{2}+1)a.$

$|-\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = a\begin{pmatrix} 1 \\ -(\sqrt{2}+1) \end{pmatrix}$, etc.

Resulting into, after normalization in the above expression for $|-\rangle$.

Check:

$\langle +|-\rangle = \frac{1}{\sqrt{4+2\sqrt{2}}}\frac{1}{\sqrt{4-2\sqrt{2}}}[\langle 1| + (\sqrt{2}-1)\langle 2|][|1\rangle - (\sqrt{2}+1)|2\rangle] = 0 .$

Furthermore:

$|+\rangle\langle +| = \frac{1}{4-2\sqrt{2}}\{[|1\rangle + (\sqrt{2}-1)|2\rangle][\langle 1| + (\sqrt{2}-1)\langle 2|]\} =$

$= \frac{1}{4-2\sqrt{2}}\{|1\rangle\langle 1| + (\sqrt{2}-1)^2|2\rangle\langle 2| + (\sqrt{2}-1)|1\rangle\langle 2| + (\sqrt{2}-1)|2\rangle\langle 1|\}.$

Similarly $|-\rangle\langle -|$, is derived. See Boccio.

### 4.22.8 Functions of operators

Suppose that we have some operator $\hat{Q}$ such that $\hat{Q}|q\rangle = q|q\rangle$ , i.e., $|q\rangle$ is an eigenvector of $\hat{Q}$ with eigenvalue $q$. Show that $|q\rangle$ is also an eigenvector of $\hat{Q}^2$, $\hat{Q}^n$ and $e^{\hat{Q}}$. Determine the corresponding eigenvalues.

First Boccio showed

$\hat{Q}^2|q\rangle = \hat{Q}\hat{Q}|q\rangle = \hat{Q}\, q|q\rangle = q\hat{Q}|q\rangle = q^2|q\rangle.$

Hence, the eigenvalue of $\hat{Q}^2$ is $q^2$.

By induction it is shown , the eigenvalue of $\hat{Q}^n$ to be $q^n$.

I used a slightly different order for this induction procedure:

$\hat{Q}^n|q\rangle = \hat{Q}\hat{Q}^{n-1}|q\rangle = \hat{Q}q^{n-1}|q\rangle = \cdots = q^n|q\rangle.$

The induction procedure stated with the assumption: $\hat{Q}^{n-1}|q\rangle = q^{n-1}|q\rangle.$

Next, the eigenvalues of $e^{\hat{Q}}$ are obtained from the series expansion of $e$, with the interesting result of the eigenvalue to be: $e^q$.

### 4.22.9 A Symmetric Matrix

Let $A$ be a $4 \times 4$ matrix. Assume that the eigenvalues are given by 0, 1, 2, 3 with corresponding normalized eigenvectors

$$|\lambda_0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}, |\lambda_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}, |\lambda_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix}, \text{ and } |\lambda_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}.$$

Then, Boccio used the symmetry of $A$ to use the existence of an orthogonal matrix $U$, such that $D = UAU^T$,

where $D$ is the diagonal matrix with eigenvalues 0, 1, 2, 3 .

The matrix $U^T$, is given by the normalized eigenvectors of $A$, i.e.,

$$U^T = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 0 & 1\\1 & 0 & 0 & -1\\0 & 1 & 1 & 0\\0 & 1 & -1 & 0\end{pmatrix}.$$

With $U^T = U^{-1} \Longrightarrow A = U^{-1}D(U^T)^{-1}$, $A$ is obtained.

However,

I used a different approach, than used by Boccio. An approach by brute force:

$A|\lambda_i\rangle = \lambda_i|\lambda_i\rangle$,

with

$$A = \begin{pmatrix}a_{11} & a_{12} & a_{13} & a_{14}\\a_{21} & a_{22} & a_{23} & a_{24}\\a_{31} & a_{32} & a_{33} & a_{34}\\a_{41} & a_{42} & a_{43} & a_{44}\end{pmatrix}.$$

Consequently, there are 16 equations resulting from $A|\lambda_i\rangle = \lambda_i|\lambda_i\rangle$. The equations are given in the two tables below. To be solved in one glance:

| | | | | |
|---|---|---|---|---|
| $\lambda_0 = 0$ | $a_{11} + a_{14} = 0$ | $a_{21} + a_{24} = 0$ | $a_{31} + a_{34} = 0$ | $a_{41} + a_{44} = 0$ |
| $\lambda_1 = 1$ | $a_{11} - a_{14} = 1$ | $a_{21} - a_{24} = 0$ | $a_{31} - a_{34} = 0$ | $a_{41} - a_{44} = 1$ |
| | $a_{11} = \frac{1}{2}$ ; $a_{14} = -\frac{1}{2}$ | $a_{21} = 0$ ; $a_{24} = 0$ | $a_{31} = 0$ ; $a_{34} = 0$ | $a_{41} = -\frac{1}{2}$ ; $a_{44} = \frac{1}{2}$ |

So, we have already 8 elements of the matrix $A$.

The next 8:

| | | | | |
|---|---|---|---|---|
| $\lambda_2 = 2$ | $a_{12} + a_{13} = 0$ | $a_{22} + a_{23} = 2$ | $a_{32} + a_{33} = 2$ | $a_{42} + a_{43} = 0$ |
| $\lambda_3 = 3$ | $a_{12} - a_{13} = 0$ | $a_{22} - a_{23} = 3$ | $a_{32} - a_{33} = -3$ | $a_{42} - a_{43} = 0$ |
| | $a_{12} = 0$ ; $a_{13} = 0$ | $a_{22} = \frac{5}{2}$ ; $a_{23} = -\frac{1}{2}$ | $a_{32} = -\frac{1}{2}$ ; $a_{33} = \frac{5}{2}$ | $a_{42} = 0$ ; $a_{43} = 0$ |

We have here all the elements of $A$:

$$A = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 5 & -1 & 0 \\ 0 & -1 & 5 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}.$$

Brute force was not that brute. The zero's in the eigenvectors were helpful.

### 4.22.10 Determinants and Traces

Let $A$ be an $n \times n$ matrix. Show that

det(exp($A$))=exp($Tr(A)$).

This is about matrix analysis.

The key is any $n \times n$ matrix can be brought into triangular form by a similarity transformation.

To me, the other solution method as presented by Boccio is more attractive.

There, the trace of the matrix(the sum of the diagonal elements) is used in a direct way.

The result of Problem 4.22.8, Functions of Operators,

$e^{\hat{Q}}|q\rangle = e^{q}|q\rangle$ ,

can be used.

### 4.22.11 Function of a Matrix

Let

$$A = \begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix}.$$

Calculate exp($\alpha A$), where $\alpha$ is a real number.

See also exercises 4.22.8 and 4.22.9.

First the eigenvalues and eigenvectors of $\alpha A$.

The eigen values of $\alpha A$:

$$\begin{vmatrix} -\alpha - q & 2\alpha \\ 2\alpha & -\alpha - q \end{vmatrix} = 0,$$

we have $q_{1,2} = \alpha, -3\alpha$.

The eigen vectors, $|q_{1,2}\rangle$ of $\alpha A$:

$A|q_i\rangle = q_i|q_i\rangle$.

Just represent $|q_i\rangle$ as 2-D column vector and the two column vectors are obtained:

$$|q_1\rangle = \begin{pmatrix} \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} \end{pmatrix}, \text{ and } |q_2\rangle = \begin{pmatrix} \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} \end{pmatrix}.$$

The key equation is, see Problem 4.22.8(Boccio):

$e^{\alpha A}|q_i\rangle = e^{q_i}|q_i\rangle$.

Now again, I use a different approach than Boccio(See Problem 4.22.9 above).

I represent $e^{\alpha A}$ by a $2 \times 2$ matrix:

$$e^{\alpha A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}.$$

Consequently, there are 4 equations resulting from $e^{\alpha A}|q_i\rangle = e^{q_i}|q_i\rangle$. The equations and solutions are given in the table below.

| | | |
|---|---|---|
| $q_1 = -3\alpha$ | $a_{11}\frac{\sqrt{2}}{2} - a_{12}\frac{\sqrt{2}}{2} = e^{-3\alpha}\frac{\sqrt{2}}{2}$ | $a_{21}\frac{\sqrt{2}}{2} - a_{22}\frac{\sqrt{2}}{2} = -e^{-3\alpha}\frac{\sqrt{2}}{2}$ |
| $q_2 = \alpha$ | $a_{11}\frac{\sqrt{2}}{2} + a_{12}\frac{\sqrt{2}}{2} = e^{\alpha}\frac{\sqrt{2}}{2}$ | $a_{21}\frac{\sqrt{2}}{2} + a_{22}\frac{\sqrt{2}}{2} = e^{\alpha}\frac{\sqrt{2}}{2}$ |
| | $a_{11} = \frac{1}{2}(e^{\alpha} + e^{-3\alpha})$ | $a_{21} = \frac{1}{2}(e^{\alpha} - e^{-3\alpha})$ |
| | $a_{12} = \frac{1}{2}(e^{\alpha} - e^{-3\alpha})$ | $a_{22} = \frac{1}{2}(e^{\alpha} + e^{-3\alpha})$ |

Hence,

$$e^{\alpha A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} e^{\alpha} + e^{-3\alpha} & e^{\alpha} - e^{-3\alpha} \\ e^{\alpha} - e^{-3\alpha} & e^{\alpha} + e^{-3\alpha} \end{pmatrix} = \frac{e^{-\alpha}}{2}\begin{pmatrix} \cosh 2\alpha & \sinh 2\alpha \\ \sinh 2\alpha & \cosh 2\alpha \end{pmatrix}.$$

### 4.22.12 More Gram-Schmidt

Let $A$ be the symmetric matrix:

$$A = \begin{pmatrix} 5 & -2 & -4 \\ -2 & 2 & 2 \\ -4 & 2 & 5 \end{pmatrix}.$$

Determine the eigenvalues and eigen vectors of $A$.

The eigenvalues:

$$\begin{vmatrix} 5-q & -2 & -4 \\ -2 & 2-q & 2 \\ -4 & 2 & 5-q \end{vmatrix} = 0,$$

with the general expression for the $3 \times 3$ determinant(Chisholm and Morris, page 423) the resulting cubic equation is:

$$q^3 - 12q^2 + 21q - 10 = 0.$$

The roots of this cubic equation are, with the WolframAlpha-app or Abramowitz and Stegun or give Cardano a try,

$q_1 = 1$, $q_2 = 1$, and $q_3 = 10$.

Then with:

$A|q_i\rangle = q_i|q_i\rangle$, the vectors can be obtained.

First with $q_3 = 10 \Longrightarrow$represent $|q_i\rangle$ by the column vector $\begin{pmatrix} a \\ b \\ c \end{pmatrix}$

After some algebra and normalization, we have

$$|q_3\rangle = \frac{1}{3}\begin{pmatrix} 2 \\ -1 \\ -2 \end{pmatrix}.$$

Now the eigenvectors with the same eigenvalue equal 1.

I use the same representation. In this case we obtain: $2a - b - 2c = 0 \Longrightarrow b = 2a - 2c$.

Orthogonality: $(a\ (2a - 2c)\ c))\begin{pmatrix} 2 \\ -1 \\ -2 \end{pmatrix} = 0 \Longrightarrow$ inconclusive. I choose $c = 0$. For $|q_1\rangle$ we obtain:

$$|q_1\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix}-1\\-2\\0\end{pmatrix}.$$

What about $|q_2\rangle$? We still have $2a - b - 2c = 0$. Now, if I choose $b = 0$, orthogonality with $|q_3\rangle$ , and normalization: $|q_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\0\\-1\end{pmatrix}$.

As demonstrated by Boccio: $\langle q_1|q_2\rangle \neq 0$.

Next the Gram-Schmidt procedure is used. With the projection operator $|q_1\rangle\langle q_1|$:

$$|q_2'\rangle = |q_2\rangle - |q_1\rangle\langle q_1|q_2\rangle = \frac{4}{5}\frac{1}{\sqrt{2}}\begin{pmatrix}-1\\2\\-1\end{pmatrix}.$$

My results differ from Boccio's result due to the normalization factor.

### 4.22.13 Infinite Dimensions

Let $A$ be a square finite-dimensional matrix with real elements such that $AA^T = I$.

a) Show that $A^T A = I$.

$A$ be a square finite-dimensional matrix with real elements, so the inverse exist.

Well, if we assume $AA^T = I$, then by definition $A^T$ is the inverse of $A \Longrightarrow A^{-1}$, since $AA^{-1} = I$ .

Now, with $AA^{-1} = I$,

$$AA^{-1}A = IA = A \Longrightarrow A^{-1}A = I \Longrightarrow A^T A = I.$$

b) Doe this result hold for infinite dimensional matrices?

The answer is no (Boccio).

Boccio illustrated this with a counterexample on page 38 of the problems.

### 4.22.14 Spectral Decomposition.

Find the eigenvalues and eigenvectors of the matrix

$$M = \begin{pmatrix}0 & 1 & 0\\1 & 0 & 1\\0 & 1 & 0\end{pmatrix}.$$

The eigenvalues:

$$\begin{vmatrix}-q & 1 & 0\\1 & -q & 1\\0 & 1 & 0-q\end{vmatrix} = 0,$$

with the general expression for the $3 \times 3$ determinant(Chisholm and Morris, page 423) the resulting cubic equation is:

$$-q^3 + 2q = 0 \Longrightarrow q_i = 0, \pm\sqrt{2}.$$

Then with:

$M|q_i\rangle = q_i|q_i\rangle$, the vectors can be obtained.

$$q_1 = 0 \Longrightarrow |q_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix}.$$

I reproduce the result for $|q_2\rangle$, Boccio,

$|q_2\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$.

I present the $|q_3\rangle$, where I represent the ket in column representation $\begin{pmatrix} a \\ b \\ c \end{pmatrix}$:

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = -\sqrt{2}\begin{pmatrix} a \\ b \\ c \end{pmatrix}.$$

Then,

$b = -a\sqrt{2}$,

$a + c = -b\sqrt{2}$,

$b = -c\sqrt{2}$.

Normalization,

$a^2 + b^2 + c^2 = 1 \Rightarrow \frac{b^2}{2} + b^2 + \frac{b^2}{2} = 1 \Rightarrow b = \pm\frac{1}{2}\sqrt{2}$.

I choose $b = \frac{1}{2}\sqrt{2}$.

Hence

$|q_3\rangle = \frac{1}{2}\begin{pmatrix} -1 \\ \sqrt{2} \\ -1 \end{pmatrix}$. Apparently, Boccio choose $b = -\frac{1}{2}\sqrt{2}$. A phase difference of $e^{i\pi}$.

The projection operators in matrix representation, using matrix multiplication of the ket and bra representation of the projection operators:

$$\hat{P}_i = |q_i\rangle\langle q_i| = \begin{pmatrix} a_i \\ b_i \\ c_i \end{pmatrix}(a_i, b_i, c_i) = \begin{pmatrix} a_i a_i & a_i b_i & a_i c_i \\ b_i a_i & b_i b_i & b_i c_i \\ c_i a_i & c_i b_i & c_i c_i \end{pmatrix}.$$

The results are presented by Boccio, with $|q_3\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$

The matrix can be written in terms of its eigenvalues and eigenvectors. Well, to be a bit more precise, in terms of eigenvalues and projection operators, we have,

$M|q_i\rangle = q_i|q_i\rangle$.

Multiply this expression to the left and the right with the bra $\langle q_i|$:

$M|q_i\rangle\langle q_i| = q_i|q_i\rangle\langle q_i|$ .

Sum this expression over the complete basis set:

$M\sum_i |q_i\rangle\langle q_i| = \sum_i q_i|q_i\rangle\langle q_i|$ .

Et voila, with $\sum_i |q_i\rangle\langle q_i| = I$, we have

$M = \sum_i q_i|q_i\rangle\langle q_i| = \sum_i q_i \hat{P}_i$.

The result is presented at the bottom of page 39, Boccio.

This Dirac Algebra is elegant, to say the least.

### 4.22.15 Measurement Results

Given particles in state:

$|\alpha\rangle = \frac{1}{\sqrt{83}}[-3|1\rangle + 5|2\rangle + 7|3\rangle$,

where $\{|1\rangle, |2\rangle, |3\rangle\}$, form an orthonormal basis, what are the possible experimental results for a measurement of

$$\hat{Y} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -6 \end{pmatrix},$$

written in this basis and with probabilities do they occur?

We met the state $|\alpha\rangle$ in Problem 4.22.6 *Projection Operator Representation.*

The eigenvalues of the operator(observable) $\hat{Y}$ follow from a measurement of a particle in a state $|\alpha\rangle$. The eigenvalues are respectively: $2, 3, -6$, resulting from

$(q-2)(q-3)(q+6) = 0$.

It follows that $2$, to be the eigenvalue with the eigenvector $|1\rangle$.

$3$, to be the eigenvalue with the eigenvector $|2\rangle$,

and

$-6$, to be the eigenvalue with the eigenvector $|3\rangle$.

So the probabilities of the observables are:

$|\langle 1|\alpha\rangle|^2 \Longrightarrow$ the $|1\rangle$ state is projected out, the probability of the observable with eigenvalue equal 2,

$|\langle 2|\alpha\rangle|^2 \Longrightarrow$ the $|2\rangle$ state is projected out the probability of the observable with eigenvalue equal 3,

and

$|\langle 3|\alpha\rangle|^2 \Longrightarrow$ the $|3\rangle$ state is projected out the probability of the observable with eigenvalue equal -6.

The probabilities are presented by Boccio, page 40.

### 4.22.16 Expectation Values.

Let

$$R = \begin{pmatrix} 6 & -2 \\ -2 & 9 \end{pmatrix}$$

represent an observable, and

$$|\Psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix},$$

be an arbitrary normalized state.

The expectation value of $R^2$:

$\langle R^2\rangle = \langle\Psi|R^2|\Psi\rangle$.

Plug into this expression the observable and the given state:

$$\langle\Psi|R^2|\Psi\rangle = (a^* b^*) \begin{pmatrix} 6 & -2 \\ -2 & 9 \end{pmatrix} \begin{pmatrix} 6 & -2 \\ -2 & 9 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}.$$

The resulting expectation value is presented by Boccio page 41.

Boccio presented another approach, an indirect way.

First find the eigenvalues and eigenvectors of the observable $R$.

The eigenvalues:

$$\begin{vmatrix} 6-r & -2 \\ -2 & 9-r \end{vmatrix} = 0 \Longrightarrow r^2 - 15r + 50 = 0 \Longrightarrow (r-5)(r-10) = 0.$$

The eigenvectors:

$R|r_i\rangle = r_i|r_i\rangle$, and normalization, the eigenvectors are obtained.

$|r_1\rangle = \begin{pmatrix} 2/\sqrt{5} \\ 1/\sqrt{5} \end{pmatrix}$, and $|r_2\rangle = \begin{pmatrix} 1\sqrt{5} \\ -2/\sqrt{5} \end{pmatrix}$.

Now, Boccio used these eigenvectors as a basis for $|\Psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$,

$|\Psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix} = d_1|r_1\rangle + d_2|r_2\rangle = \sum_j d_j\,|r_j\rangle$.

Hence,

$d_1 = \langle r_1|\Psi\rangle = (\left(2/\sqrt{5}\;\; 1/\sqrt{5}\right)\begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\sqrt{5}}(2a+b)$.

Similarly:

$d_2 = \langle r_2|\Psi\rangle = \left(1/\sqrt{5}\;\; -2/\sqrt{5}\right)\begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\sqrt{5}}(a-2b)$.

Then $|\Psi\rangle = \frac{1}{\sqrt{5}}(2a+b)|r_1\rangle + \frac{1}{\sqrt{5}}(a-2b)|r_2\rangle$.

Let's use the approach of problem 4.22.14: the projection operators.

$R = \sum_i r_i|r_i\rangle\langle r_i|$,

and

$R^2 = \sum_i r_i^2|r_i\rangle\langle r_i|$.

Then,

$\langle\Psi|R^2|\Psi\rangle = \sum_i r_i^2\,\langle\Psi|r_i\rangle\langle r_i|\Psi\rangle$.

With $|\Psi\rangle = \sum_j d_j\,|r_j\rangle$ ,

$\langle\Psi|R^2|\Psi\rangle = \sum_{i,j} r_i^2\,|d_j|^2|\langle r_j|r_i\rangle|^2 = \sum_{i,j} r_i^2\,|d_j|^2\delta_{ij}$.

So, the projection operators projected out:

$\langle\Psi|R^2|\Psi\rangle = \sum_i r_i^2\,|d_i|^2 = 25\cdot\frac{|2a+b|^2}{5} + 100\cdot\frac{|a-2b|^2}{5}$ ,

giving the result, presented by Boccio, page 41.

Obviously,

$\langle\Psi|R^2|\Psi\rangle = \sum_i r_i^2\,P_i$,

the usual representation of the expectation/mean value with probabilities $P_i = |d_i|^2$.

### 4.22.17 Eigenket Properties

Consider a 3-dimensional ket space. If a certain set of orthonormal kets, say $|1\rangle, |2\rangle$ and $|3\rangle$ are used as the basis kets, the operators $\hat{A}$ and $\hat{B}$ are represented by the $3\times 3$ matrices:

$$\hat{A} = \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix} \Rightarrow \begin{vmatrix} a-\lambda & 0 & 0 \\ 0 & -a-\lambda & 0 \\ 0 & 0 & -a-\lambda \end{vmatrix} = 0 \Rightarrow (a-\lambda)(a+\lambda)(a+\lambda) = 0.$$

$\hat{A}$ has a degenerate spectrum: two equal eigenvalues.

$$\hat{B} = \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix} \Rightarrow \begin{vmatrix} b-\lambda & 0 & 0 \\ 0 & -\lambda & -ib \\ 0 & ib & -\lambda \end{vmatrix} = 0 \Rightarrow (b-\lambda)(\lambda^2-b^2) = 0\ .$$

It is clear from the determinant for the eigenvalues of $\hat{B}$ to have a degenerate spectrum: two equal eigenvalues.

Show that $\hat{A}$ and $\hat{B}$ commute:

$$\hat{A}\hat{B} - \hat{B}\hat{A} = \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix}\begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix} - \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix}\begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix} =$$

$$= \begin{pmatrix} ab & 0 & 0 \\ 0 & 0 & iab \\ 0 & -iab & 0 \end{pmatrix} - \begin{pmatrix} ba & 0 & 0 \\ 0 & 0 & iba \\ 0 & -iba & 0 \end{pmatrix} = 0,$$

since $a$ en $b$ are real numbers.

We learned that commuting operators have a common set of eigenvectors.

Find a new set of orthonormal kets which are simultaneously eigenkets of both $\hat{A}$ and $\hat{B}$.

I use the notation of Boccio.

Let $|u^i\rangle$ be an eigenvector of $\hat{A}$ with eigenvalue $\lambda_i$: $\hat{A}|u^i\rangle = \lambda_i|u^i\rangle$.

With $(a-\lambda)(a+\lambda)(a+\lambda) = 0$

$$\begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & a \end{pmatrix}\begin{pmatrix} u_1^1 \\ u_2^1 \\ u_3^1 \end{pmatrix} = a\begin{pmatrix} u_1^1 \\ u_2^1 \\ u_3^1 \end{pmatrix} \Longrightarrow au_1^1 = au_1^1 \Longrightarrow u_1^1 = ?\,,\ -au_2^1 = au_2^1 \Longrightarrow u_2^1 = 0\ ,$$

$-au_3^1 = au_3^1 \Longrightarrow u_3^1 = 0.$

Consequently, with normalization

$|u_1^1|^2 + |u_2^1|^2 + |u_3^1|^2 = 1$, and

$$u_2^1 = u_3^1 = 0, \Longrightarrow u_1^1 = 1 \Longrightarrow |u^1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

With the usual notation, it follows $|u^1\rangle = |1\rangle$ .

What about the degenerate eigenvalue $-a$ and the eigenvector $|u^2\rangle$?

$$\begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix}\begin{pmatrix} u_1^2 \\ u_2^2 \\ u_3^2 \end{pmatrix} = -a\begin{pmatrix} u_1^2 \\ u_2^2 \\ u_3^2 \end{pmatrix} \Longrightarrow au_1^2 = -au_1^2 \Longrightarrow u_1^2 = 0\ ,$$

$-au_2^2 = -au_2^2 \Longrightarrow u_2^2 = ?$, $-au_3^2 = -au_3^2 \Longrightarrow u_3^2 = ?$

Normalization gives:

$|u_1^2|^2 + |u_2^2|^2 + |u_3^2|^2 = 1 \Longrightarrow |u_2^2|^2 + |u_3^2|^2 = 1.$

So, here stops the buck for $\hat{A}$. The new eigenvector $|u^1\rangle = |1\rangle$, is found. The element $u_1^2 = 0$, is obtained and the normalization relation $|u_2^2|^2 + |u_3^2|^2 = 1$. Then for the second eigenvector we have: $|u^2\rangle = \begin{pmatrix} 0 \\ u_2^2 \\ u_3^2 \end{pmatrix}$.

Next, we evaluate $\hat{B}$, with the eigen values $\pm b$.

$$\begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix}\begin{pmatrix} 0 \\ u_2^2 \\ u_3^2 \end{pmatrix} = b\begin{pmatrix} 0 \\ u_2^2 \\ u_3^2 \end{pmatrix} \Longrightarrow -ibu_3^2 = bu_2^2\,, ibu_2^2 = bu_3^2 \Longrightarrow iu_2^2 = u_3^2.$$

Using normalization:

$|u_1^2|^2 + |u_2^2|^2 + |u_3^2|^2 = 1 \Longrightarrow 2|u_3^2|^2 = 1 \Longrightarrow u_3^2 = \frac{1}{\sqrt{2}}$, and $u_2^2 = -i\frac{1}{\sqrt{2}}$.

Hence

$$|u^2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(-i|2\rangle + |3\rangle).$$

One eigenvector to be evaluated. Let’s use the eigenvalue $-b$.

Then,

$$\begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix}\begin{pmatrix} u_1^3 \\ u_2^3 \\ u_3^3 \end{pmatrix} = -b\begin{pmatrix} u_1^3 \\ u_2^3 \\ u_3^3 \end{pmatrix} \Longrightarrow bu_1^3 = -bu_1^3 \Longrightarrow u_1^3 = 0\,, -ibu_3^3 = -bu_2^3$$ , and $ibu_2^3 = -bu_3^3$ .

So, for $|u^3\rangle$, we have: $|u^3\rangle = \begin{pmatrix} 0 \\ u_2^3 \\ -iu_2^3 \end{pmatrix}$.

Again, with normalization $|u_1^3|^2 + |u_2^3|^2 + |u_3^3|^2 = 1 \Longrightarrow 2|u_2^3|^2 = 1 \Longrightarrow u_2^3 = \frac{1}{\sqrt{2}}$.

Finally

$$|u^3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -i \end{pmatrix} = \frac{1}{\sqrt{2}}(|2\rangle - i|3\rangle).$$

We found a new orthonormal set $|u^i\rangle$.

Obviously, I need not to demonstrate:

$\langle u^1|u^2\rangle = 0$ , $\langle u^1|u^2\rangle = 0$, and $\langle u^2|u^3\rangle = 0$ .

Remark 1:

$|u^1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |1\rangle$ , is an eigenvector.

After inspection, it appears $|2\rangle$ and $|3\rangle$, are eigenvectors too.

My results differ not essentially from the results of Boccio. Furthermore, I did not choose any elements. The eigenvectors followed from the basic rules.

**Remark 2:**

A $3 \times 3$ matrix and a $3 \times 3$ determinant are the usual suspects. For that reason I used the following Memoria Technica:

$$\begin{vmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{vmatrix} = b_{11}\begin{vmatrix} b_{22} & b_{23} \\ b_{32} & b_{33} \end{vmatrix} - b_{12}\begin{vmatrix} b_{21} & b_{23} \\ b_{31} & b_{33} \end{vmatrix} + b_{13}\begin{vmatrix} b_{21} & b_{22} \\ b_{31} & b_{32} \end{vmatrix},$$ or

$$\begin{vmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{vmatrix} = \begin{vmatrix} \boldsymbol{b_{11}} & 0 & 0 \\ 0 & \boldsymbol{b_{22}} & \boldsymbol{b_{23}} \\ 0 & \boldsymbol{b_{32}} & \boldsymbol{b_{33}} \end{vmatrix} - \begin{vmatrix} 0 & \boldsymbol{b_{12}} & 0 \\ \boldsymbol{b_{21}} & 0 & \boldsymbol{b_{23}} \\ \boldsymbol{b_{31}} & 0 & \boldsymbol{b_{33}} \end{vmatrix} + \begin{vmatrix} 0 & 0 & \boldsymbol{b_{13}} \\ \boldsymbol{b_{21}} & \boldsymbol{b_{22}} & 0 \\ \boldsymbol{b_{31}} & \boldsymbol{b_{32}} & 0 \end{vmatrix}.$$

### 4.22.18 The World of Hard/Soft Particles

Let us define a state using a *hardness* basis $\{|h\rangle, |s\rangle\}$, where

$\hat{O}_H|h\rangle = |h\rangle$, and $\hat{O}_H|s\rangle = -1|s\rangle$ .

Suppose that the system is in a state

$|A\rangle = \cos\theta\,|h\rangle + e^{i\varphi}\sin\theta\,|s\rangle$.

**a)** Is this state normalized?

Boccio showed the result of $\langle A|A\rangle$ to be 1.

It is about the calculation of the inner product:

$[\cos\theta\,\langle h| + e^{-i\varphi}\sin\theta\,\langle s|][\cos\theta\,|h\rangle + e^{i\varphi}\sin\theta\,|s\rangle]$.

**b)** Find a state $|B\rangle$ orthonormal to $|A\rangle$.

We expand $|B\rangle$ in the basis $\{|h\rangle, |s\rangle\}$: $|B\rangle = c_1|h\rangle + c_2|s\rangle$.

With $\langle A|B\rangle = 0$, and $\langle B|B\rangle = 1$, the state $|B\rangle$ is found:
- $\langle A|B\rangle = 0 \Longrightarrow\ c_2 = -e^{i\varphi}\cot\theta$,
- $\langle B|B\rangle = 1$, and with $c_2 = -e^{i\varphi}\cot\theta \Longrightarrow\ c_1 = \sin\theta$.
Hence,
$|B\rangle = \sin\theta\,|h\rangle - e^{i\varphi}\cos\theta\,|s\rangle$ .
**c)** Express $|h\rangle$, and $|s\rangle$, in the $\{\,|A\rangle, |B\rangle\}$ basis.
$|h\rangle = h_1|A\rangle + h_2|B\rangle$.
Then,
$h_1 = \langle A|h\rangle = \cos\theta\,\langle h|h\rangle + e^{-i\varphi}\sin\theta\,\langle s|h\rangle = \cos\theta$ ,
and
$h_2 = \langle B|h\rangle = \sin\theta\,\langle h|h\rangle - e^{-i\varphi}\cos\theta\,\langle s|h\rangle = \sin\theta$ .
So,
$|h\rangle = \cos\theta\,|A\rangle + \sin\theta\,|B\rangle$ .
Next,
$|s\rangle = s_1|A\rangle + s_2|B\rangle$.
Then,
$s_1 = \langle A|s\rangle = \cos\theta\,\langle h|s\rangle + e^{-i\varphi}\sin\theta\,\langle s|s\rangle = e^{-i\varphi}\sin\theta$ ,
and
$s_2 = \langle B|s\rangle = \sin\theta\,\langle h|s\rangle - e^{-i\varphi}\cos\theta\,\langle s|s\rangle = -e^{-i\varphi}\cos\theta$.
So,
$|s\rangle = e^{-i\varphi}\{\sin\theta\,|A\rangle - \cos\theta\,|B\rangle\} \Longrightarrow \sin\theta\,|A\rangle - \cos\theta\,|B\rangle$ .
**d)** What are the possible outcomes of a hardness measurement on state $|A\rangle$ and with what probabilities?
The outcomes are:
$P(h|A) = |\langle h|A\rangle|^2$, with probability $\cos^2\theta$,
and
$P(s|A) = |\langle s|A\rangle|^2$, with probability $\sin^2\theta$ .
e) Express the hardness operator the $\{\,|A\rangle, |B\rangle\}$ basis.
The hardness operator in the $\{|h\rangle, |s\rangle\}$ basis:
$\hat{O}_H = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.
We expressed the operator in its projection operators as we have done before in Problem 4.22.14:
$O_h = \alpha|h\rangle\langle h| + \beta|s\rangle\langle s|$,
where the eigenvalue $\alpha = 1$, and the eigenvalue $\beta = -1$.
So, the old $\hat{O}_H$ observable
$\hat{O}_H = |h\rangle\langle h| - |s\rangle\langle s|$ .
Boccio presented two methods two express the new matrix $\hat{O}_H$ . I present here one of them.
With $\hat{O}_H = |h\rangle\langle h| - |s\rangle\langle s|$, and $|h\rangle$, and $|s\rangle$, in the $\{\,|A\rangle, |B\rangle\}$ basis:
$\hat{O}_H = |h\rangle\langle h| - |s\rangle\langle s| \Longrightarrow (\cos\theta\,|A\rangle + \sin\theta\,|B\rangle)(\cos\theta\langle A| + \sin\theta\,\langle B|) -$
$-(\sin\theta\,|A\rangle - \cos\theta\,|B\rangle)(\sin\theta\,\langle A| - \cos\theta\,\langle B|)$.
Then, Boccio used the most basic column representation for the $\{\,|A\rangle, |B\rangle\}$ basis:
$|A\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, and $|B\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ .

In this way the matrix representation of the projection operators
$|A\rangle\langle A|$, $|A\rangle\langle B|$, $|B\rangle\langle A|$ and $|B\rangle\langle B|$ ,
are obtained.

**Remark: $|A\rangle\langle B|$ , and $|B\rangle\langle A|$, are no projection operators at all!**

This results in the new matrix for $\hat{O}_H$. I think this matrix is meaningless.
There is a problem?
We try to find a $2 \times 2$ matrix in the $\{\ |A\rangle, |B\rangle\}$ basis, with unknown eigenvalues $\alpha_{1,2}$.
Then
$\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \alpha_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow a = \alpha_1$ and $c = 0$ .
Furthermore
$\begin{pmatrix} \alpha_1 & b \\ 0 & d \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \alpha_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \Rightarrow d = \alpha_2$ and $b = 0$ .
So, the matrix reads:
$\begin{pmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{pmatrix}$.
This matrix differs from what Boccio obtained:
$\hat{O}_H = \begin{pmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{pmatrix}$.
Now, use the $\{\ |A\rangle, |B\rangle\}$ basis and you will find the element $\sin 2\theta = 0$ , and
$\hat{O}_H = \begin{pmatrix} \cos 2\theta & 0 \\ 0 & -\cos 2\theta \end{pmatrix}$.
That is the problem.
The eigenvalues of $\begin{pmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{pmatrix}$ are $\pm 1$. That is correct in the $\{|h\rangle, |s\rangle\}$ basis with
$\hat{O}_H = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.
Let's pay some more attention to the matrix:
$\begin{pmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{pmatrix}$, with the eigenvalues $\pm 1$, the eigenvectors are $\begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix}$, and $\begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$ .
Then
$\begin{pmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{pmatrix} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}(\cos\theta\ \ \sin\theta) - \begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix}(\sin\theta\ \ \cos\theta)$.
These eigenvectors are orthonormal⟹a basis. Well, I leave this problem, with some problems left. The major one is, page 44 Boccio, $|B\rangle\langle A|$, and $|A\rangle\langle B|$, are used as projection operators. These two are just outer products! When you get rid of these, the operator is:
$\hat{O}_H = \begin{pmatrix} \cos 2\theta & 0 \\ 0 & -\cos 2\theta \end{pmatrix}$.
Note: The eigenvalues $\lambda_i$ of $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ are obtained from the determinant:
$\begin{vmatrix} a-\lambda & b \\ c & d-\lambda \end{vmatrix} = 0 \Rightarrow \lambda_{1,2} = \frac{1}{2}(a+d) \pm \sqrt{\frac{1}{4}(a-d)^2 - bc}$ .

### 4.22.19 Things in Hilbert Space

For all parts of this problem, let $\mathcal{H}$ be a Hilbert space spanned by the basis kets $\{|0\rangle, |1\rangle, 2\rangle, 3\rangle\}$, and let $a$ and $b$ be arbitrary complex constants.

**a)** Which of the following operators are Hermitian operators on $\mathcal{H}$?

- $|0\rangle\langle 1| + i|1\rangle\langle 0| \Longrightarrow$ take the complex conjugate of these outer products of bras and kets. The conclusion is not Hermitian.
- $|0\rangle\langle 0| + |1\rangle\langle 1| + |2\rangle\langle 3| + |3\rangle\langle 2|$ . A combination of projection operators being Hermitian and a symmetric combination of outer products being Hermitian.
- $(a|0\rangle + |1\rangle)^\dagger(a|0\rangle + |1\rangle) = (a^*\langle 0| + \langle 1|)(a|0\rangle + |1\rangle) = a^*a + 1$, a real number. Consequently Hermitian. A number as operator.
- $[(a|0\rangle + b^*|1\rangle)^\dagger(b|0\rangle - a^*|1\rangle)]|2\rangle\langle 1| + |3\rangle\langle 3| =$

$= [(a^*\langle 0| + b\langle 1|)(b|0\rangle - a^*|1\rangle)]|2\rangle\langle 1| + |3\rangle\langle 3| =$

$(a^*b - ba^*)|2\rangle\langle 1| + |3\rangle\langle 3| = |3\rangle\langle 3|$. The operator is Hermitian.

- $|0\rangle\langle 0| + i|1\rangle\langle 0| - i|0\rangle\langle 1| + |1\rangle\langle 1|$ .

Then,

$(|0\rangle\langle 0| + i|1\rangle\langle 0| - i|0\rangle\langle 1| + |1\rangle\langle 1|)^\dagger = |0\rangle\langle 0| - i|0\rangle\langle 1| + i|1\rangle\langle 0| + |1\rangle\langle 1|$.

The operator is Hermitian.

**b)** Find the spectral decomposition of the following operator on $\mathcal{H}$:

$\hat{K} = |0\rangle\langle 0| + 2|1\rangle\langle 2| + 2|2\rangle\langle 1| - |3\rangle\langle 3|$.

From this operator follows the $4 \times 4$ matrix.

Then,

$$\hat{K} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}(1\;0\;0\;0) + 2\begin{pmatrix}0\\1\\0\\0\end{pmatrix}(0\;0\;1\;0) + 2\begin{pmatrix}0\\0\\1\\0\end{pmatrix}(0\;1\;0\;0) - \begin{pmatrix}0\\0\\0\\1\end{pmatrix}(0\;0\;0\;1) =$$

$$= \begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix} + \begin{pmatrix}0&0&0&0\\0&0&2&0\\0&0&0&0\\0&0&0&0\end{pmatrix} + \begin{pmatrix}0&0&0&0\\0&0&0&0\\0&2&0&0\\0&0&0&0\end{pmatrix} - \begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&1\end{pmatrix}.$$

Hence,

$$\hat{K} = \begin{pmatrix}1&0&0&0\\0&0&2&0\\0&2&0&0\\0&0&0&-1\end{pmatrix}.$$

The eigenvalues follows from:

$$\begin{vmatrix}1-\lambda&0&0&0\\0&-\lambda&2&0\\0&2&-\lambda&0\\0&0&0&-1-\lambda\end{vmatrix} = 0.$$

A $4 \times 4$ determinant with a lot of zero's .

This gives the following polynomial in $\lambda$:

$$(1-\lambda)\Big(-\lambda\big(-\lambda(-1-\lambda)\big) - 2\cdot 2(-1-\lambda)\Big) = 0 \Longrightarrow (1-\lambda)(1+\lambda)(4-\lambda^2) =$$

$$= (1-\lambda)(1+\lambda)(2-\lambda)(2+\lambda) = 0,$$

four eigenvalues.

The eigenvectors are:

for $\lambda = 1, |\lambda_1\rangle = |0\rangle$,

for $\lambda = -1, |\lambda_2\rangle = |3\rangle$, for $\lambda = 2, |\lambda_3\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}[|1\rangle + |2\rangle]$,

and for $\lambda = -2, |\lambda_4\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}[|1\rangle - |2\rangle]$.

So:

$\hat{K} = 1 \cdot |\lambda_1\rangle - 1 \cdot |\lambda_2\rangle + 2 \cdot |\lambda_3\rangle - 2 \cdot |\lambda_4\rangle$.

**c)** Let $|\Psi\rangle$ be a normalized ket in $\mathcal{H}$, and let $\hat{I}$ denote the identity operator on $\mathcal{H}$. Is the operator

$\hat{B} = \frac{1}{\sqrt{2}}(\hat{I} + |\Psi\rangle\langle\Psi|)$

a projection operator?

Boccio showed by calculating the square of $\hat{B}$, $\hat{B}$ not to be a projection operator since $\hat{B}^2 \neq \hat{B}$. This is an elegant way using the property of projection operators. It is basically about:

$|\Psi\rangle\langle\Psi|\Psi\rangle\langle\Psi| = |\Psi\rangle\langle\Psi|$.

**d)** Find the spectral decomposition of $\hat{B} = \frac{1}{\sqrt{2}}(\hat{I} + |\Psi\rangle\langle\Psi|)$.

Boccio showed $|\Psi\rangle$ to be an eigen vector of $\hat{B}$, with eigenvalue $\sqrt{2}$.

This was shown in the following way:

$\hat{B}|\Psi\rangle = \frac{1}{\sqrt{2}}(\hat{I} + |\Psi\rangle\langle\Psi|)|\Psi\rangle = \frac{1}{\sqrt{2}}\left[\hat{I}|\Psi\rangle + |\Psi\rangle\langle\Psi|\Psi\rangle\right] = \frac{1}{\sqrt{2}}[|\Psi\rangle + |\Psi\rangle] = \sqrt{2}|\Psi\rangle$.

Now,

$|\Psi\rangle\langle\Psi| = 2|\Psi\rangle\langle\Psi| - |\Psi\rangle\langle\Psi| \Rightarrow \frac{1}{\sqrt{2}}|\Psi\rangle\langle\Psi| = \sqrt{2}|\Psi\rangle\langle\Psi| - \frac{1}{\sqrt{2}}|\Psi\rangle\langle\Psi|$.

So, using the preceding expression, $\hat{B}$ is decomposed

$\hat{B} = \frac{1}{\sqrt{2}}(\hat{I} + |\Psi\rangle\langle\Psi|) = \sqrt{2}|\Psi\rangle\langle\Psi| - \frac{1}{\sqrt{2}}|\Psi\rangle\langle\Psi| + \frac{1}{\sqrt{2}}\hat{I} = \sqrt{2}|\Psi\rangle\langle\Psi| + \frac{1}{\sqrt{2}}(\hat{I} - |\Psi\rangle\langle\Psi|)$.

Hence , the operator is decomposed in the projection operator times the eigenvalue $\sqrt{2}$ plus $\frac{1}{\sqrt{2}}(\hat{I} - |\Psi\rangle\langle\Psi|)$ .

$\frac{1}{\sqrt{2}}(\hat{I} - |\Psi\rangle\langle\Psi|)$ needs to be decomposed into eigenvalues times projection operators.

Notice $(\hat{I} - |\Psi\rangle\langle\Psi|)$ to be a projection operator. And eigenvalue $\frac{1}{\sqrt{2}}$ .

How to decompose this projection operator? Hilbert space is still 4-dimensional, I suppose.

So, I need to decompose $(\hat{I} - |\Psi\rangle\langle\Psi|)$.

Hidden in plain sight, $(\hat{I} - |\Psi\rangle\langle\Psi|)$ consists of three projection operators with the same eigenvalue $\frac{1}{\sqrt{2}}$ .

Define an orthonormal basic set $|q_i\rangle$, one of the kets is $|\Psi\rangle$, with eigenvalue $\sqrt{2}$ .The other three are $|q_i\rangle$, with eigen value $\frac{1}{\sqrt{2}}$ .

So,

$\hat{I} = |q_1\rangle\langle q_1| + |q_2\rangle\langle q_2| + |q_3\rangle\langle q_3| + |\Psi\rangle\langle\Psi|$.

Hence
$\hat{I} - |\Psi\rangle\langle\Psi| = |q_1\rangle\langle q_1| + |q_2\rangle\langle q_2| + |q_3\rangle\langle q_3|$.
Consequently
$\hat{B} = \frac{1}{\sqrt{2}}(\hat{I} + |\Psi\rangle\langle\Psi| = \sqrt{2}|\Psi\rangle\langle\Psi| + \frac{1}{\sqrt{2}}(|q_1\rangle\langle q_1| + |q_2\rangle\langle q_2| + |q_3\rangle\langle q_3|)$.
That is all there is to find out about the spectral decomposition.
The basis kets $\{|0\rangle, |1\rangle, 2\rangle, 3\rangle\}$ could do the job.

### 4.22.20 A 2-Dimensional Hilbert Space

Consider a 2-dimensional Hilbert space. Spanned by an orthonormal basis $\{|\uparrow\equiv u\rangle, |\downarrow\equiv d\rangle\}$.
This corresponds to spin up/down for spin ½ , presented in Chapter 9. In the following, I will use $\{|u\rangle, |d\rangle\}$ to prevent 'arrow clutter'.
There are three operators:
$\hat{S}_x = \frac{\hbar}{2}(|u\rangle\langle d| + |d\rangle\langle u|)$ , $\hat{S}_y = \frac{\hbar}{2i}(|u\rangle\langle d| - |d\rangle\langle u|)$, and $\hat{S}_z = \frac{\hbar}{2}(|u\rangle\langle u| - |d\rangle\langle d|)$.
**a)** Boccio proved, page 259 Section 4.10. *More about Vectors, Linear Functional, Operators*, Eqs. (4.92)-(4.96), the outer product: $|q\rangle\langle p|$ to be Hermitian. I will use this.
**Remark**:
However, let's pay some attention. A question with respect to Eq.(4.92): $|q\rangle$ and $|p\rangle$ are orthogonal? Assume this to be so, then, in Eq.(4.94), $\langle p|q\rangle = 0$. Consequently, $(|q\rangle\langle p|)^\dagger = |q\rangle\langle p|$ , is meaningless. So, in order to make it work $|q\rangle$ and $|p\rangle$ are not orthogonal. One way or the other, we run into trouble with the basis set $\{|\uparrow\equiv u\rangle, |\downarrow\equiv d\rangle\}$. The kets are orthogonal.
In Eq.(4.94), Boccio used the dagger symbol for complex conjugate and transposition, I suppose. Then, $(|q\rangle\langle p|)^\dagger$is the complex conjugate of a transposed matrix.
With Dirac, $(|q\rangle\langle p|)^\dagger = |p\rangle\langle q|$. Plug this into Eq. (4.94) and the question arises whether new information is created. I am confused.

**Note**: I do not know how to relate this with Dirac, page 28 Eq. (7), where Dirac showed the conjugate imaginary of the outer product $|A\rangle\langle B|$ : $\overline{|A\rangle\langle B|} = |B\rangle\langle A|$.
Susskind mentioned the projection operator to be Hermitian: $A = B$.

So, I will use the outer product to be Hermitian.

- $\hat{S}_x{}^\dagger = \frac{\hbar}{2}(|u\rangle\langle d| + |d\rangle\langle u|)^\dagger = \frac{\hbar}{2}\left[(|u\rangle\langle d|)^\dagger + (|d\rangle\langle u|)^\dagger\right] = \frac{\hbar}{2}(|u\rangle\langle d| + |d\rangle\langle u|) = \hat{S}_x$.
As far as I am concerned, in this case there is no confusion. Since, using Dirac,
$\hat{S}_x{}^\dagger = \frac{\hbar}{2}(|u\rangle\langle d| + |d\rangle\langle u|)^\dagger = \frac{\hbar}{2}(|d\rangle\langle u| + |u\rangle\langle d|) = \hat{S}_x$ .
- $\hat{S}_y{}^\dagger = (\frac{\hbar}{2i}(|u\rangle\langle d| - |d\rangle\langle u|))^\dagger = \frac{\hbar}{2}i[|d\rangle\langle u| - |u\rangle\langle d|] = \frac{\hbar}{2i}(|u\rangle\langle d| - |d\rangle\langle u|) = \hat{S}_y$.
There is no need to use the outer product to be Hermitian. I used $\overline{|A\rangle\langle B|} = |B\rangle\langle A|$, Dirac.
Finally,
$(\hat{S}_z)^\dagger = \frac{\hbar}{2}(|u\rangle\langle u| - |d\rangle\langle d|)^\dagger$.
We have two projection operators. Projection operators are Hermitian. Consequently,

$(\hat{S}_z)^\dagger = \frac{\hbar}{2}(|u\rangle\langle u| - |d\rangle\langle d|)^\dagger = \frac{\hbar}{2}(|u\rangle\langle u| - |d\rangle\langle d|) = \hat{S}_z$.

**b)** Matrix representations of the operators $\hat{S}_x$ , $\hat{S}_y$ and $\hat{S}_z$.

There are two ways to proceed:

- the method presented by Boccio, page 46, e.g.,

$$\hat{S}_x = \begin{pmatrix} \langle u|\hat{S}_x|u\rangle & \langle u|\hat{S}_x|d\rangle \\ \langle d|\hat{S}_x|u\rangle & \langle d|\hat{S}_x|d\rangle \end{pmatrix},$$

with $\hat{S}_x = \frac{\hbar}{2}(|u\rangle\langle d| + |d\rangle\langle u|)$, $\langle u|\hat{S}_x|u\rangle = 0$, $\langle d|\hat{S}_x|d\rangle = 0$, $\langle d|\hat{S}_x|u\rangle = 1$, and $\langle u|\hat{S}_x|d\rangle = 1$.

- by choosing the column representation of $|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

I have chosen the latter method.

Through this choice of $|u\rangle \Longrightarrow |d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ . The two kets being orthonormal.

- $\hat{S}_x = \frac{\hbar}{2}(|u\rangle\langle d| + |d\rangle\langle u|) \Longrightarrow \hat{S}_x|u\rangle = \frac{\hbar}{2}|d\rangle$ .

- $\hat{S}_x = \frac{\hbar}{2}(|u\rangle\langle d| + |d\rangle\langle u|) \Longrightarrow \hat{S}_x|d\rangle = \frac{\hbar}{2}|u\rangle$ .

With $\hat{S}_x = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, and the preceding two equations: $\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ .

Simarlily:

$\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and $\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

**c)** The commutator $[\hat{S}_x, \hat{S}_y] = \frac{\hbar^2}{4i}[(|u\rangle\langle d| + |d\rangle\langle u|)(|u\rangle\langle d| - |d\rangle\langle u|) -$

$-(|u\rangle\langle d| - |d\rangle\langle u)(|u\rangle\langle d| + |d\rangle\langle u)] = \frac{\hbar^2}{4i}[|d\rangle\langle d| - |u\rangle\langle u| + |d\rangle\langle d| - |u\rangle\langle u|] = -\frac{\hbar^2}{4i}\frac{4}{\hbar}\hat{S}_z$.

Hence,

$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z, \Longrightarrow\ [\hat{S}_y, \hat{S}_z] = i\hbar\hat{S}_x$ , and $[\hat{S}_z, \hat{S}_x] = i\hbar\hat{S}_y$ .

The same result is obtained by using the matrix representation in the commutators.

An example of this is given by Boccio on page 47. It is about matrix multiplication.

**d)** Two vectors:

$|+\rangle = \frac{1}{\sqrt{2}}(|u\rangle + |d\rangle)$, and $|-\rangle = \frac{1}{\sqrt{2}}(|u\rangle - |d\rangle)$.

Boccio made the remark $|+\rangle$ and $|-\rangle$ to be eigenvectors of $\hat{S}_x$. I could show this by using the matrix representation of $\hat{S}_x$ and the column representation of $|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, and $|d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

And also in the outer product representation of $\hat{S}_x$:

$\hat{S}_x = \frac{\hbar}{2}(|u\rangle\langle d| + |d\rangle\langle u|)$ and, e.g., $|+\rangle = \frac{1}{\sqrt{2}}(|u\rangle + |d\rangle) \Longrightarrow$

$\Longrightarrow (|u\rangle\langle d| + |d\rangle\langle u|)(|u\rangle + |d\rangle) = |d\rangle + |u\rangle$.

Show these vectors, $|+\rangle$ and $|-\rangle$, form a new orthonormal basis.

Then,

$\langle +|+\rangle = 1$ , and $\langle +|-\rangle = 0$ .

$\langle +|+\rangle = \frac{1}{\sqrt{2}}(\langle u| + \langle d|)\frac{1}{\sqrt{2}}(|u\rangle + |d\rangle) = \frac{1}{2}[\langle u|u\rangle + 2\langle u|d\rangle + \langle d|d\rangle] = 1$.

$\langle +|-\rangle = \frac{1}{\sqrt{2}}(\langle u| + \langle d|)\frac{1}{\sqrt{2}}(|u\rangle - |d\rangle) = \frac{1}{2}[\langle u|u\rangle + 2\langle u|d\rangle - \langle d|d\rangle] = 0$.

Hence, they form an orthonormal basis.

We can also write:

$|u\rangle = \frac{1}{\sqrt{2}}[\ |+\rangle + |-\rangle]$,

and

$|d\rangle = \frac{1}{\sqrt{2}}[\,|+\rangle - |-\rangle].$

**e)** Find the matrix representations of these operators in the $\{|+\rangle, |-\rangle\}$ basis.

$\hat{S}_x = \frac{\hbar}{2}(|u\rangle\langle d| + |d\rangle\langle u|)$, with

$|u\rangle = \frac{1}{\sqrt{2}}[\,|+\rangle + |-\rangle]$ and $|d\rangle = \frac{1}{\sqrt{2}}[\,|+\rangle - |-\rangle]$, the result in the $\{|+\rangle, |-\rangle\}$ basis is:

$\hat{S}_x = \frac{\hbar}{2}[|+\rangle\langle+| - |-\rangle\langle-|].$

So, we obtained the expression for the operator in the representation of projection operators with eigen values $+\frac{\hbar}{2}$, and $-\frac{\hbar}{2}$.

The representation in projection operators can be transferred into a matrix.

For this I use:

$|+\rangle = \frac{1}{\sqrt{2}}(|u\rangle + |d\rangle)$, and $|-\rangle = \frac{1}{\sqrt{2}}(|u\rangle - |d\rangle)$.

Boccio calculated the matrix elements of, e.g.,

$$\hat{S}_x^{\pm} = \frac{\hbar}{2}\begin{pmatrix} \langle+|\hat{S}_x^{ud}|+\rangle & \langle+|\hat{S}_x^{ud}|-\rangle \\ \langle-|\hat{S}_x^{ud}|+\rangle & \langle-|\hat{S}_x^{ud}|-\rangle \end{pmatrix} = \hat{S}_z^{ud},$$

and $\hat{S}_y^{\pm} = -\hat{S}_y^{ud}$, $\hat{S}_z^{\pm} = \hat{S}_x^{ud}$.

Well, from a geometrical point of view, the $x$-axis is rotated to the $z$-axis and the $y$-axis is rotated to the $-y$-axis. In this way the $z$-axis is rotated to the $x$-axis.

**f)** The matrices found in **b)** and **e)** are related through a similarity transformation given by a unitary matrix $U$, such that

$\hat{S}_x^{ud} = U^\dagger \hat{S}_x^{\pm} U, \qquad \hat{S}_y^{ud} = U^\dagger \hat{S}_y^{\pm} U,$ and $\hat{S}_z^{ud} = U^\dagger \hat{S}_z^{\pm} U$,

or

$\hat{S}_x^{ud} = U^\dagger \hat{S}_z^{ud} U, \qquad \hat{S}_y^{ud} = -U^\dagger \hat{S}_y^{ud} U,$ and $\hat{S}_z^{ud} = U^\dagger \hat{S}_x^{ud} U.$

The superscripts denotes the basis in which the operator is represented. Find $U$ and show that it is unitary.

Let us look into

$\hat{S}_y^{ud} = U^\dagger \hat{S}_y^{\pm} U$, with $\hat{S}_y^{\pm} = -\hat{S}_y^{ud}$, (as shown by Boccio).

Then,

$\hat{S}_y^{ud} = -U^\dagger \hat{S}_y^{ud} U \Longrightarrow -U^\dagger \hat{S}_y^{ud} U = (-U^\dagger)^2 \hat{S}_y^{ud} U^2 = \hat{S}_y^{ud}.$

Hence, in general,

$\hat{S}_y^{ud} = (-)^n (U^\dagger)^n \hat{S}_y^{ud} U^n.$

For $n$ is even I think $(U^\dagger)^n$ and $U^n$ are unitary. Let us find out.

$U$ to be unitary needs to satisfy:

$U^\dagger U = I.$

Now, to find out about the matrix elements of $U$, I will use brute force.

In general:

$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, so $U^\dagger = \begin{pmatrix} a & c^* \\ b^* & d \end{pmatrix}$.

Then, with the matrix representations of $\hat{S}_x^{ud}, \hat{S}_y^{ud}$, and $\hat{S}_z^{ud}$, in addition with $\hat{S}_x^{\pm} = \hat{S}_z^{ud}$, $\hat{S}_y^{\pm} = -\hat{S}_y^{ud}$, $\hat{S}_z^{\pm} = \hat{S}_x^{ud}$, you will find a set of 12 equations.

Let us start, I leave out the details, and present the equations I need.

$\hat{S}_x^{ud} = U^\dagger \hat{S}_z^{ud} U \Rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} a & c^* \\ b^* & d \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Rightarrow$

$\Rightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} a^2 - c^*c & ab - c^*d \\ b^*a - dc & b^*b - d^2 \end{pmatrix}.$

$\hat{S}_y^{ud} = -U^\dagger \hat{S}_y^{ud} U \Rightarrow \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = -\begin{pmatrix} a & c^* \\ b^* & d \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Rightarrow$

$\Rightarrow \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} -ac + c^*a & -ad + c^*b \\ -b^*c + da & -b^*d + db \end{pmatrix}.$

$\hat{S}_z^{ud} = U^\dagger \hat{S}_x^{ud} U \Rightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} a & c^* \\ b^* & d \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Rightarrow$

$\Rightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} ac + c^*a & ad + c^*b \\ b^*c + da & b^*d + db \end{pmatrix}.$

The first set of equations to be analysed:

$a^2 - c^*c = 0$ ,

$-ac + c^*a = 0,$

$ac + c^*a = 1.$

This results into:

$2ac = 1$ , $2c^*a = 1$, and $a(c - c^*) = 0$ .

I conclude $a \neq 0 \therefore c = c^*$.

Then, with $a^2 - c^*c = 0 \Rightarrow a = \pm\frac{1}{2}\sqrt{2}$ , and $c = \pm\frac{1}{2}\sqrt{2}$ .

The second set of equations to be analysed:

$b^*b - d^2 = 0$ ,

$-b^*d + db = 0,$

$b^*d + db = -1.$

This results into:

$2db = -1$ , $2b^*d = -1$, and $d(b - b^*) = 0$.

I conclude $d \neq 0 \therefore b = b^*$.

Then, $b^*b - d^2 = 0 \Rightarrow b = \pm\frac{1}{2}\sqrt{2}$ , and $d = \mp\frac{1}{2}\sqrt{2}$ .

So, to summarize the result:

$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \frac{1}{2}\sqrt{2}\begin{pmatrix} \pm 1 & \pm 1 \\ \pm 1 & \mp 1 \end{pmatrix}.$

We can do a bit more: there are 6 other equations of which 3 are different.

$b^*a - dc = 1 \Rightarrow ba - dc = 1$ , this leads to the conclusion:

$U = \frac{1}{2}\sqrt{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$

This $U$ is unitary:

$U^\dagger U = I \Rightarrow \frac{1}{2}\sqrt{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\frac{1}{2}\sqrt{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$

Boccio showed, pages 49 and 50, the unitary matrix to be correct by calculating the matrix multiplication:

$U^\dagger \hat{S}_z^{\pm} U$ to be equal to $\hat{S}_x^{ud}$ ,etc.

**g)** Now let

$\hat{S}_\pm = \frac{1}{2}(\hat{S}_x^{ud} \pm i\hat{S}_y^{ud}).$

Express $\hat{S}_\pm$ as outer products in the $\{|u\rangle, |d\rangle\}$ basis and show that $\hat{S}_+^\dagger = \hat{S}_-$. May be the $\pm$ subscript is a bit confusing. Here, the $\pm$ is not the indication of the $\{|+\rangle, |-\rangle\}$ basis.

$\hat{S}_{\pm} = \frac{\hbar}{4}[(|u\rangle\langle d| + |d\rangle\langle u|) \pm (|u\rangle\langle d| - |d\rangle\langle u|)]$.
Then,
$\hat{S}_{+} = \frac{\hbar}{2}|u\rangle\langle d|$, and $\hat{S}_{-} = \frac{\hbar}{2}|d\rangle\langle u|$, $\Longrightarrow \hat{S}_{+}^{\dagger} = \frac{\hbar}{2}|d\rangle\langle u| = \hat{S}_{-}$, and $(\hat{S}_{+}^{\dagger})^{\dagger} = \frac{\hbar}{2}|u\rangle\langle d| = \hat{S}_{-}^{\dagger}$.
**h)** With the results of **g)** :
$\hat{S}_{+}|d\rangle = \frac{\hbar}{2}|u\rangle\langle d|d\rangle = \frac{\hbar}{2}|u\rangle$ ,
$\hat{S}_{-}|u\rangle = \frac{\hbar}{2}|d\rangle\langle u|u\rangle = \frac{\hbar}{2}|d\rangle$ ,
$\hat{S}_{-}|d\rangle = \frac{\hbar}{2}|d\rangle\langle u|d\rangle = 0$ ,
and
$\hat{S}_{+}|u\rangle = \frac{\hbar}{2}|u\rangle\langle d|u\rangle = 0$ .
Then,
$\langle u|\hat{S}_{+} = \frac{\hbar}{2}\langle u|d\rangle\langle u| = 0$ ,
$\langle d|\hat{S}_{+} = \frac{\hbar}{2}\langle d|d\rangle\langle u| = \frac{\hbar}{2}\langle u|$,
$\langle u|\hat{S}_{-} = \frac{\hbar}{2}\langle u|u\rangle\langle d| = \frac{\hbar}{2}\langle d|$ ,
and
$\langle d|\hat{S}_{-} = \frac{\hbar}{2}\langle d|u\rangle\langle d| = 0$.

### 4.22.21. Find the Eigenvalues

The three matrices $M_x, M_y, M_z$, each with 256 rows and columns, obey the commutation rules
$[M_i, M_j] = i\hbar\varepsilon_{ijk}M_k$ .
The eigenvalues of $M_z$ are $\pm 2\hbar$ (each once), $\pm 2\hbar$ (each once), $\pm 3\hbar/2$ (each 8 times), $\pm\hbar$ (each 28 times), $\pm\hbar/2$ (each 56 times), and 0 (70 times). State the 256 eigenvalues of the matrix $M^2 = M_x^2 + M_y^2 + M_z^2$.
The matrices $M_i$ represent the $i^{th}$ component of some angular momentum operator $\vec{J}$ in some basis $\{\alpha, j, m\}$. For each set of values $(\alpha, j)$ there are $2j+1$ different values of $m$. There can be basis vectors with the same value of $j$ but different values of $m$.

**Questions**: is this about quantum mechanics and orbital angular momentum (without spin)? As far as I can see it, spin has not been the subject matter so far. Boccio refers to chapter 9. When it has been the subject matter, which course? When it is about quantum mechanics , why $\alpha$ instead of $n$?
However, $n$ is usually considered to be the radial quantum number. So, in this case I assume spin is represented by the quantum number $\alpha$? Well, this problem is about total angular momentum. So, $\alpha$ has to be the spin quantum number.
A question with respect of the formulation of the problem: why "*The eigenvalues of $M_z$ are $\pm 2\hbar$ (each once), $\pm 2\hbar$ (each once)*….." instead of "$M_z$ are $\pm 2\hbar$ (each twice),….?"
$\vec{J}$ , the total angular momentum? If so, then spin is included.
The commutation relations:
$[M_x, M_y] = i\hbar M_z$,

$[M_y, M_z] = i\hbar M_x,$
and
$[M_z, M_x] = i\hbar M_y.$
Well, I leave this problem. Too many questions.

### 4.22.22. Operator properties

**a)** If $O$ is a quantum-mechanical operator, what is the definition of the corresponding Hermitian conjugate operator, $O^\dagger$? I use the dagger the for conjugate Hermitian symbol. In section 4.11 the definition of the Hermitian conjugate operator is given in Eq. 4.117.
**b)** An operator $\hat{Q}$ is Hermitian when
$\hat{Q}^\dagger = \hat{Q}.$
**c)** Show $\frac{d}{dx}$ not to be Hermitian. Let's denote this operator $\hat{D}$.
For this we use the matrix elements of the operator.
The matrix element is $\langle\Psi|\hat{D}|\Phi\rangle$. When $\hat{D}$ is Hermitian, we have
$\langle\Psi|\hat{D}|\Phi\rangle = \langle\Phi|\hat{D}|\Psi\rangle^*.$
As shown by Boccio:
$\langle\Psi|\hat{D}|\Phi\rangle = \int_{-\infty}^{\infty} \psi^* \frac{d\phi}{dx} dx,$
and
$\langle\Phi|\hat{D}|\Psi\rangle = \int_{-\infty}^{\infty} \phi^* \frac{d\psi}{dx} dx = \phi^*\psi|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d\phi^*}{dx}\psi dx.$
With $\phi^*\psi|_{-\infty}^{\infty} \to 0,$
the result is:
$\langle\Psi|\hat{D}|\Phi\rangle = -\langle\Phi|\hat{D}|\Psi\rangle^*.$
Hence , the Hermitian conjugate of
$\hat{D}^\dagger = -\hat{D}$ .
**d)** Prove that for any two operators $A$ and $B$ , $(AB)^\dagger = B^\dagger A^\dagger$.
With Dirac Algebra.
We make use of Eq. (7) page 21 Dirac:
$\langle\Psi|\Phi\rangle = \langle\Phi|\Psi\rangle^*.$
Now, pages 27 and 28, Dirac:
$\langle\Psi_1| = \langle\Psi_2|A \Longrightarrow |\Psi_1\rangle = A^\dagger|\Psi_2\rangle,$
and
$\langle\Phi_1| = \langle\Phi_2|B^\dagger \Longrightarrow |\Phi_1\rangle = B|\Phi_2\rangle.$
Then,
$\langle\Phi_2|B^\dagger A^\dagger|\Psi_2\rangle = \langle\Psi_2|AB|\Phi_2\rangle^\dagger = \langle\Phi_2|(AB)^\dagger|\Psi_2\rangle.$
Dirac: "This holds for any $|\Phi_2\rangle$, and $|\Psi_2\rangle$, we can infer
$B^\dagger A^\dagger = (AB)^\dagger.$

### 4.22.23 Ehrenfest's Relations

**a)** Show that the following relation applies for any operator $O$ that lacks an explicit dependence on time:
$\frac{\partial}{\partial t}\langle O\rangle = \frac{i}{\hbar}\langle[H, O]\rangle.$

Assume at a time $t$ the state of the system is represented by $|\Psi\rangle$.
So, with the product rule, $O$ not dependent explicitly on time and Schrödinger's equation,
$\frac{\partial|\Psi\rangle}{\partial t} = -\frac{i}{\hbar}H|\Psi\rangle$,
$\frac{\partial}{\partial t}\langle O\rangle \equiv \frac{\partial}{\partial t}\langle\Psi|O|\Psi\rangle = \left\langle\frac{\partial}{\partial t}\Psi\middle|O\middle|\Psi\right\rangle + \left\langle\Psi\middle|O\middle|\frac{\partial}{\partial t}\Psi\right\rangle = \frac{i}{\hbar}\langle\Psi|HO|\Psi\rangle - \frac{i}{\hbar}\langle\Psi|OH|\Psi\rangle =$
$= \frac{i}{\hbar}\langle\Psi|HO - OH|\Psi\rangle = \frac{i}{\hbar}\langle\Psi|[H,O]|\Psi\rangle \equiv \frac{i}{\hbar}\langle[H,O]\rangle$.
**b)** Use the result under **a)** to derive Ehrenfest's relations, which show that classical physics still applies to expectation values:
$m\frac{\partial}{\partial t}\langle\vec{x}\rangle = \langle\vec{p}\rangle$ ,
and
$\frac{\partial}{\partial t}\langle\vec{p}\rangle = -\langle\nabla V\rangle$ .
We will make use of $\frac{\partial}{\partial t}\langle O\rangle = \frac{i}{\hbar}\langle[H,O]\rangle$, for the position operator:
$\frac{\partial}{\partial t}\langle x\rangle = \frac{i}{\hbar}\langle[H,x]\rangle = \frac{i}{\hbar}\langle\left(\frac{p_x^2}{2m}+V\right)x - x\left(\frac{p_x^2}{2m}+V\right)\rangle = \frac{i}{\hbar}\langle\frac{p_x^2}{2m}x - x\frac{p_x^2}{2m}\rangle =$
$\frac{i}{2m\hbar}\langle p_x p_x x - x p_x p_x\rangle = \frac{i}{2m\hbar}\langle p_x p_x x - p_x x p_x + p_x x p_x - x p_x p_x\rangle =$
$= \frac{i}{2m\hbar}\langle p_x[p_x,x] + [p_x,x]p_x\rangle$.
With $[p_x,x] = -i\hbar$ , we obtain:
$m\frac{\partial}{\partial t}\langle\vec{x}\rangle = \langle\vec{p}\rangle$,
since we will find similar results for $y$ and $z$.
Now,
$\frac{\partial}{\partial t}\langle\vec{p}\rangle = -\langle\nabla V\rangle$.
For the $x$-coordinate, using the commutation of the Hamiltonian and $\frac{p_x^2}{2m}$, we have
$\frac{\partial p_x}{\partial t} = \frac{i}{\hbar}\langle[V,p_x]\rangle = \frac{i}{\hbar}\langle i\hbar\frac{\partial V}{\partial x}\rangle = -\langle\frac{\partial V}{\partial x}\rangle$,
where use has been made of an operator always operates on something.
$[V,p_x]\Psi = Vp_x\Psi - p_xV\Psi = Vp_x\Psi - (p_xV)\Psi - Vp_x\Psi - (p_xV)\Psi$ ,
$\Longrightarrow [V,p_x] = -p_xV$.
Finally,
$\frac{\partial}{\partial t}\langle\vec{p}\rangle = -\langle\nabla V\rangle$,
since we will find similar results for $y$ and $z$.

### 4.22.24 Solutions of Coupled Linear ODE's

Consider the set of coupled linear differential equations $\dot{x} = Ax$, where $x = (x_1, x_2, x_3) \in R^3$, and
$$A = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$
We need the eigenvalues of $A$:
$$\begin{vmatrix} -\lambda & 1 & 1 \\ 1 & -\lambda & 1 \\ 1 & 1 & -\lambda \end{vmatrix} = 0 \Longrightarrow -\lambda^3 + 3\lambda + 2 = 0 \Longrightarrow \lambda^3 + 2\lambda^2 + \lambda - 2\lambda^2 - 4\lambda - 2 = 0.$$

So, we have

$$\lambda(\lambda^2+2\lambda+1)-2(\lambda^2+2\lambda+1)=(\lambda+1)^2(\lambda-2)=0.$$

There are 3 eigenvalues: $\lambda=-1$, twice and $\lambda=2$.

Then, the eigenvectors are found from,

$$Ax=\lambda x,$$

$$\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}\begin{pmatrix}x_1\\x_2\\x_3\end{pmatrix}=\lambda\begin{pmatrix}x_1\\x_2\\x_3\end{pmatrix}.$$

With $\lambda=-1$:

$$x_2+x_3=-x_1,$$
$$x_1+x_3=-x_2,$$
$$x_1+x_2=-x_3.$$

All three equations leading to: $x_1+x_2+x_3=0$ . Then, we have 6 unknowns, the three elements of the 2 column vectors and 5 equations:

$x_1+x_2+x_3=0$ (twice), orthogonality (one) and normalization (two).

This expression creates sufficient possibilities for two elegant and simple vectors, as shown by Boccio, one denoted by $v_{-1,1}$ and the other by $v_{-1,2}$, orthonormal.

So, let us choose one element of the eigenvector equal to zero: $x_1=0$.

Then we have, with $x_1+x_2+x_3=0$

$$x_2=-x_3.$$

Normalization, assuming $(x_1,x_2,x_3)\in R^3$ to be real numbers, gives us the other elements:

$$x_1^2+x_2^2+x_2^2=1\Longrightarrow 2x_3^2=1\Longrightarrow x_3=\tfrac{1}{\sqrt{2}}\Longrightarrow x_2=-\tfrac{1}{\sqrt{2}}.$$

Remark:

Then,

$$v_{-1,2}=\begin{pmatrix}0\\-\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{pmatrix}=\tfrac{1}{\sqrt{2}}\begin{pmatrix}0\\-1\\1\end{pmatrix}\text{, or, phase ambiguity } e^{i\pi}\text{ , } v_{-1,2}=\tfrac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\end{pmatrix}.$$

Now the other eigenvector with eigen value $\lambda=-1$ is completely determined.

Again

$$x_1+x_2+x_3=0\text{ ,}$$
$$x_1^2+x_2^2+x_3^2=1,$$

and

$$(x_1,x_2,x_3)\tfrac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\end{pmatrix}=0\Longrightarrow x_2-x_3=0\Longrightarrow x_2=x_3.$$

With $x_2=x_3$, and $x_1+x_2+x_3=0\Longrightarrow x_1=-2x_3$.

Plugging these results into $x_1^2+x_2^2+x_3^2=1$

$$4x_3^2+2x_3^2=1\Longrightarrow x_3=\tfrac{1}{\sqrt{6}}.$$

For the second eigenvector with $\lambda=-1$, we have

$$v_{-1,1}=\tfrac{1}{\sqrt{6}}\begin{pmatrix}-2\\1\\1\end{pmatrix}.$$

*Intermezzo*

Being curious, let us choose one element of the eigenvector, with eigenvalue $\lambda=-1$ :

$x_1 = 1.$
Then , $x_2 = -1 - x_3$.
$x_1^2 + x_2^2 + x_3^2 = 1 \Longrightarrow 1 + (-1 - x_3)^2 + x_3^2 = 1 \Longrightarrow 2x_3^2 + 2x_3 + 1 = 0$ .
Now, $x_3$, appears to be a complex number. So? With hindsight, meaning given vector $v_{-1,1}$, this will not produce results.
Having chosen the first element equal to zero, the vector is:
$$\begin{pmatrix} 1 \\ x_2 \\ x_3 \end{pmatrix}.$$
This using orthogonality with $v_{-1,1}$, you will find:
$-2 + x_2 + x_3 = 0$ .
We have already:
$1 + x_2 + x_3 = 0$ .
So the choice of $x_1 = 1$ for vector $v_{-1,2}$ is not allowed.
*End of Intermezzo.*
Now the other eigenvalue $\lambda = 2$:
$x_2 + x_3 = 2x_1$,
$x_1 + x_3 = 2x_2$,
$x_1 + x_2 = 2x_3$.
These three equations has as a solution: $x_1 = x_2 = x_3$.
With normalization the vector is:
$$v_2 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix},$$
orthogonal with the other two eigenvectors.
*A Hermitian matrix, $A$, can be diagonalized by a transformation $P^\dagger AP$, where $P$ is a unitary matrix whose columns are the normalized eigenvectors of $A$.*
With the eigenvectors of $A$ the unitary matrix, $P$, which diagonalize $A$, is obtained, given by Boccio on page 54:
$$P = \frac{1}{\sqrt{6}}\begin{pmatrix} -2 & 0 & \sqrt{2} \\ 1 & \sqrt{3} & \sqrt{2} \\ 1 & -\sqrt{3} & \sqrt{2} \end{pmatrix}.$$
The diagonalized $A$, denoted by $A_d$, is
$$A_d = P^\dagger AP = P^T AP = \frac{1}{6}\begin{pmatrix} -2 & 1 & 1 \\ 0 & \sqrt{3} & -\sqrt{3} \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{pmatrix}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}\begin{pmatrix} -2 & 0 & \sqrt{2} \\ 1 & \sqrt{3} & \sqrt{2} \\ 1 & -\sqrt{3} & \sqrt{2} \end{pmatrix} =$$
$$= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$
In addition:
$A_d = P^\dagger AP \Longrightarrow PA_d = PP^\dagger AP = AP \Longrightarrow PA_dP^\dagger = APP^\dagger = A.$
So,
$$A = PA_dP^\dagger = \frac{1}{6}\begin{pmatrix} -2 & 0 & \sqrt{2} \\ 1 & \sqrt{3} & \sqrt{2} \\ 1 & -\sqrt{3} & \sqrt{2} \end{pmatrix}\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}\begin{pmatrix} -2 & 1 & 1 \\ 0 & \sqrt{3} & -\sqrt{3} \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{pmatrix}.$$

This expression is presented by Boccio.
The solution for $x(t)$ with the initial condition $x(t=0)$:

$x(t) = e^{At}x(0)$.

For the analysis the series expansion of the exponential is used.
With $A$ and $e^{At}$ presented by Boccio, $x(0)$ is expanded in eigenvectors of $A$:

$x(t) = e^{-t}c_1\, v_{-1,1} + e^{-t}c_2 + e^{2t}c_3 v_2$.

The resulting expression for $x(t)$ is presented on page 55.

### 4.22.25 Spectral Decomposition Practice

Find the spectral decomposition of the matrix

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & o \end{pmatrix}.$$

The eigenvalues of matrix $A$

$$\begin{vmatrix} 1-\lambda & 0 & 0 \\ 0 & -\lambda & i \\ 0 & -i & -\lambda \end{vmatrix} = 0 \Longrightarrow (1-\lambda)(\lambda^2 - 1) = 0.$$

So, the eigenvalues are $\lambda = 1$, (twice) and $\lambda = -1$.
The first eigen vector is chosen as simple as possible:
with the eigenvector $\begin{pmatrix} a \\ b \\ c \end{pmatrix}$, we can choose $a = 1, b = 0,$ and $c = 0 \Longrightarrow$

$$\Longrightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

Then for the other eigenvector and $\lambda = 1$:
the first element of this eigenvector $a = 0$ , applying orthogonality.
For the other two elements we have:

$ic = b$, and $-ib = c$.

Normalization gives:

$|b|^2 + |c|^2 = 1 \Longrightarrow |c| = \frac{1}{\sqrt{2}}$.

Hence, the most simple eigenvector is:

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ i \\ 1 \end{pmatrix}.$$

The eigen vector with eigenvalue $\lambda = -1$:
the first element is zero, since $a = -a \Longrightarrow a = 0$.
The relation between the other two elements: $ic + b = 0$, and $-ib + c = 0$.
Again $|c| = \frac{1}{\sqrt{2}}$.
Using orthogonality, the eigenvector with $\lambda = -1$ becomes

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix}.$$

With the eigenvectors we can compose the spectral decomposition by the projection operators.

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & o \end{pmatrix} = \lambda_1|\lambda_1\rangle\langle\lambda_1| + \lambda_2|\lambda_2\rangle\langle\lambda_2| + \lambda_3|\lambda_3\rangle\langle\lambda_3|.$$

With the eigen values and the eigenvectors in column representation, the preceding expressions reads:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & o \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}(1\,,0\,,0) + \frac{1}{2}\begin{pmatrix} 0 \\ i \\ 1 \end{pmatrix}(0\,,-i\,,1) - \frac{1}{2}\begin{pmatrix} 0 \\ -i \\ 1 \end{pmatrix}(0\,,i\,,1) =$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & i \\ 0 & -i & 1 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & 1 \end{pmatrix}.$$

### 4.22.26 More on Projection Operators

The basis definition of a projection operator is that it must satisfy $P^2 = P$. If $P$ satisfies $P = P^\dagger$ we say that $P$ is an orthogonal projector. As derived in the course, the eigenvalues of an orthogonal projector are all equal to either zero or one.

**a)** Show that if $P$ is an projection operator, then so is $I - P$.

So, by using the basic definition, we need to find out about $(I - P)^2$:

$(I - P)^2 = I - 2IP + P^2 = I - 2IP + IP = I - IP = I - P.$

**b)** Show that for any orthogonal projector $P$ (meaning projection operator?) and normalized state: $0 \le \langle P\rangle \le 1$.

Any orthogonal projector leads to the choice of a simple and elegant projection operator:

$P = |1\rangle\langle 1|$.

The vector $|1\rangle$, is an eigenvector of $P$, with eigenvalue 1

$|1\rangle\langle 1|\,|1\rangle = 1|1\rangle$ .

Then, any orthogonal eigenvector orthogonal to $|1\rangle$ is an eigenvector with eigenvalue zero. Let us denote one of these eigenvectors: $|0\rangle$,

$|1\rangle\langle 1|\,|0\rangle = 0|1\rangle = 0.$

The normalized state, denoted by $|\Psi_a\rangle$ , is decomposed into the eigenvectors of $P$:

$|\Psi_a\rangle = c_0|0\rangle + c_1|1\rangle.$

Then

$\langle\Psi_a|\Psi_a\rangle = |c_0|^2 + |c_1|^2 = 1.$

So,

$\langle\Psi_a|P|\Psi_a\rangle = (\langle 1|c_1^* + \langle 0|c_0^*)|1\rangle\langle 1|(c_0|0\rangle + c_1|1\rangle) = (\langle 1|c_1^*)(c_1|1\rangle) = |c_1|^2.$

As mentioned $|\Psi_a\rangle$, is normalized. So, $0 \le c_0 \le 1$, and $0 \le c_1 \le 1$.

Consequently

$0 \le \langle\Psi_a|P|\Psi_a\rangle \le 1.$

**c)** Show that the singular values of an orthogonal projector are also equal to zero or to one.

Definition: The singular values of an arbitrary matrix $A$ are given by the square roots of the eigenvalues of

$A^\dagger A$.

It follows that for every singular value $\sigma_i$ of a matrix $A$ there exist some unit normalized vector $u_i$ such that

$u_i^* A^\dagger A u_i = \sigma_i^2$.

Using this part of matrix theory for the projection operator(matrix), we have

$P^\dagger P = P^2 = P,$

or

$= (|\psi\rangle\langle\psi|)^\dagger(|\psi\rangle\langle\psi|) = (|\psi\rangle\langle\psi|)^2 = |\psi\rangle\langle\psi|\,|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi|.$

Hence, the singular values are 0 and 1.

So,

$u_i^* P^\dagger P u_i = \sigma_i^2,$

with $\sigma_i$ equal 1 or zero, depending on $u_i = |\psi\rangle$ or $u_i \neq |\psi\rangle$.

The projection operator never lengthens a vector.

**d)** Consider the example of a non-orthogonal projection operator

$N = \begin{pmatrix} 0 & 0 \\ -1 & 1 \end{pmatrix}.$

The eigenvalues of $N$.

$\begin{vmatrix} -\lambda & 0 \\ -1 & 1-\lambda \end{vmatrix} = 0 \Rightarrow \lambda(1-\lambda) = 0 \Rightarrow \lambda = 0{,}1.$

The corresponding eigenvectors are found from:

$\begin{pmatrix} 0 & 0 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}.$

With normalization

$\lambda = 0 \Rightarrow |\lambda_0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix},$

and

$\lambda = 1 \Rightarrow |\lambda_1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$

These two vectors are not orthogonal.

The projection operators

$P_0 = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}(1\,,1) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},$

$P_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}(0\,,\ 1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$

It appears:

$\sum_i \lambda_i P_i = 0 \cdot \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + 1 \cdot \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \neq \begin{pmatrix} 0 & 0 \\ -1 & 1 \end{pmatrix} = N.$

**e)** Find the singular values of $N$.

For this we need:

$N^\dagger N = \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$

The eigenvalues:

$\begin{vmatrix} 1-\lambda & -1 \\ -1 & 1-\lambda \end{vmatrix} = 0 \Rightarrow (1-\lambda)^2 - 1 = 0 \Rightarrow \lambda(\lambda - 2) = 0.$

The eigenvalues are 0, and 2.

The singular values are given by the square roots of the eigenvalues of $N^\dagger N$.

Hence, these singular values are: 0 and $\sqrt{2}$.

There exist a unit vector that gets lengthened by the action of the matrix $N$.

So, we use the normalized eigenvector of $N^\dagger N$, with eigenvalue 2, $|u_2\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$:

$\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 2\begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow a = -b\,,$

and

$|u_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix}$.

The norm of this vector $|u_2\rangle$:

$(\langle u_2|N^\dagger N|u_2\rangle)^{1/2} = \sqrt{2}$ .

# 5. Probability

## 5.1 Probability Concepts

Quantum mechanics will necessarily involve probability in order to make the connection with experiments.

The quantity to be obtained is:

$P(A|B) \Longrightarrow$ *probability of event $A$ given that event $B$ is true.*

### 5.1.1 Standard Thinking

The standard mathematical formalism are presented, with $A$ and $B$ are given sets.

- $A \cap B$, represents the intersection of the two sets. Language: $A$ cap $B$.

Thus: $A \cap B \Longrightarrow \{\exists x: x \in A$ and $x \in B\}$.

- $A \cup B$ , represents the union of the two sets. Language: $A$ cup $B$. The set of elements which belong to $A$ alone or to $B$ alone or to both $A$ and $B$.

Thus: $A \cap B \Longrightarrow \{\exists x: x \in A$ and $x \in B\}$.

Boolean logic is presented with an example of a truth table at page 324.

Then the axioms for a theory of probability is given.

An example of the use of axioms is shown in the Eqs. (5.5)-(5.15).

Evaluate $P(X \cap Y|C) + P(X \cap \sim Y|C)$,

reminder $\sim Y$ =NOT $Y$ =nonoccurrence of $Y$(denotes that proposition $Y$ is false).

Axiom 4 will be used:

$P(A \cap B|C) = P(A|C)P(B|A \cap C)$,

where Boccio made the remark this equality to make sense if you think the events $A$ and $B$ happening in sequence.

$P(X \cap Y|C) + P(X \cap \sim Y|C) =$

$P(X|C)P(Y|X \cap C) + P(X|C)P(\sim Y|X \cap C)$.

Now Axiom 3:

$P(A|B) + P(\sim A|B) = 1 \Longrightarrow P(\sim A|B) = 1 - P(A|B)$.

Then,

$P(X|C)P(Y|X \cap C) + P(X|C)P(\sim Y|X \cap C) = P(X|C)[P(Y|X \cap C) + P(\sim Y|X \cap C)]$.

Hence,

$P(X \cap Y|C) + P(X \cap \sim Y|C) = P(X|C)$, Eq. (5.6) page 325,

Plug $X = \sim A, Y = \sim B$, into Eq.(5.6) :

$P(\sim A \cap \sim B|C) + P(\sim A \cap \sim\sim B|C) = P(\sim A|C)$,

with Axiom 3:

$P(\sim A \cap \sim B|C) + P(\sim A \cap B|C) = 1 - P(A|C) \Longrightarrow$

$\Longrightarrow P(\sim A \cap \sim B|C) = 1 - P(A|C) - P(\sim A \cap B|C)$, Eq. (5.9) page 325.

Now plug into

$P(X \cap Y|C) + P(X \cap \sim Y|C) = P(X|C)$, Eq. (5.6),
$X = B$ and $Y = \sim A \Longrightarrow\ P(B \cap \sim A|C) + P(B \cap A|C) = P(B|C)$ , Eq.(5.10).
With $P(B \cap \sim A|C) = P(\sim A \cap B|C)$ , EQ. (5.10) gives
$P(\sim A \cap B|C) = P(B|C) - P(B \cap A|C)$, Eq.(5.11).
Eq. (5.9):
$P(\sim A \cap \sim B|C) = 1 - P(A|C) - \ P(\sim A \cap B|C)$ .
So,
$P(\sim A \cap B|C) = 1 - P(A|C) - \ P(\sim A \cap \sim B|C)$.
Plug the preceding expression into Eq. (5.11):
$P(\sim A \cap \sim B|C) = 1 - \ P(A|C) - P(B|C) + \ P(B \cap A|C)$ , Eq. (5.12).
With Axiom 3
$P(A \cup B|C) + P[\sim(A \cup B|C] = 1 \Longrightarrow P(A \cup B|C) = 1 - P[\sim(A \cup B|C] =$
$= 1 - P[(\sim A \cap \sim B)|C]$, Eq.(5.13),
where use has been made of $\sim(A \cup B) = \sim A \cap \sim B$.
Boccio showed with the truth Table 5.2, the expression $\sim(A \cup B) = \sim A \cap \sim B$, to be correct. This could have been shown by means of a Venn Diagram.
Now plug Eq. (5.13) into Eq. (5.12) giving Eq. (5.15), called the rule of *addition for exclusive events*.
Then with Eq. (5.18) Baye's theorem is presented:
$P(B|A \cap C) = P(A|B \cap C)\frac{P(B|C)}{P(A|C)}$.
Now, with $B$ independent of $A$, we have Eq.(5.19)
$P(B|A \cap C) = P(B|C)$.
Use axiom 4,
$P(A \cap B|C) = P(A|C)P(B|A \cap C)$.
Plug into Axiom 4, $P(B|A \cap C) = P(B|C)$,
$P(A \cap B|C) = P(A|C)P(B|C)$.
This is called *statistical independence*.

### 5.1.2 Bayesian Thinking …….

**Two Axiom**s are presented, more or less illustrating the subjective character of Baye's Statistics.
Boccio noticed *this subjectivity(*beliefs, Nz*) works only then when the real numbers we attach to our beliefs in the various propositions could be transformed to another set of real positive numbers which obeys the usual rules of probability theory.*
The rules are: axiom 3 the sum rule, Eq. (5.22) and axiom 4 the product rule, Eq. (5.23).
**Baye's Theorem and Marginalization**
Eq. (5.28) represents Baye's Theorem.
The, Boccio explained the fundamental importance of Baye's Theorem, Eq. (5.28), to data analysis where $X$ and $Y$ in Eq.(5.28) are replaced by hypothesis and data.
Then the various terms in Baye's theorem are explained by their formal names, page 329.
With Eq.(5.40),
$\sum_{k=1}^{M} p(Y_k \cap X|I) = \hat{I}$,
we have

$p(X|I) = \sum_{k=1}^{M} p(X \cap Y_k|I)$.
Note: I use $p$ instead of $prob$.
For $M \to \infty$ , the preceding equation gives Eq.(5.41),
As mentioned by Boccio, the integrand of Eq. (5.41) is a probability density function, defined by Eq. (5.42).

## 5.2 Probability Interpretation.

The concept of limit frequency linked to probability is defined in Eq. (5.45) page 331
$P(A|C) = \lim_{n\to\infty} \frac{m}{n}$,
for $n$ repetitions, $A$ occurs $m$ times.
An experiment is presented comparing with flipping a coin. Leading to the binomial probability distribution presented in Eq.(5.52):
$P(n_A = r|M^n) = \binom{n}{r} p^r q^{n-r}$,
where is the number of experiments, $P(A|M) = p$ , and $P(\sim A|M) = q$.
Hence binomial.
Next the expectation value if $n_A$, the number of times $A$ occurs.
With the binomial expansion, Newton's binomium, the expectation value is obtained by differentiating the Binomial expansion with respect to $p$, together with the frequency, Eqs. (5.60) and (5.61).
Then, Boccio evaluated an experiment where the outcome of a measurement is some continuous variable, Eq. (5.62).

## 5.3 First hints of "subversive" or "Bayesian" thinking.....

Boccio discussed some basic thinking about probability.
**Example:**
An urn that contains 5 red balls and 7 green balls.
Random selection:
- the probability of picking a red ball 5/12,
- the probability of picking a green ball 7/12.
The ball is not returned to the urn: The probability on picking red or a green ball depends on the outcome of the first pick.
This is illustrated by Boccio with only two balls a red and a green one in the urn. Then, the result is calculated for 5 and 7 balls:
Start with
$Y$ =Pick is Green($2^{nd}$ pick),
$X$ =Pick is Red ($1^{st}$ pick).
$p(X|Y \cap I) \times p(Y|I) = p(Y|X \cap I) \times P(X|I)$.
Initial values $I$ : Green $m$ and Red $n$.
Then,
$p(X|I) = \frac{n}{n+m}$,
$p(Y|I) = \frac{n}{n+m}(\frac{m}{n+m-1} + \frac{m-1}{n+m-1})$,

$p(Y|X \cap I) = \frac{m}{n+m-1}$

Bayesian: $\frac{n}{n+m-1} = 5/11$, Eq. (5.72),
Non-Bayesian: $\frac{n}{n+m} = 5/12$, Eq. (5.73).
In discussing the difference, the subject of subjectivity, as mentioned earlier, is introduced.
Boccio explained this is not the same as subjectivity, it is about probabilities to be conditional.
**Another Example-Is this a fair coin?**
4 heads are observed in 11 flips.
A fair coin is well understood.
Denote Tail and Head ⟹Tail=0 means Head =1 and Tail=1 means Head=0.
So, it is about hypotheses on fairness.
At the top of page 337, Boccio presented various hypotheses.
Assuming flipping the coin to be independent events, then the probability of obtaining the data $R$ heads in $N$ flips is given by the binomial distribution as presented in Eq. (5.77) page 337.
Then, Boccio presented three distinct and very different prior probabilities used in a computer simulation. As mentioned, the prior probabilities represent very different initial knowledge.
It appears the posterior probabilities are all the same. Consequently they are independent of the three prior probabilities.

### 5.3.1 The Problem of Prior Probabilities

How to design probabilities based on prior information?
It is about the *principle of insufficient reason* also denoted the *principle of indifference*.
Boccio illustrated this principle for flipping a legitimate coin, Eq. (5.78).
Then some examples are given:
**Example 1 :** Assume $W$ white balls and $R$ red balls in an urn. The balls are randomly drawn from the urn.
The prior probability is given in Eq. (5.80):
$prob(j|I) = \frac{1}{R+W}, j = 1, 2,3, \ldots, R + W.$
Then,
$prob(red|I) = \sum_{j=1}^{R+W} prob(red \cap j|I = \sum_{j=1}^{R+W} prob(j|I) prob(red|j \cap I) =$
$= \frac{1}{R+W} \sum_{j=1}^{R+W} prob(red|j \cap I)$, Eq. (5.82).
The product rule has been used.
Finally,
$prob(red|I) = \frac{R}{R+W}$, Eq. (5.83)
Now repeat the experiment that after each draw the ball is returned to the urn.
The conclusion: the expected frequency of red balls, in repetitions of the urn experiment, is equal to the probability of picking one red ball in a single trial, Eq. (5.92).

**Example 2 :**
A location parameter. The complete ignorance about a location parameter is represented by the assignment of a uniform probability distribution function.
A scale parameter.
If we have no idea about length scale $L$ involved, then the probability distribution is invariant to scale.
It follows, Eq. (5.104), the assignment of a uniform probability distribution function for $\log L$ is the way to represent ignorance about a scale parameter.

## 5.4 Testable Information: The Principle of Maximum Entropy.

Now, the case is considered where there cannot be ignorance.
This case is illustrated with the role of a die. The die was rolled a very large number with the average result of 4.5. Then the question was posed: what probability to assign for a outcome $\{X_i\}$ with the face on top showing $i$ dots?
For a uniform distribution the average is 7/2.
Then, Boccio introduced the principle of maximum entropy as a decision tool.
The maximization equation is presented in Eq.(5.113).
Boccio raised the question about why the entropy function in Eq.( 5.123) to be the choice for a selection criterion. To find out about this question, two examples are analysed.
**Example 1** The Kangaroo Problem, page 347.
I summarize the problem: 1/3 of all kangaroos have blue eyes and 1/3 of all kangaroos are left-handed. Question: what proportion of kangaroos are both blue-eyed and left-handed?
The problem is dealt wit on the pages 347-349. The conditions of marginal probabilities are used.
The choice was made for independence. Then, it follows the entropy function presented in Eq. (5.123) gives the correct independent result as given in Eq. (132).
**Example 2** The Team of Monkeys Problem, page 350.
There are $M$ distinct possibilities $\{X_i\}$. How to assign truth tables $(prob(X_i|I = p_i)$ to the mentioned possibilities given some testable information $I$ (experimental results)?
Boccio described an experiment where the monkeys distributed a large number of coins into boxes. The process is repeated many times. Then, various distribution are obtained. The one that occurs most frequently can be chosen for $(prob(X_i|I = p_i)$.
Now, what about maximum entropy $S = -\sum p_i \log_e p_i$ ?
Considered the experiment, it is to be expected the probability distribution function(pdf) to be $\{p_i\}$ :
$p_i = \frac{n_i}{N}$,
where $n_i$ is the number of coins in box $i$ , and $N = \sum_{i=1}^{M} n_i$, the total number of coins.
Since $M$ is the number of boxes, there are $M^N$ number of possibilities to distribute the coins among the boxes.
The expected frequency with which a set $\{p_i\}$ arises is presented in Eqs. (5.136)- (5.139).
Then, finally the it is shown , the maximum entropy function to be the choice for a selection criterion.

## 5.5 Discussion

Boccio concluded this chapter by observations of Bayesian methods.
"The use of Bayesian methods in quantum mechanics presents a very different view of quantum probability than normally appears in quantum theory textbooks. It is becoming increasingly important in discussions of measurement.

## 5.6 Problems Boccio-1

### 5.6.1 Simple probability concepts

14 problems are in this section.

**a)** Two dices are rolled, one after the other. Let $A$ be the event that the second number is greater than the first. Find the probability $P(A)$. This is about counting.
With two dices there are $6^2 = 36$ possibilities, of which $N_A = 15$ :
$(5{,}6), (4{,}6), (3{,}6), (2{,}6), (1{,}6), (4{,}5), (3{,}5), (2{,}5), (1{,}5), (3{,}4), (2{,}4), (1{,}4), (2{,}3), (1{,}3), (1{,}2)$.
Hence,
$P(A) = \frac{N_A}{N} = \frac{15}{36}$.

**b)** Three dices are rolled and scores added. Are you likely to get 9 than 10, or the other way around?
Now there are $6^3 = 216$ possible outcomes.
A counting problem:
- 9 eyes : (1,2,6),(1,3,5),(1,4,4),(1,5,3),(1,6,2), (2,1,6),(2,2,5),(2,3,4),(2,4,3),(2,5,2),(2,6,1), (3,1,5),(3,2,4),(3,3,3),(3,4,2),(3,5,1),(4,1,4),(4,2,3),(4,3,2),(4,4,1), (5,1,3),(5,2,2), (5,3,1),(6,1,2),(6,2,1).

So, you find 25 triples. In addition, you may wonder how to distinguish, e.g., (1,2,6),(1,6,2), (2,1,6),(2,6,1),(6,1,2), and (6,2,1): 3! possibilities.
In the formulation of the problem nothing about this issue is mentioned. I am of the opinion, the possibilities to distinguish is by means of coloured dices or the dices are rolled one after another as mentioned under **a).**
-10 eyes: (1,3,6),(1,4,5),(1,5,4),(1,6,3),(2,2,6),(2,3,5),(2,4,4),(2,5,3),(2,6,2),(3,1,6),(3,2,5), (3,3,4),(3,4,3),(3,5,2),(3,6,1),(4,1,5),(4,2,4),(4,3,3),(4,4,2), (4,5,1),(5,1,4),(5,2,3), (5,3,2),(5,4,1),(6,1,3),(6,2,2),(6,3,1).
The, 27 triples are found. I assume the dices are rolled in the way as mentioned under **a).**
So,
$P(9) = \frac{25}{216}$,
and
$P(10) = \frac{27}{216}$.

**c)** Which of these two following events is more likely?
- four rolls of a die yield at least one six, event $A$,
- four rolls of two dice yield at least one double six, event $B$.

$A$. With four rolls of a die there are $6^4$ possibilities. The formulation: *at least one six* indicates the use of the negation of $A \rightarrow \sim A$: $P(A) = 1 - P(\sim A) = 1 - \left(\frac{5}{6}\right)^4 = 0.518$, since there are $5^4$possibilities with an outcome of no six.

$B$. Again, we will use $\sim B$. With one roll of two dices there are $6^2 = 36$ possibilities. The probability of two sixes in one roll is $\frac{1}{36}$ . The possibilities with four rolls are $36^4$ and consequently, $35^4$ show no double six.
Now, the probability *at least one double six* **:**
$P(B) = 1 - P(\sim B) = 1 - \left(\frac{35}{36}\right)^4 = 0.491.$
Hence, $A$ is more likely than $B$.
Remark: in the formulation of case $B$ twenty-four rolls are mentioned: a typo.

**d)** From meteorological records it is known for a certain island at its winter solstice, it is wet with a probability 30%, windy with probability 40% and both wet and windy with a probability of 20% .
Find:
- Prob(dry). Dry means not wet.
So,
$P(dry) = P(\sim wet) = 1 - P(wet) = 1 - 0.3 = 0.7$ .
Find:
-Prob(dry AND windy), AND≡∩ .
We need again to get wet instead of dry.
So,
$P(dry \cap windy) = P(windy) - P(\sim dry \cap windy) = P(windy) - P(wet \cap windy) =$
$= 0.4 - 0.2 = 0.2$ .
Find:
- Prob(wet OR windy), OR≡∪.
$P(wet \cup windy)$.
We have another expression for the preceding expression, visualized by a Venn diagram,
$P(wet \cup windy) = P(wet) + P(windy) - P(wet \cap windy) = 0.4 + 0.3 - 0.2 = 0.5.$

**e)** Another application of the rule:
$P(A \cup B) = P(A) + P(B) - P(A \cap B).$
So,
$P(A\ OR\ B) = P(A) + P(B) - P(A\ AND\ B).$
A kitchen contains two fire alarms: one activated by smoke and the other by heat. The probability of the smoke alarm to react within one minute is 0.95, the probability of the heat alarm to react within one minute is 0.91, and the probability of both alarms sounding within one minute is 0.88. What is the probability of at least one alarm to react within one minute? This is the OR probability. We have all the information for the right hand side of the preceding expression.
So, the probability is
$P(A \cup B) = 0.91 + 0.95 - 0.88 = 0.98.$
**f)** Roll, two dice, one from each hand. What is the probability that your right-hand die shows a larger number than your left-hand die?
With two dice there are 36 outcome/possibilities. See under **a)**. There I denoted it a

counting problem. Well, it is. However a reduced one. See Figure below.

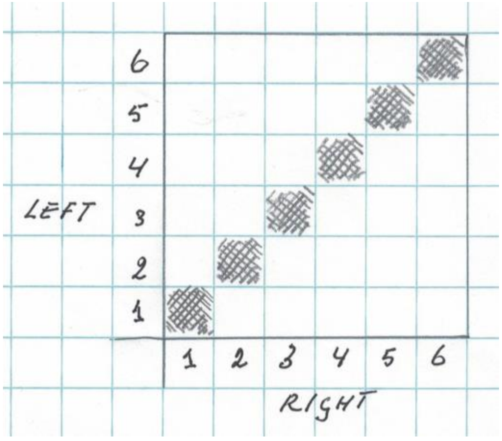



Figure 1 Problem 5.6.1 f)

36 outcomes of which 6 are excluded in the case the roll showed equal faces like (1,1). So, 30 outcomes are allowed. As illustrated in Figure1, 15 possibilities for a higher score for the right-hand.
Consequently, the probability for a higher score is
$P(RH\ larger) = \frac{15}{36}$.
Obviously, the same applies for the left-hand.
Now, suppose you roll the left-hand die first and it shows a 5. For the right-hand to be larger than 5, the probability is not $\frac{15}{36}$. Since, only one face will do: a 6, of which the probability is $\frac{1}{6}$.
As mentioned by Boccio, this is a special case of the general observation that, if conditions change, then results change.
We have learned the rule:
$P(A \cap B) = P(A|B)P(B) \Longrightarrow P(A|B) = \frac{P(A\cap B)}{P(B)}$.
Hence
$P(Rlarger|Lshows5) = \frac{P(Rshows6ANDLshows5)}{P(Lshows5)} = \frac{1/36}{1/6} = \frac{1}{6}$.

**g)** A coin is flipped three times. Let $A$ be the event that the first flip gives a head, H, and $B$ be the event that there are two heads overall.
- Determine $P(A|B)$.
There are three possibilities to get two heads, with two of the possibilities making $A$ true:
HHT, HTH,THH.
Hence: $P(A|B) = \frac{2}{3}$.
- Determine $P(B|A)$.
There are four possibilities to get the first flip H: HHH, HHT, HTH, HTT. Two of them making $B$ true.
Hence: $P(B|A) = \frac{2}{4}$.
**h)** A box contains a double headed coin, a double-tailed coin and a conventional coin. A coin is picked at random and flipped. It shows a head. What is the probability that it is a double-headed coin?

The three coins have 6 faces. The total number of outcomes is 6. Let $D$ be the event that the coin is double-headed. $A$ is the event that the coin shows a head. So, 3 faces yield $A$.
The probability of showing the face head
$P(A) = \frac{1}{2}$.
Two faces yield $A$ . When $A$ is shown, you do not know whether it is the head of the double-headed coin or of the conventional coin. So,
$P(A \cap D) = \frac{1}{3}$.
With the rule we learned
$P(A \cap D) = P(D|A) \cdot P(A) \Longrightarrow P(D|A) = \frac{P(A \cap D)}{P(A)} = \frac{\frac{1}{3}}{\frac{1}{2}} = \frac{2}{3}$.
Boccio explained that the usual reasoning goes as follows:
If the coin shows a head, it is either double-headed or the conventional coin. Since the coin was picked at random, these are equally likely, so
$P(D|A) = \frac{3}{6} = \frac{1}{2}$.
**i)** A box contains 5 red socks and 3 blue socks. I you remove 2 socks at random, what is the probability that you are holding a blue pair?
Let $B$ be the event that the first sock is blue and $A$ the event that you have a pair od blue socks. If you have one blue sock, the probability that the second sock is blue is the chance of drawing one of the 2 remaining blue socks from the total remaining 7 socks.
Hence,
$P(A|B) = \frac{2}{7}$.
Now $A = A \cap B \Longrightarrow$ The Venn diagram where $A$ is completely contained in $B$.
Furthermore, with 8 socks,
$P(B) = \frac{3}{8}$.
Finally, the probability of the event to have 2 blue socks, using the rule
$P(A \cap B) = P(A|B) \cdot P(B)$
$P(A) = P(A \cap B) = P(A|B) \cdot P(B) = \frac{2}{7} \cdot \frac{3}{8}$.
**j)** An expensive electronic toy made by Acme Gadgets Inc. is defective with probability 0.001. These toys are so popular that they are copied and sold illegally but cheaply. Pirate versions capture 10% of the market and any pirated copy is defective with probability 0.5. If you buy a toy, wat is the chance that the toy is defective?
Let $A$ be the event that you buy a genuine article and let $D$ be the event that your purchase is defective.
Information:
$P(A) = 0.9$ , $P(\sim A) = 0.1$ , $P(D|A) = 0.001$, and $P(D|\sim A) = 0.5$ .
The chance of buying a defective one is the sum of two chances:
$P(D) = P(D \cap A) + P(D \cap \sim A)$.
Again, we use the general rule
$P(A \cap B) = P(A|B) \cdot P(B)$,
$P(D) = P(D \cap A) + P(D \cap \sim A) = P(D|A) \cdot P(A) + P(D|\sim A) \cdot P(\sim A)$.
We have all the ingredients
$P(D) = 0.9 \cdot 0.001 + 0.5 \cdot 0.1 = 0.0509$.
**k)** Patients may be treated with any number of drugs, each of which may give rise to side effects. A certain drug $C$ has a 99% success rate in the absence of side effects and side effects only arise in 5% of the cases. However, if the side effects do arise, the $C$ has a 30%

success rate. If $C$ is used, what is the probability of the event $A$ that a cure is effected?
Let $B$ the event that no side effects occur. We know:
$P(A|B \cap C) = 0.99$ , $P(B|C) = 0.95$ ,
and
$P(\sim A|\sim B \cap C) = 0.3$ , $P(\sim B|C) = 0.05$ .
The probability that a cure is effected, is the probability of success plus the probability of side effects:
$P(A|C) = P(A|B \cap C) \cdot P(B|C) + P(\sim A|\sim B \cap C) \cdot P(\sim B|C)$ .
Hence,
$P(A|C) = 0.99 \cdot 0.95 + 0.3 \cdot 0.05 = 0.9555$ .

**l)** Suppose a multiple choice question has $c$ available choices. A student either knows the answer with probability $p$ or guesses at random with probability $1 - p$ . Given that the answer selected is correct,, what is the probability that the student knew the answer?
Let $A$ be the event that the question is answered correctly and $S$ the event that the student knew the answer.
We require the probability the student knew the answer under the assumption that the question is answered correctly: $P(S|A)$.
The probability that the question is answered correctly, $P(A)$, is the sum of the probabilities of knowing the answer and the probability of guessing the answer:
$P(A) = P(A|S) \cdot P(S) + P(A|\sim S) \cdot P(\sim S)$.
Under the condition the student knew the answer,
$P(A|S) = 1$, and $P(S) = p$.
Under the condition the student does not know the answer with $c$ available choices,
$P(A|\sim S) = 1/c$, and $P(S) = 1 - p$ .
Hence
$P(A) = P(A|S) \cdot P(S) + P(A|\sim S) \cdot P(\sim S) = p + \frac{1-p}{c}$ .
We need to know the probability the student knew the answer under the assumption that the question is answered correctly: $P(S|A)$.
So, with
$P(A|S) \cdot P(S) = P(S|A) \cdot P(A)$, we have, with the ingredients above:
$P(S|A) = \frac{P(A|S) \cdot P(S)}{P(A)} = \frac{p}{p + \frac{1-p}{c}}$ .
The larger $c$, $P(S|A) \to 1$.
**m)** Common PINs do not begin with zero. They have four digits. A computer assigns you pain at random. What is the probability that all four digits are different?
Since the first position can not be a zero , there are nine numbers. For the other three positions there are 10 numbers.
Hence, the total number of possibilities
$N = 9 \cdot 10 \cdot 10 \cdot 10 = 9000$.
$A$ is the event that no digit is repeated. Hence the number of possibilities results from permutation without repetition:
$9 \cdot \left(\frac{9!}{6!}\right) = 9 \cdot 9 \cdot 8 \cdot 7 = 4536$.
At first sight, this l seems to be a bit confusing. However, keep in mind, think of the first 9 as $10 - 1$ .

The probability of four digits being different is:

$P(A) = \frac{4536}{9000} = 0.504$ .

**n)** You are dealt with a hand of 5 cards from a conventional deck(52 cards). A full house comprises 3 cards of one value and 2 of another value. If that hand has 4 cards of one value , this is called four of a kind. Which is more likely?

The number $N$ of possible choices of 5 cards from 52 cards is:

$N = \binom{52}{5}$ possibilities.

- The full house:

The value can be chosen from 13(=52/4) or 13 ways.

Since this done for three suits out of the four colours(suits), the possibilities are

$\binom{4}{3}$.

The other two cards of the full house can be chosen in 12(=13-1) ways>

The possibilities for two suits are,

$\binom{4}{2}$.

So, the probability for a full house is:

$P(full\ house) = \frac{13 \cdot \binom{4}{3} \cdot 12 \cdot \binom{4}{2}}{\binom{52}{5}}$ .

So, it does not matter whether you did start with the choice of the double or the triple:

$P(full\ house) = \frac{12 \cdot \binom{4}{3} \cdot 13 \cdot \binom{4}{2}}{\binom{52}{5}}$ .

- Four of a kind:

You can choose 13 different sets in one way.

For the last card there are $4 \cdot 12$ possibilities.

$P(Four\ of\ a\ kind) = \frac{13 \cdot 48}{\binom{52}{5}}$ .

Hence,

$\frac{P(Four\ of\ a\ kind)}{P(full\ house)} = \frac{13 \cdot 48}{12 \cdot \binom{4}{3} \cdot 13 \cdot \binom{4}{2}} = \frac{1}{12}$ .

### 5.6.2 Playing Cards

Two cards are drawn at random from a shuffled deck and laid aside without being examined. Then a third card is drawn. Show that the probability that the third card is a spade is equal to the probability as the spade was the first card drawn.

*Hint*: consider all the mutually exclusive possibilities, i.e., two discarded cards spades, third card spade or not spade, etc.

Let $S$ is spade and $N$ is not spade.

Then the symbol $N_1S_2S_3$ means: 1st card drawn is not a spade, 2nd card drawn is a spade and 3rd card drawn is a spade.

With the third card to be a spade, we have four possible draws:

$S_1S_2S_3$, $S_1N_2S_3$, $N_1S_2S_3$, and $N_1N_2S_3$ .

With mutually exclusive possibilities, in general notation,

$P(A \cup B) = P(A) + P(B)$,

the probabilities are added.

To compute the probability of, say, $S_1N_2S_3$, we use the general equation

$P(A \cap B) = P(A) \cdot P(B)$.

With 52 cards the probability of

$S_1 = \frac{13}{52}$ .
The probability of, with one card out of the deck and 39 are not spades
$N_2 = \frac{39}{51}$.
The last probability, with 50 cards in the deck of which twelve are spades
$S_3 = \frac{12}{50}$ .
Hence
$P(S_1 N_2 S_3) = \frac{13}{52} \cdot \frac{39}{51} \cdot \frac{12}{50}$ .
Next
with $P(S_1 S_2 S_3)$ we are dealing with the deck of spades, so
$P(S_1 S_2 S_3) = \frac{13}{52} \cdot \frac{12}{51} \cdot \frac{11}{50}$ .
The other two probabilities
$P(N_1 S_2 S_3) = \frac{39}{52} \cdot \frac{13}{51} \cdot \frac{12}{50}$ ,
and
$P(N_1 N_2 S_3) = \frac{39}{52} \cdot \frac{38}{51} \cdot \frac{13}{50}$ .
Consequently, collecting the various factors in an efficient way
$P(third\ card\ is\ a\ spade) = P(S_1 N_2 S_3) + P(S_1 S_2 S_3) + P(N_1 S_2 S_3) + P(N_1 N_2 S_3) =$
$= \frac{13}{52}\left[\frac{12(11+39)+39(12+38)}{(51 \cdot 50)}\right] = \frac{13}{52}\frac{(51 \cdot 50)}{(51 \cdot 50)} = \frac{13}{52} = \frac{1}{4}$ .

### 5.6.3 Birthdays

-What is the probability that you and your friend have different birthdays? A classic one. For simplicity let a year have 365 days.
- What is the probability that three people have different birthdays?
- Show that the probability that $n$ people have different birthdays is
$p = \left(1 - \frac{1}{365}\right)\left(1 - \frac{2}{365}\right) \ldots . (1 - \frac{n-1}{365})$ .
Estimate this probability for $n \ll 365$.
- Find the smallest integer $N$ for which $p < \frac{1}{2}$ .
Hence show that for a group of $N$ people or more, the probability is greater than ½ that two of them have the same birthday.
- Start with one person. The probability that another person, your friend, has its birthday on the same day is $\frac{1}{365}$ . So, the probability for the second person to have its birthday on another day is $1 - \frac{1}{365} = \frac{364}{365}$ .
- The probability that a third person has its birthday on the same day as either of the first two is $\frac{2}{365}$ . So, the probability that the third person has a different birthday from either of the two is $1 - \frac{2}{365} = \frac{363}{365}$ .
- We have the product rule:
$P(A \cap B) = P(A) \cdot P(B)$.
Hence, the chance that three people have different birthdays is:
$P(three\ people\ different\ birtdays) = \frac{364}{365} \cdot \frac{363}{365}$ .
Then for $n$ people :
$P(all\ different\ birtdays) = \left(1 - \frac{1}{365}\right)\left(1 - \frac{2}{365}\right) \ldots . (1 - \frac{n-1}{365})$.
This probability becomes for $n \ll 365$, using the first term of the Taylor expansion

$\ln(1-x) \approx -x$ for $x \ll 1$,
$\ln P = \ln\left(1-\frac{1}{365}\right) + \ln\left(1-\frac{2}{365}\right) + \cdots + \ln\left(1-\frac{n-1}{365}\right)$.
Now, we use $n \ll 365$
$\ln P = -\frac{1}{365} - \frac{2}{365} - \cdots - \frac{n-1}{365}$.
The preceding expression is an arithmetic series:
$\ln P = \left(-\frac{1}{365} - \frac{n-1}{365}\right)\frac{n-1}{2} = -\frac{n(n-1)}{730}$.
- Find the smallest integer $n$ for which $P < \frac{1}{2}$.
$\ln P < \ln\frac{1}{2} = -\ln 2$.
So,
$-\ln 2 > \ln P = -\frac{n(n-1)}{730} \Longrightarrow \frac{n(n-1)}{730} > \ln 2 \Longrightarrow n \geq 23 = N$.
Hence, for a group of $N$ people or more, the probability is greater than ½ that two of them have the same birthday.
Remark:
You could have used your pocket calculator to find that the expression
$P(all\ different\ birtdays) = \left(1-\frac{1}{365}\right)\left(1-\frac{2}{365}\right)\dots.(1-\frac{n-1}{365})$,
leads to the conclusion that with $n = 23$, the probability of no one having the same birthday is 0.4927. Consequently, the opposite at least two people have the same birthday is $1 - 0.4927 = 0.5073$.
A classical one. You do not expect this. Intuitively, the thinking is the probability to be much smaller. Since, usually people think about a particular person's birthday.
The probability that a particular person has its birthdate not together with anyone of the group of $n-1$ people is
$\left(\frac{364}{365}\right)^{n-1}$.
Hence, the opposite is
$1 - \left(\frac{364}{365}\right)^{n-1}$.
Then, for $n = 23$, the preceding probability is $0.061151$.
Now, the probability is about 6% that another person has its birthday on the same day as the above mentioned particular person.

### 5.6.4 Is there Life?

The numbers of stars, $N$, in our galaxy is about $N = 10^{11}$. Assume that the probability that a star has planets is $p = 10^{-2}$, the probability that the conditions on the planet are suitable for life is $q = 10^{-2}$, and the probability of life evolving, given suitable conditions, is $r = 10^{-2}$. These are arbitrary numbers.
**a)** What is the probability of life existing in an arbitrary solar system, i.e., a star and planets?
We may assume that the above mentioned probabilities are independent. Consequently, the probability of life in an arbitrary solar system is:
$p \cdot q \cdot r = 10^{-6}$.
**b)** What is the probability that life exists in at least one solar system?
The probability $P$ that life exists in the vicinity of at least one star, is given by
$P = 1 - P_0$,
where $P_0$ is the probability that no stars have life about them.
The probability of no life about some arbitrary star is
$1 - p \cdot q \cdot r$.

Hence with the number of stars in our galaxy $N$, and the independence of the probabilities
$P_0 = (1 - p \cdot q \cdot r)^N$.
Now with $p \cdot q \cdot r \ll 1$, we approximate $P_0$:
$\ln P_0 = N \ln(1 - p \cdot q \cdot r) \approx -N \cdot p \cdot q \cdot r = -10^5$.
The approximation of $P_0$
$P_0 = e^{-10^5} \approx 0$.
So,
$P = 1 - P_0 \approx 1$.
Boccio: *This says that even a very rare event is almost certain to occur in a large enough sample.*
Furthermore, Boccio makes the note that the possibility of life is sometimes based on the probability $p \cdot q \cdot r = 10^{-6}$. However, it is about $P \approx 1$.

### 5.6.5 Law of Large Numbers

This problem is about the illustration of this law.
**a)** Assuming the probability of obtaining *heads* in a coin toss is 0.5, compare the probability of obtaining *heads* in 5 out of 10 tosses with the probability of obtaining *heads* in 50 out of 100 tosses and with the probability of obtaining *heads* I 5000 out of 10000 tosses.
With tossing a coin we have the binomial distribution for the probability of the stochast to be a success.
The probability of $n_H$ heads in $n$ trials is
$P = \binom{n}{n_H} p^{n_H}(1-p)^{n-n_H}$,
where $p$ is the success rate of *heads*.
So
$P(n_H|M^n) = \binom{n}{n_H} p^{n_H}(1-p)^{n-n_H} = \binom{n}{n_H}\left(\frac{1}{2}\right)^n$, Eq. (5.52) page 332,
for $p = \frac{1}{2}$,
and $M^n$ is the label representing any sequence of $n$ independent measurements.
- $P(5|M^{10}) = \frac{10!}{5!5!}\left(\frac{1}{2}\right)^{10} = 0.246$,
- $P(50|M^{100}) = \frac{100!}{50!50!}\left(\frac{1}{2}\right)^{100} = 0.0796$,
- $P(500|M^{1000}) = 0.0252$,
- $P(5000|M^{10000}) = 0.00798$.

This demonstrates for $n \to \infty$, $P(n_H|M^n) \to 0$, for $p = \frac{1}{2}$. See Eq.(5.68).
Is this the same as the probability goes to zero in a probability density? Since the probability is the integral or summation over an interval. The interval goes to zero, the probability goes to zero.
**b)** For a set of 10 tosses, a set of 100 tosses and a set of 10000 tosses, calculate the probability that the fraction of heads will between 0.445 and 0.555.
Here, we have a given interval.
The cumulative probability $binomial(k, n, p)$ is defined as(or better 1− cumulative probability):
$binomial(k, n, p) = P(x \geq k) = \sum_{x=k}^{n} \binom{n}{x} p^x (1-p)^{n-x}$.
Next we consider an increasing value of $n_H$ and the meaning of $n_H + 1$.
So with the cumulative expression, we can rewrite

$P(n_H|M^n) = binomial\left(n_H, n, \frac{1}{2}\right) - binomial\left(n_H + 1, n, \frac{1}{2}\right)$,
where $p = \frac{1}{2}$.
Since,
$P(n_H|M^n) = \binom{n}{n_H}\left(\frac{1}{2}\right)^n = \sum_{k=n_H}^{n}\binom{n}{n_H}(\frac{1}{2})^n - \sum_{k=n_H+1}^{n}\binom{n}{n_H+1}(\frac{1}{2})^n$,
where
$\sum_{k=n_H+1}^{n}\binom{n}{n_H+1}p^n = \sum_{k=n_H}^{n}\binom{n}{n_H}(\frac{1}{2})^n - \binom{n}{n_H}\left(\frac{1}{2}\right)^n$.
So, for the interval $m \le n_H \le s$, we find
$P(m \le n_H \le s|M^n) = binomial\left(m, n, \frac{1}{2}\right) - binomial\left(s + 1, n, \frac{1}{2}\right)$.
The given interval $m \le n_H \le s$
- $P(4.45 \le n_H \le 5.5|M^{10}) = binomial\left(4,10,\frac{1}{2}\right) - binomial\left(6,10,\frac{1}{2}\right)$.
$binomial\left(4.45,10,\frac{1}{2}\right) = \sum_{x=4}^{n}\binom{n}{4}p^x(1-p)^{10-x}$,
and
$binomial\left(6,10,\frac{1}{2}\right) = \sum_{x=6}^{n}\binom{n}{4}p^x(1-p)^{10-x}$.
Giving: $P(4.45 \le n_H \le 5.55|M^{10}) = 0.246$,
- $P(44.5 \le n_H \le 55.5|M^{100}) = binomial\left(44,100,\frac{1}{2}\right) - binomial\left(56,100,\frac{1}{2}\right)$.
Then, similarly
$P(44.5 \le n_H \le 55.5|M^{100}) = 0.729$.
- $P(445 \le n_H \le 555|M^{1000}) = binomial\left(445,1000,\frac{1}{2}\right) - binomial\left(555,1000,\frac{1}{2}\right) =$
$= 0.9996$.
- $P(4450 \le n_H \le 5550|M^{10000}) = binomial\left(4450,10000,\frac{1}{2}\right) -$
$+binomial\left(5550,10000,\frac{1}{2}\right) = 1.000$.
Hence, the probability in an interval near $\frac{1}{2}$, goes to 1 for $n \to \infty$.

### 5.6.6 Bayes

Suppose you have 3 nickels and 4 dimes in your right pocket and 2 nickels and a quarter in your left pocket. You pick a pocket at random and from that pocket select a coin at random. If it is a nickel, what is the probability that it came from the right pocket?
It is about Bayes formula.
Concise notation: Let $A$ mean nickel and $B$ means right pocket.
So, we have the conditional probability: $P(B|A)$.
Bayes Theorem:
$P(B|A) = \frac{P(B \cap A)}{P(A)} = \frac{P(B) \cdot P(A|B)}{P(A)}$.
In words: $P(B) \cdot P(A|B) \Rightarrow$probability of selecting the right pocket and then selecting a nickel from it.
So,
$P(B) = \frac{1}{2}$, the choice between two pockets.
In the right pocket 7 coins of which 3 nickels:
$P(A|B) = \frac{3}{7}$.
Hence,
$P(B) \cdot P(A|B) = \frac{1}{2} \cdot \frac{3}{7} = \frac{3}{14}$.

Next, we must find $P(A)$. We have two probabilities: the nickels in the right pocket and the nickels in the left pocket.
So,
$P(A) = P(A|B) \cdot P(B) + P(A|{\sim}B)P({\sim}B)$.
Plug in to this expression the given probabilities:
$P(A) = \frac{3}{7} \cdot \frac{1}{2} + \frac{2}{3} \cdot \frac{1}{2} = \frac{23}{42}$.
Finally,
$P(B|A) = \frac{P(B \cap A)}{P(A)} = \frac{P(B) \cdot P(A|B)}{P(A)} = \frac{3/14}{23/42} = \frac{9}{23}$.

### 5.6.7 Psychological Tests

Two psychologists reported on tests in which subjects were given the *prior information:*
$I =$ In a certain city, 85% of the taxicabs are blue and 15% are green,
and the data:
$D =$ A witness to a crash who is 80% reliable(i.e., who in the lighting conditions prevailing can distinguish between green and blue 80% of the time) reports that the taxicab was actually green.
The subjects in the tests were then asked to judge the probability that the taxicab was actually blue.
What is the correct answer?
Let $B =$ event that the taxicab was actually blue.
Now we use Bayes theorem, Eq. (5.69):
$prob(X|Y \cap I) = \frac{prob(Y|X \cap I) \cdot prob(X|I)}{prob(Y|I)}$.
So,
$P(B|D \cap I) = \frac{P(D|B \cap I) \cdot P(B|I)}{P(D|I)}$.
Under the condition the taxicab was actually blue,
$P(D|B \cap I) = 1 - 0.8 = 0.2$ ,
and
$P(B|I) = 0.85$.
Furthermore, we need $P(D|I)$.Somethinh similar was encountered in the foregoing problem (5.6.6):
$P(D|I) = P(D|B \cap I) \cdot P(B|I) + P(D|{\sim}B \cap I) \cdot P({\sim}B|I)$.
Then, we need to determine
$P(D|{\sim}B \cap I) \cdot P({\sim}B|I)$.
So, the observation the taxicab was not blue,
$P(D|{\sim}B \cap I) = 0.8$ ,
and not blue from the prior information
$P({\sim}B|I) = 0.15$ .
Now, we have all the ingredients
$P(B|D \cap I) = \frac{P(D|B \cap I) \cdot P(B|I)}{P(D|I)} = \frac{P(D|B \cap I) \cdot P(B|I)}{P(D|B \cap I) \cdot P(B|I) + P(D|{\sim}B \cap I) \cdot P({\sim}B|I)} = \frac{0.2 \cdot 0.85}{0.2 \cdot 0.85 + 0.8 \cdot 0.15} = 0.59$ .
Boccio paid some attention to what the usual errors are by guessing influenced by prior opinions:
*This is easiest to reason out in one's head using odds; since the statement of the problem told us that the witness was equally likely to err in either direction (G → B or B → G), Bayes' theorem reduces to simple multiplication of odds. The prior odds in favour of blue are 85 : 15, or nearly 6 : 1; but the odds on 70the witness being right are only 80 : 20 = 4 : 1, so the posterior odds on blue are 85 : 60 = 17 : 12. Yet most people tend to guess P(B|D ∧ I) as about 0.2, corresponding to the odds of 4 : 1 in*

*favour of green, thus ignoring the prior information. For these guesses, the data come first with a vengeance, even though the prior information implies many more observations than the single datum. The opposite error - clinging irrationally to prior opinions in the face of massive contrary evidence - is equally familiar to us that is the stuff of which fundamentalist religious/political stances are made. In general, the intuitive force of prior opinions depends on how long we have held them.*

### 5.6.8 Bayes Rules, Gaussians and Learning

Let us consider a classical problem(no quantum uncertainty). Suppose we are trying to measure the position of a particle and we assign a prior probability function,

$$p(x) = \frac{1}{\sqrt{2\pi\sigma_0^2}} e^{-\frac{(x-x_0)^2}{2\sigma_0^2}} .$$

Our measuring device is not perfect. Due to noise it can measure only with a resolution $\Delta$ . That is, when we measure the position, we must assume error bars of this size. Thus, if the detector registers the position $y$, we assign the likelihood that the position was $x$ by a Gaussian,

$$p(y|x) = \frac{1}{\sqrt{2\pi\Delta^2}} e^{-\frac{(y-x)^2}{2\Delta^2}} .$$

Use Bayes theorem to show that, given the new data, we must now update the probability assignment of the position to a new Gaussian,

$$p(x|y) = \frac{1}{\sqrt{2\pi\sigma'^2}} e^{-\frac{(y-x')^2}{2\sigma'^2}}$$

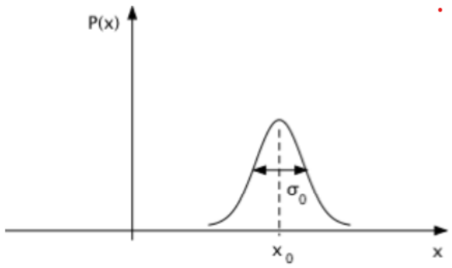
where

$$x' = x_0 + K_1(y - x_0) \, , \sigma'^2 = K_2\sigma_0^2 \, , K_1 = \frac{\sigma_0^2}{\sigma_0^2+\Delta^2} \, , K_2 = \frac{\Delta^2}{\sigma_0^2+\Delta^2} .$$

Now, we are trying to determine the position of a particle along one dimension.
The prior probability distribution given above:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma_0^2}} e^{-\frac{(x-x_0)^2}{2\sigma_0^2}} .$$

This distribution is presented in the following figure(Boccio):




Next, we measure the position and find the value $y$ in the detector. As mentioned, the detector has finite resolution meaning detecting $y$ do not give you the true position of $x$ . Given an uncertainty $\Delta$ in the detector with a Gaussian distribution, let the likelihood distribution be

$$p(y|x) = \frac{1}{\sqrt{2\pi\Delta^2}} e^{-\frac{(y-x)^2}{2\Delta^2}} .$$

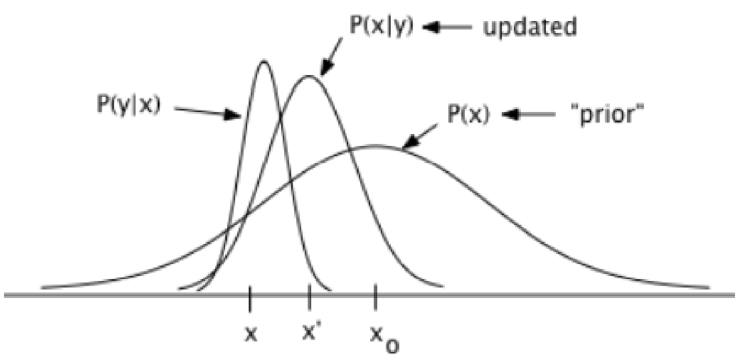
Bayes rule

$$p(x|y) = Np(y|x)p(x),$$

where $N^{-1}$ is a normalization factor.

$$p(y|x)p(x) = \frac{1}{\sqrt{2\pi\Delta^2}} e^{-\frac{(y-x)^2}{2\Delta^2}} \cdot \frac{1}{\sqrt{2\pi\sigma_0^2}} e^{-\frac{(x-x_0)^2}{2\sigma_0^2}} = \frac{1}{2\pi\Delta\sigma_0} e^{-\frac{(y-x)^2}{2\Delta^2}} e^{-\frac{(x-x_0)^2}{2\sigma_0^2}} .$$

Rearranging:
$\frac{(x-x_0)^2}{\sigma_0^2}+\frac{(y-x)^2}{\Delta^2}=\frac{x^2-2xx_0+x_0^2}{\sigma_0^2}+\frac{x^2-2xy+y^2}{\Delta^2}$.
We use:
$\sigma'^2=K_2\sigma_0^2=\frac{\Delta^2}{\sigma_0^2+\Delta^2}\cdot\sigma_0^2\Longrightarrow\frac{1}{\sigma'^2}=\frac{\sigma_0^2+\Delta^2}{\Delta^2\sigma_0^2}=\frac{1}{\sigma_0^2}+\frac{1}{\Delta^2}\Longrightarrow\frac{x^2}{\sigma'^2}=\frac{x^2}{\sigma_0^2}+\frac{x^2}{\Delta^2}$.
Then
$\frac{x^2-2xx_0+x_0^2}{\sigma_0^2}+\frac{x^2-2xy+y^2}{\Delta^2}=\frac{x^2}{\sigma'^2}-2x\left(\frac{x_0}{\sigma_0^2}+\frac{y}{\Delta^2}\right)+\frac{x_0^2}{\sigma_0^2}+\frac{y^2}{\Delta^2}$,
with
$A(y)=\frac{x_0}{\sigma_0^2}+\frac{y}{\Delta^2}$, and $B(y)=$ ,
$\frac{x^2}{\sigma'^2}-2x\left(\frac{x_0}{\sigma_0^2}+\frac{y}{\Delta^2}\right)+\frac{x_0^2}{\sigma_0^2}+\frac{y^2}{\Delta^2}=\frac{x^2}{\sigma'^2}-2xA(y)+B(y)$.
$2xA(y)=2x\left(\frac{x_0}{\sigma_0^2}+\frac{y}{\Delta^2}\right)=\frac{2x}{\Delta^2\sigma_0^2}(x_0\Delta^2+y\sigma_0^2)=\frac{2x}{\sigma'^2}\left[\frac{x_0(\sigma_0^2+\Delta^2)+\sigma_0^2y-x_0\sigma_0^2}{\sigma_0^2+\Delta^2}\right]=$
$=\frac{2x}{\sigma'^2}\left[x_0+\frac{\sigma_0^2}{\sigma_0^2+\Delta^2}(y-x_0)\right]=\frac{2x}{\sigma'^2}[x_0+K_1(y-x_0)]=\frac{2xx'}{\sigma'^2}$.
Then,
$\frac{x^2}{\sigma'^2}-2xA(y)=\frac{x^2}{\sigma'^2}-\frac{2xx'}{\sigma'^2}=\frac{(x-x')^2}{\sigma'^2}-\frac{x'^2}{\sigma'^2}$.
To summarize
$\frac{(x-x_0)^2}{\sigma_0^2}+\frac{(y-x)^2}{\Delta^2}=\frac{(x-x')^2}{\sigma'^2}-\frac{x'^2}{\sigma'^2}+\frac{x_0^2}{\sigma_0^2}+\frac{y^2}{\Delta^2}$.
The updated probability assignment:
$p(y|x)p(x)=\frac{1}{2\pi\Delta\sigma_0}e^{-\frac{(y-x)^2}{2\Delta^2}}e^{-\frac{(x-x_0)^2}{2\sigma_0^2}}=\frac{1}{2\pi\Delta\sigma_0}e^{-\frac{1}{2}\frac{(x-x')^2}{\sigma'^2}}\cdot F(y,x_0,\Delta,\sigma_0,\sigma')$.
Now, use normalization for the preceding exponential,
applying the integral of the Gaussian function $\int_{-\infty}^{\infty}e^{-x^2}dx=\sqrt{\pi}$,
$p(x|y)=\frac{1}{\sqrt{2\pi\sigma'^2}}e^{-\frac{1}{2}\frac{(x-x')^2}{\sigma'^2}}$ .
Note: $\frac{F(y,x_0,\Delta,\sigma_0,\sigma')}{2\pi\Delta\sigma_0}$ does not depend on $x$, and $e^{-\frac{x'^2}{\sigma'^2}+\frac{x_0^2}{\sigma_0^2}+\frac{y^2}{\Delta^2}}$ is included in $F(y,x_0,\Delta,\sigma_0,\sigma')$.
Furthermore, $\frac{F(y,x_0,\Delta,\sigma_0,\sigma')}{2\pi\Delta\sigma_0}\equiv\frac{1}{\sqrt{2\pi\sigma'^2}}$.
Below I reproduce the graphics of Boccio:




*After the measurement, the new distribution is a narrower Gaussian peaked closer to the actual position. That is called Bayes 'learning.*

### 5.6.9 Berger's Burgers-Maximum Entropy Ideas.

A fast food restaurant offers three meals: burger, chicken and fish.
The price, Caloric count, and probability of each meal being delivered cold are listed in Table 5.1 (Boccio):

| Item | Entree | Cost | Calories | Prob(hot) | Prob(cold) |
|---|---|---|---|---|---|
| Meal 1 | burger | \$1.00 | 1000 | 0.5 | 0.5 |
| Meal 2 | chicken | \$2.00 | 600 | 0.8 | 0.2 |
| Meal 3 | fish | \$3.00 | 400 | 0.9 | 0.1 |

Table 5.1: Berger's Burgers Details

The state of the system needs to be identified:
-Prob(burger)= $P(B)$,
-Prob(chicken)= $P(C)$,
-Prob(fish)= $P(F)$.
Even though the problem has been set up, we do not know which state is the actual state of the system.
To express what we do know despite this ignorance, or uncertainty, we assume that each of the possible states $A_i$ has some probability of occupancy $P(A_i)$ , where $i$ is an index running over the possible states.
As stated above, for the restaurant model, we have three such possibilities, which we have labelled $P(B)$, $P(C)$, and $P(F)$ .
A probability distribution $P(A_i)$ has the property that each of the probabilities is in the range $0 \le P(A_i) \le 1$ and since the events are mutually exclusive and exhaustive, the sum of all the probabilities is given by
$\sum_i P(A_i) = 1$ , Eq.(5.1).
Since probabilities are used to cope with our lack of knowledge and since one person may have more knowledge than another, it follows that two observers, because of their different knowledge, may use different probability distributions. In this sense probability, and all quantities that are based on probabilities are subjective.
The uncertainty is expressed quantitatively by the information which we do not have about the state occupied. This information is represented by Eq.(5.123), Part 1. Here presented as:
$S = -\sum_i P(A_i)\log_2[P(A_i)] = \sum_i P(A_i)\log_2[1/P(A_i)]$, Eq. (5.2).
This information is measured in bits because logarithms to base 2, are used.
In physical systems, this uncertainty is known as the entropy. Note that the entropy, because it is expressed in terms of probabilities, depends on the observer.
The principle of maximum entropy (**MaxEnt**) is used to discover the probability distribution which leads to the largest value of the entropy (a maximum), thereby assuring that no information is inadvertently assumed.
If one of the probabilities is equal to 1, all the other probabilities are equal to 0, and the entropy is equal to 0.
It is a property of the above entropy formula that it has its maximum when all the probabilities are equal (for a finite number of states), which is the state of maximum ignorance.
If we have no additional information about the system, then such a result seems reasonable. However, if we have additional information, then we should be able to find a probability distribution which is better in the sense that it has less uncertainty.
In this problem we will impose only one constraint. The particular constraint is the known average price for a meal at Berger's Burgers, namely \$1.75. This constraint is an example of

an expected value.
**a)** Express the constraint in terms of the unknown probabilities and the prices for the three types of meals.
Constraints take the form
$G$ =expected value= $\sum_i P(A_i)g(A_i)$ .
The constraints are:
$P(B) + P(C) + P(F) = 1$,
and, see Table 5.1,
$1.00P(B) + 2.00P(C) + 3.00)P(F) = 1.75$.
Two equations and three unknowns $P(B), P(C), P(F)$.
The amount of uncertainty about the probability distribution is, as mentioned before, the entropy, given by Eq.(5.2)
$S = P(B)\log_2\frac{1}{P(B)} + P(C)\log_2\frac{1}{P(C)} + P(F)\log_2\frac{1}{P(F)}$ .
Boccio presented two examples as a solution for the problem. These seem no to be appropriate, since information is used which cannot be known.

*The only way to find the probability distribution that uses no further assumptions beyond what can be known is to use the MaxEnt principle.*
This principle states that the selection of the probability distribution that gives maximum entropy is consistent with the constraints. So, no additional assumptions are introduced.
**b)** Using the above presented constraints, gives ranges for the three probabilities:
$a \le P(B) \le b$ ,
$c \le P(C) \le d$ ,
$e \le P(F) \le f$ .
Use
Subtract $P(B) + P(C) + P(F) = 1$, from $1.00P(B) + 2.00P(C) + 3.00)P(F) = 1.75 \Longrightarrow$
$\Longrightarrow 0.75 = P(C) + 2P(F)$.
Multiply $P(B) + P(C) + P(F) = 1$ by 2, and subtract
$1.00P(B) + 2.00P(C) + 3.00)P(F) = 1.75 \Longrightarrow 0.25 = P(B) - P(F)$.
Hence, with $P(C) = 0.75 - 2P(F)$
we learn: $0 \le P(F) \le \frac{0.75}{2}$.
With $0.25 = P(B) - P(F)$,
we have : $0.25 \le P(B) \le 0.25 + \frac{0.75}{2}$.
Finally, $P(C) = 0.75 - 2P(F)$,
$0 \le P(C) \le 0.75$ .
In summary:
$0 \le P(F) \le 0.375$,
$0 \le P(C) \le 0.75$,
$0.25 \le P(B) \le 0.625$.
**c)** Using these constraints, the total probability equal to 1, the entropy formula and the MaxEnt rule to obtain the three probabilities which maximise the entropy.
The entropy is
$S = P(B)\log_2\frac{1}{P(B)} + P(C)\log_2\frac{1}{P(C)} + P(F)\log_2\frac{1}{P(F)}$ ,
and plug into this expression the probabilities given above expressed in $P(F)$:
$S = [0.25 + P(F)]\log_2[\frac{1}{0.25+P(F)}] + [0.75 - 2P(F)\log_2[\frac{1}{0.75-P(F)}] + P(F)\log_2\frac{1}{P(F)}$ .

From $\frac{dS}{dP(F)} = 0$, the value of $P(F)$ and hence the values of $P(B)$, and $P(C)$ can be obtained.
The numbers are given by Boccio:
$P(F) = 0.216, P(B) = 0.466 , P(C) = 0.318$, and $S = 1.517$ bits.
Note: use could have been made of $\log_2 z = \ln z \,/\, \ln 2$ .
**d)** With these numbers the average calorie count and average meal cold can be calculated, se table 5.1 above:
- average meals cold: $1000P(B) + 600P(C) + 400P(F)$,
- average meals cold: $0.5P(B) + 0.2P(C) + 0.1P(F)$.

### 5.6.10 Extended Menu at Berger's Burgers

Suppose now that Berger's extends its menu with Tofu($T$), see table 5.2, Boccio page 77.

| Entree | Cost | Calories | Prob(hot) | Prob(cold) |
|---|---|---|---|---|
| burger | \$1.00 | 1000 | 0.5 | 0.5 |
| chicken | \$2.00 | 600 | 0.8 | 0.2 |
| fish | \$3.00 | 400 | 0.9 | 0.1 |
| tofu | \$8.00 | 200 | 0.6 | 0.4 |

Table 5.2: Extended Berger's Burgers Menu Details

Given: the average meal price is \$2.50.
Determine the state of the system, $P(B), P(C), P(F), P(T)$, using Lagrange multipliers.
The constraints
$P(B) + P(C) + P(F) + P(T) = 1$,
and
$1.00P(B) + 2.00P(C) + 3.00P(F) + 8.00P(T)$.
With the entropy function
$S = P(B)\log_2 \frac{1}{P(B)} + P(C)\log_2 \frac{1}{P(C)} + P(F)\log_2 \frac{1}{P(F)} + P(T)\log_2 \frac{1}{P(T)}$ .
The analytical method will not work. There are 2 equations and 4 unknowns. This require gradient search techniques.
A more general procedure is the Lagrange multipliers.
Define the Lagrange multipliers $\alpha$ and $\beta$. The Lagrange function $L$:
$L = S - (\alpha - \log_2 e)\,[P(B) + P(C) + P(F) + P(T)] +$
$-\beta[1.00P(B) + 2.00P(C) + 3.00P(F) + 8.00P(F) - 2.50]$.
$\log_2 e$ is plugged into this equation, since use will be made of
$\log_2 P(B) = \ln P(B) \,/\, \ln 2$.
Differentiate the preceding expression with respect to $P(B)$:
$\frac{d}{dP(B)} \log_2 P(B) = \frac{1}{\ln 2}\frac{1}{P(B)}$,
and
$\log_2 e = \frac{\ln e}{\ln 2} = \frac{1}{\ln 2}$.
So,
$\frac{d}{dP(B)} \log_2 P(B) = \frac{1}{\ln 2}\frac{1}{P(B)} = \frac{1}{P(B)}\log_2 e$.
Using this expression and the expression for $S$, differentiate $L$ with respect to $P(B)$ while keeping all the other probabilities, $\alpha$ and $\beta$ constant:
$\frac{\partial L}{\partial P(B)} = \frac{\partial S}{\partial P(B)} - (\alpha - \log_2 e) - \beta = \log_2 \frac{1}{P(B)} - P(B)\frac{d}{dP(B)}\log_2 P(B) - (\alpha - \log_2 e) - \beta =$
$= \log_2 \frac{1}{P(B)} - \log_2 e - (\alpha - \log_2 e) - \beta = 0$.
This results into
$\log_2 \frac{1}{P(B)} = \alpha + \beta$.
Similarly

$\log_2 \frac{1}{P(C)} = \alpha + 2\beta$ , $\log_2 \frac{1}{P(F)} = \alpha + 3\beta$ , $\log_2 \frac{1}{P(T)} = \alpha + 8\beta$.

Then, Boccio pages 78 and 79, two equations for $\alpha$ and $\beta$ are obtained

$$P(B) = 2^{-\alpha}2^{-\beta}$$
$$P(C) = 2^{-\alpha}2^{-2\beta}$$
$$P(F) = 2^{-\alpha}2^{-3\beta}$$
$$P(T) = 2^{-\alpha}2^{-8\beta}$$

With the constraints:

$$P(B) + P(C) + P(F) + P(T) = 1$$
$$2^{-\alpha}(2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta}) = 1$$
$$\log_2\left(2^{-\alpha}(2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta})\right) = 0$$
$$\alpha = \log_2\left(2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta}\right)$$

and the average

$$2^{\alpha}\left(1.00P(B) + 2.00P(C) + 3.00P(F) + 8.00P(T)\right) = 2.50 \times 2^{\alpha}$$
$$1 \times 2^{-\beta} + 2 \times 2^{-2\beta} + 3 \times 2^{-3\beta} + 8 \times 2^{-8\beta} = 2.50 \times 2^{\alpha}$$
$$1 \times 2^{-\beta} + 2 \times 2^{-2\beta} + 3 \times 2^{-3\beta} + 8 \times 2^{-8\beta} = 2.50 \times (2^{-\beta} + 2^{-2\beta} + 2^{-3\beta} + 2^{-8\beta})$$
$$1.50 \times 2^{-\beta} + 0.50 \times 2^{-2\beta} - 0.50 \times 2^{-8\beta} - 5.50 \times 2^{-8\beta} = 0$$

Finding the zeroes of the last equation gives us $\beta$ and the value of $\beta$ gives us $\alpha$, which then determine the probabilities and the entropy. The computed values are

$$\beta = 0.2586\ bits/dollar$$
$$\alpha = 1.2371\ bits$$
$$P(B) = 0.3546$$
$$P(C) = 0.2964$$
$$P(F) = 0.2478$$
$$P(T) = 0.1011$$
$$S = 1.8835\ bits$$

Note: I used the results of Boccio. However, the equation for $\beta$, with the WolframAlpha app,
$1.50 \cdot 2^{-\beta} + 0.50 \cdot 2^{-2\beta} - 0.50 \cdot 2^{-8\beta} - 5.50 \cdot 2^{-8\beta} = 0$,
gives as a solution: $\beta = 0.2339$.

### 5.6.11 The Poisson Probability Distribution

Boccio: "*The arrival time of rain drops on the roof or photons from a laser beam on a detector are completely random, with no correlation from count to count. If we count for a certain time interval we won't always get the same number - it will fluctuate from shot-to-shot. This kind of noise is sometimes known as shot noise or counting statistics*."

Suppose, the particles arrive at an average rate $R$. In a small time interval $\Delta t \ll \frac{1}{R}$, no more than one particle can arrive. Now we seek the probability for $n$ particles to arrive after time $t$, $P(n, t)$.

The probability for a particle to be in the interval $\Delta t$ is
$P_{\Delta t} = R\Delta t \ll 1$ .

**a)** Show that the probability to detect zero particles exponentially decays:
$P(0, t) = e^{-Rt}$.

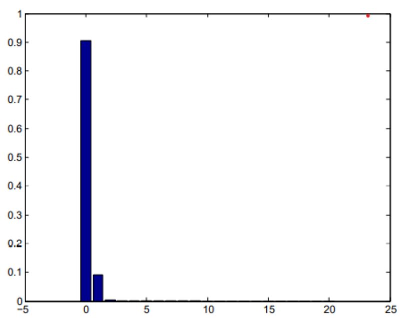
Consider a finite time interval $[0, t]$.

There are $N = \frac{t}{\Delta t}$ slices in the interval.

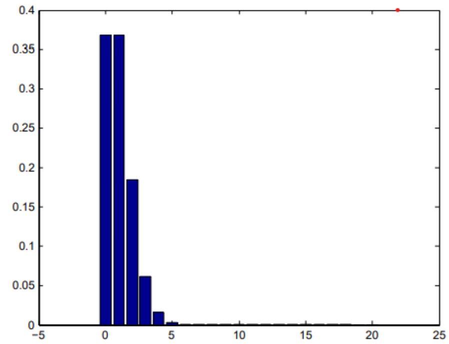
Let $q_{\Delta t} = 1 - P_{\Delta t}$, to be the probability of no particle in the slice.

The different slices are statistically independent. Hence, the probability of no detection in the interval $[0, t]$ is given by

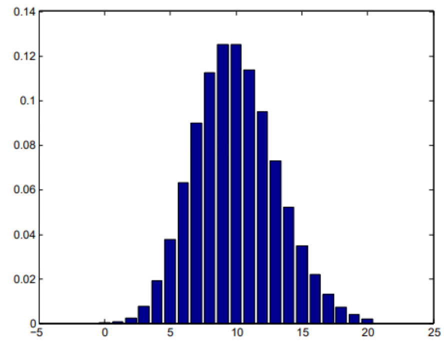
$(q_{\Delta t})^N = (1 - P_{\Delta t})^N = (1 - R\Delta t)^{\frac{t}{\Delta t}}$.
Consequently,
$P(0,t) = \lim_{\Delta t \to 0} (1 - R\Delta t)^{\frac{t}{\Delta t}} = e^{-Rt}$ .
**b)** Obtain a differential equation as a recursion relation.
In the time interval $t \to t + \Delta t$, either no particles or one particle is detected, with $n$ the number of particles, the sum of two products of independent probabilities:
$P(n, t + \Delta t) = P(n,t) \cdot P(0, \Delta t) + P(n-1,t) \cdot P(1, \Delta t) =$
$= P(n,t) \cdot (1 - P_{\Delta t}) + P(n-1,t) \cdot P(1,\Delta t) = P(n,t) \cdot (1 - R\Delta t) + P(n-1,t) \cdot R\Delta t.$
Then,
$P(n, t + \Delta t) - P(n,t) = -P(n,t) \cdot R\Delta t + P(n-1,t) \cdot R\Delta t \Longrightarrow$
$\Longrightarrow \frac{P(n,t+\Delta t) - P(n,t)}{\Delta t} = R[P(n-1,t) - P(n,t)].$
So,
$\frac{d}{dt} P(n,t) = \lim_{\Delta t \to 0} \frac{P(n,t+\Delta t) - P(n,t)}{\Delta t} = R[P(n-1,t) - P(n,t)].$
In this way a differential equation as a recursion relation has been derived.
**c)** Solve the preceding recursion relation:
$\frac{d}{dt} P(n,t) = R[P(n-1,t) - P(n,t)].$
Start with $n = 0$:
$\frac{d}{dt} P(0,t) = R[-P(0,t)] \Longrightarrow P(0,t) = e^{-Rt},$
where use has been made at $t = 0$, $P(0,0) = 1$. No particles decayed.
$n = 1$ :
$\frac{d}{dt} P(1,t) = R[P(0,t) - P(1,t)] = R[e^{-Rt} - P(1,t)] = -RP(1,t) + Re^{-Rt},$
a nonhomogeneous differential equation of first order.
The solution is
$P(1,t) = Rte^{-Rt},$
where use has been made of the decay of one particle$\Longrightarrow$ $P(1,0) = 0$.
$n = 2$:
$\frac{d}{dt} P(2,t) = R[P(1,t) - P(2,t)] = R[te^{-Rt} - P(2,t)] = -RP(2,t) + Rte^{-Rt}.$
The solution is
$P(2,t) = \frac{1}{2}(Rt)^2 e^{-Rt}.$
Applying induction, the Poisson distribution is
$P(n,t) = \frac{1}{n!}(Rt)^n e^{-Rt}.$
Note: assume this expression to be correct and solve the differential equation for $n + 1$.
A histogram for $Rt = 0.1$, Boccio:



A histogram for $Rt = 1$, Boccio




A histogram for $Rt = 10$, Boccio




For $Rt \to \infty$, the Gaussian distribution is recovered.

**d)** The mean and the standard deviation.

- the mean

The expectation value definition, use $\lambda \equiv Rt$

$$\langle n \rangle = \sum_{n=0}^{\infty} nP(n,t) = \sum_{n=0}^{\infty} \frac{n}{n!}(\lambda)^n e^{-\lambda} = 1 \cdot \frac{\lambda}{1!} \cdot e^{-\lambda} + 2 \cdot \frac{\lambda^2}{2!} \cdot e^{-\lambda} + 3 \cdot \frac{\lambda^3}{3!} \cdot e^{-\lambda} + \cdots =$$

$$= \lambda \cdot e^{-\lambda}\left(1 + \lambda + \frac{\lambda^2}{2!} + \frac{\lambda^3}{3!} + \cdots \frac{\lambda^n}{n!} + \cdots\right) = \lambda \cdot e^{-\lambda} \cdot e^{\lambda} = \lambda \equiv Rt\ .$$

- the standard deviation

$\sigma_n^2 = \langle n^2 \rangle - \langle n \rangle^2$.

$\sigma_n^2 = \langle (n - \langle n \rangle)^2 \rangle$.

Now, Boccio presented a trick.

First consider, use the result of the mean:

$$\langle n^2 \rangle - \langle n \rangle = \langle n(n-1) \rangle = \sum_{n=0}^{\infty} n(n-1)P(n,t) = \sum_{n=0}^{\infty} \frac{1}{(n-2)!}(\lambda)^n e^{-\lambda} =$$

$$\sum_{m=0}^{\infty} \frac{1}{m!}(\lambda)^{m+2} e^{-\lambda} = \lambda^2.$$

Then,

$$\sigma_n^2 = \langle n^2 \rangle - \langle n \rangle^2 = \langle n(n-1) \rangle + n - \langle n \rangle^2 = \lambda^2 + \lambda - \langle n \rangle^2 = \lambda \equiv Rt.$$

Hence,

$$\sigma_n = \sqrt{Rt} = \sqrt{n}\ .$$

**e)** An alternative way to derive the Poisson distribution is to note that the count in each small time interval is a Bernoulli trial[2] with probability $p = R\Delta t$ to detect a particle and $1 - p$ for no detection. The total number of counts is the binomial distribution. Take the limit as $\Delta t \to 0$ (thus $p \to 0$) but $\lambda \equiv Rt$ remains finite. Let the number of intervals

[2] Bernoulli Trial. https://en.wikipedia.org/wiki/Bernoulli_trial : In the theory of probability and statistics , a Bernoulli trial (or binomial trial) is a random experiment with two possible outcomes, “success” and “failure”, in which the probability of success is the same every time the experiment is conducted.

$N = \frac{t}{\Delta t} \to \infty$, while $Np = Rt \equiv \lambda$ , remains finite.
The binomial distribution in the interval $[0, t]$, with $N$ interval, for $n$ counts is

$$P(N, n) = \binom{N}{n} p^n (1-p)^{N-n}.$$

The probability of a count in $\Delta t$ is

$$p = R\Delta t = \frac{Rt}{N} \equiv \frac{\lambda}{N} .$$

So,

$$P(N, n) = \frac{N!}{n!(N-n)!} (\frac{\lambda}{N})^n \frac{(1-\frac{\lambda}{N})^N}{(1-\frac{\lambda}{N})^n} .$$

With $\lambda$ is finite

$$\lim_{N\to\infty} P(N, n) = \frac{\lambda^n}{n!} e^{-\lambda} \lim_{N\to\infty} \frac{N!}{N^n(N-n)!} ,$$

where use has been made of

$$\lim_{N\to\infty} (1 - \frac{\lambda}{N})^N = e^{-\lambda}, \text{ and } \lim_{N\to\infty} (1 - \frac{\lambda}{N})^n = 1.$$

Finally,

$$\lim_{N\to\infty} \frac{N!}{N^n(N-n)!} = \lim_{N\to\infty} \frac{N(N-1)(N-2)\ldots.(N-(n-1))(N-n)!}{N^n(N-n)!} = \lim_{N\to\infty} \left(1-\frac{1}{N}\right)\left(1-\frac{2}{N}\right)..(1-\frac{n-1}{N}) = 1.$$

With all the ingredients available

$$\lim_{N\to\infty} P(N, n) = \frac{\lambda^n}{n!} e^{-\lambda},$$

the Poisson distribution.

### 5.6.12 Modeling Dice: Observables and Expectation Values

Suppose we have a pair of six-sided dice. If these are both rolled a pair of results is obtained:
$a \in \{1,2,3,4,5,6\}$ , $b \in \{1,2,3,4,5,6\}$,
where $a$ and $b$ correspond to the number of spots of the top face of the dice. With fair dices the probability of a number of spots of the top faces is 1/6 .
Then

$$\langle a \rangle = \langle b \rangle = \sum_{i=1}^{6} i \cdot \Pr(i) = \frac{1}{6} \sum_{i=1}^{6} i = \frac{7}{2} .$$

Define two new observables

$$s = a + b \quad , \quad p = ab.$$

- $\langle s \rangle$ ,

where $s_{min} = 2$, and $s_{max} = 12$.

$$\langle s \rangle = \sum_{i=2}^{12} i \cdot \Pr(s = i).$$

This expectation value can be obtained by counting all the results. Keep in mind by rolling the dice the probability to obtain a combination, e.g., $\{1,2\}$, is $\frac{1}{6} \cdot \frac{1}{6}$ . This combination can be obtained in two ways: $\{1,2\}, \{2,1\}$ . The expression in the summation for this combination is:

$$i \cdot \Pr(i) = 3\left(\frac{1}{36} + \frac{1}{36}\right) = \frac{1}{6} . \text{ Etc.}$$

However, we know already

$$\langle s \rangle = \langle a \rangle + \langle b \rangle .$$

Hence

$$\langle s \rangle = \frac{7}{2} + \frac{7}{2} = 7.$$

Note: as mentioned by Boccio, carefully bookkeeping gives the same result as it should.
Is this bookkeeping necessary?

$$\langle s \rangle = \sum_{i=1}^{6} \sum_{j=1}^{6} (i + j) P(i, j),$$

and
$P(i,j) = \frac{1}{36}$.
$\langle s\rangle = \frac{1}{36}\sum_{i=1}^{6}\sum_{j=1}^{6}(i+j) = \frac{1}{36}\sum_{i=1}^{6}(6\cdot i + \sum_{j=1}^{6} j) = \frac{1}{6}\sum_{i=1}^{6}(i + \frac{1}{6}\sum_{j=1}^{6} j) =$
$= \frac{1}{6}\sum_{i=1}^{6}(i + \langle b\rangle) = \frac{1}{6}[(\sum_{i=1}^{6} i) + 6\cdot\langle b\rangle] = \langle a\rangle + \langle b\rangle$.
Here, I used another type of "bookkeeping" with the advantage that, in addition,
$\langle s\rangle = \langle a\rangle + \langle b\rangle$, has been proven.

- $\langle p\rangle$,
where $p_{min} = 1$, and $p_{max} = 36$. Note: prime numbers excluded: (7,11,13,17,19,23,29,31).
$\langle p\rangle = \sum_{i=1, i\neq prime}^{36} i \cdot \Pr(p=i)$,
for $prime > 5$.
Again, e.g., the combination $\{1,2\}$ is obtained in two ways,. Each with a probability of $\frac{1}{36}$.
So,
$i\cdot \Pr(p=i) = \frac{1}{36}(1\cdot 2 + 2\cdot 1) = \frac{1}{9}$.
Again, carefully bookkeeping gives $\langle p\rangle = \frac{49}{4}$, as it should be.
Rolling the dice create independent results:
$\langle p\rangle = \langle a\rangle\langle b\rangle = \frac{7}{2}\cdot\frac{7}{2} = \frac{49}{2}$.
Another approach, comparable with the approach used for $\langle s\rangle = \langle a\rangle + \langle b\rangle$.
$\langle p\rangle = \langle ab\rangle = \sum_{i=1}^{6}\sum_{j=1}^{6}(i\cdot j)P(i,j)$.
With $P(i,j) = \frac{1}{36}$,
$\langle p\rangle = \langle ab\rangle = \frac{1}{36}\sum_{i=1}^{6}\sum_{j=1}^{6}(i\cdot j) = \frac{1}{36}\sum_{i=1}^{6} i\cdot\sum_{j=1}^{6} j = \frac{1}{6}\sum_{i=1}^{6} i\cdot\langle b\rangle = \frac{\langle b\rangle}{6}\sum_{i=1}^{6} i = \langle a\rangle\langle b\rangle$.
Now, again without counting all the results of rolling the two dice, we proved.
$\langle p\rangle = \langle ab\rangle = \langle a\rangle\langle b\rangle$.

### 5.16.3 Conditional Probabilities for Dice

Use the results of problem 5.6.12.
By intuition the answers for this problem can be obtained. Without intuition, there is Baye's Rule to be used:
$\Pr(x|y) = \frac{\Pr(y|x)\cdot\Pr(x)}{\Pr(y)}$.
**a)** A pair of dice(a,b) is rolled. The only information you get is that
$s = a + b = 8$.
The question here is to find the conditional probability for $a$.
For $s = 8$, you can list the possibilities (a,b):
(2,6)(3,5)(4,4)(5,3)(6,2), 5 combinations out of a possible 36 combinations.
The forward conditional probability distribution ($\Pr(s=8|a=i)$ for $a$ is $\frac{1}{6}$.
Now Baye's rule, with $\Pr(a=i) = \frac{1}{6}$, and $\Pr(s=8) = \frac{5}{36}$,
$\Pr(a=i|s=8) = \frac{\Pr(s=8|a=i)\cdot\Pr(a=i)}{\Pr(s=8)} = \frac{\Pr(s=8|a=i)\cdot\frac{1}{6}}{\frac{5}{36}} = \frac{6}{5}\cdot\Pr(s=8|a=i)$.
The forward probabilities are
$(\Pr(s=8|a=2) = \Pr(b=6) = \frac{1}{6}$,
$(\Pr(s=8|a=3) = \Pr(b=5) = \frac{1}{6}$,
…………

$(\Pr(s = 8|a = 6) = \Pr(b = 2) = \frac{1}{6}$.
**b)** A pair of dice(a,b) is rolled. The only information you get is that and, without showing the results, you are informed $p = 12$, and $p = a \cdot b$.
What is the conditional expectation value of $\langle s \rangle = \langle a \rangle + \langle b \rangle$?
If $p = 12$, we have the following combinations of $(a, b)$:
$(2{,}6)(3{,}4)(4{,}3)(6{,}2)$.
So, with
$s = a + b$,
$s = 7(twice)$, and $s = 8(twice)$ .
Then, the conditioned probability distribution for $s$ is:
$\Pr(s = 7|p) = \Pr(s = 8|p) = \frac{2}{4} = \frac{1}{2}$.
Consequently, the conditioned expectation value is:
$\sum_i iP(i|p) = (7 + 8) \cdot \frac{1}{2} = \frac{15}{2}$.

### 5.6.14 Matrix Observables for Classical Probability

Suppose we have a biased coin, which has probability $p_h$ of landing heads-up and probability of landing tails-up. Say, we flip the biased coin but do not look at the result. This preparation procedure is represented by a classical state vector
$x_0 = \begin{pmatrix} \sqrt{p_h} \\ \sqrt{p_t} \end{pmatrix}$.
**a)** Define an observable (random variable) $r$ that takes $+1(= h)$ if the coin is heads-up and $-1(t)$ if the coin is tails-up. Find a matrix $R$ such that
$x_0^T R x_0 = \langle r \rangle$,
where $\langle r \rangle$ denotes the mean or expectation value of the defined observable.
The expectation value for this (biased) coin:
$\langle r \rangle = h \cdot p_h + t \cdot p_t = p_h - p_t$.
Note: for a fair coin $\langle r \rangle = 0$.
So,
Plug a general $2 \times 2$ matrix into
$x_0^T R x_0 = \ p_h - p_t \Rightarrow R = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.
**b)** Now, find a matrix $F$ such that the *dynamics* corresponding to turning the coin over (after having flipped it, but still without looking at the result) is represented by
$x_0 \mapsto F x_0 \ (\mapsto maps\ to)$,
and
$\langle r \rangle \mapsto x_0^T F^T R F x_0$.
Well, thinking in terms of dynamics $F = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$, is considered to be not vary dynamic.
Furthermore $F = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ maps $x_0 = \begin{pmatrix} \sqrt{p_h} \\ \sqrt{p_t} \end{pmatrix}$ onto itself. Not very dynamical again.
For the reason of dynamics, I assume
$F x_0$ to be $\begin{pmatrix} \sqrt{p_t} \\ \sqrt{p_h} \end{pmatrix} \Rightarrow F = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.
Then
$F^T R F = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$,

where

$RF = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$

Then,

$x_0^T F^T RF x_0 = p_t - p_h = \langle r \rangle.$

Hence the operator $F^T RF$ works.

Now

$$x_0^T RF x_0 = \begin{pmatrix} \sqrt{p_h} & \sqrt{p_t} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{p_h} \\ \sqrt{p_t} \end{pmatrix} = \sqrt{p_h p_t} - \sqrt{p_h p_t} = 0\ .$$

This result vanish for a fair coin and a biased coin. Consequently for any coin.

$$x_0^T F^T R x_0 = \begin{pmatrix} \sqrt{p_h} & \sqrt{p_t} \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{p_h} \\ \sqrt{p_t} \end{pmatrix} = -\sqrt{p_h p_t} + \sqrt{p_h p_t} = 0\ .$$

Again, similarly, this result vanish for a fair coin and a biased coin. Consequently for any coin.

**c)** Let us now define the algebra of flipped-coin observables to be the set $V$ of all matrices of the form

$v = aR + bR^2.$

With

$R = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$

$v = aR + bR^2 = \begin{pmatrix} a+b & 0 \\ 0 & b-a \end{pmatrix},$

And, I suppose, $a, b \in \mathbb{R}$ .

Consequently,

$v = \begin{pmatrix} c & 0 \\ 0 & d \end{pmatrix},$

and

$c, d \in \mathbb{R}$ .

Hence, all elements of $V$ can be expressed in this way.

So, $v_1, v_2 \in V$.

Now, $v_1 \cdot v_2$:

$v_1 \cdot v_2 = \begin{pmatrix} c_1 & 0 \\ 0 & d_1 \end{pmatrix} \begin{pmatrix} c_2 & 0 \\ 0 & d_2 \end{pmatrix} = \begin{pmatrix} c_1 c_2 & 0 \\ 0 & d_1 d_2 \end{pmatrix},$

and

$v_2 \cdot v_1 = \begin{pmatrix} c_1 c_2 & 0 \\ 0 & d_1 d_2 \end{pmatrix},$

since $c_i, d_i \in \mathbb{R}$ .

Set $(a, b) = (-1, 0) \Rightarrow v = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = -R.$

Then, $c$ takes the value for tails and $d$ takes the value for heads.

# 6 The formulation of Quantum Mechanics

## 6.1 Introduction

A physical theory is defined.

The process of doing theoretical physics is described.

A description of a physical system is summarized.

*In quantum mechanics we are forced to work in the world of probabilities.*

## 6.2 Two postulates: Presentation, Rationalization and Meaning

**Postulate 1**

*For each dynamical variable or observable, which is a physical concept, there corresponds a Hermitian, linear operator, which is a mathematical object.*

*The possible values of any measurement of the observable are restricted to the eigenvalues of the corresponding operator.*

*Then Boccio made the essential remark:*

*If the predictions agree with experiment, on a certain quantum system, then the postulates are valid for that class of systems.*

Some new mathematical objects are presented:

-the trace of a density operator and some properties of the trace, Eqs.(6.2)-(6.4).

In Eq.(6.6), we recognise the spectral representation of a matrix.

Next, the concept of a state in quantum mechanics is discussed. *The state description must be probabilistic*.

**-** the properties of expectation values are summarized at the end of the discussion of postulate 1, page 367.

**Postulate 2**

a) *A density operator exists for every real physical system.*

b) The expectation value of an operator $\hat{B}$ is given by, Eq.(6.16)

$\langle\hat{B}\rangle = Tr(\widehat{W}\hat{B})$,

where $\widehat{W}$ is the density operator.

Boccio chooses a 1-dimensional subspace spanned by the vector $|\alpha\rangle$ to demonstrate the meaning of this postulate.

The density operator is, Eq.(6.17).

$\widehat{W} = |\alpha\rangle\langle\alpha|$.

The trace of a projection operator is 1. This follows from the fact that the trace of a Hermitian operator is the sum of the eigenvalues. Since a Hermitian matrix can be diagonalized, the trace of this diagonalized operator is the sum of its eigenvalues. There are two eigenvalues: 1 and zero. The eigenvalue of $|\alpha\rangle$:

$|\alpha\rangle\langle\alpha|\,|\alpha\rangle = |\alpha\rangle$ ,

is one. So,

$Tr(\widehat{W}) = 1$, Eqs.(6.1) and (6.18).

Equation (6.21) is the spectral representation of the matrix $\widehat{W}$, Eq.(6.6).

Eq.(6.21) *represents a statistical mixture of the states.*

Consequently, $w_k$ in Eq.(6.21) can be considered the probability of each state occurring in the projection operator, or density matrix $|w_k\rangle\langle w_k|$. This can be concluded from, Eq.(6.20),

$0 \le w_k \le 1$ and $\sum_k w_k = 1$.

Boccio proved, Eqs. (6.22) and (6.23),

$\langle\hat{B}\rangle = Tr(\widehat{W}\hat{B})$,

see also Susskind page 196.

## 6.3 States and Probabilities

### 6.3.1 States

Among the set of all possible states there exists a special group called pure states.

The analysis of the density operator of a pure state is summarized: Eqs.(6.26)-(6.32).

The difference between a pure state and a nonpure state is discussed.

Boccio concluded this section with the assumption both pure and nonpure states are

fundamental and physical systems to be described by both types of states.
Boccio will not call a nonpure state a mixed state.

### 6.3.2 Probabilities

Postulate 2 is summarized [Eq.(6.16)], and slightly rewritten presented in Eq.(6.48).
Next, Boccio introduced the function $F(\hat{Q})$ of the operator $\hat{Q}$.
Then, $h(q)dq$ representing the probability that the measured value of the observable represented by $\hat{Q}$ lies in the interval $\{q, q + dq\}$.
With these results the general definition of the average of $F(\hat{Q})$ is given, Eq,(6.50), and same average of postulate 2 expressed in the trace of the product of the density operator and $F(\hat{Q})$.
Boccio discussed two cases:
- Discrete spectrum
- Continuous spectrum.

**Case 1: Discrete Spectrum**
Reminder Eq.(6.53**):**
given, Eq.(6.52), $\hat{Q}|q_n\rangle = q_n|q_n\rangle$, then
$\hat{Q}|q_n\rangle\langle q_n| = q_n|q_n\rangle\langle q_n| \longrightarrow \hat{Q}\sum_n|q_n\rangle\langle q_n| = \sum_n q_n|q_n\rangle\langle q_n| \longrightarrow \hat{Q} = \sum_n q_n|q_n\rangle\langle q_n|$,
where $\sum_n|q_n\rangle\langle q_n| = I$.
Next $F(\hat{Q})$ is defined as a Heaviside step function, Eqs. (6.54) and (6.55).
No surprise, the delta function appears, Eq.(6.58).

**Case 2: Continuous Spectrum**
$\hat{Q}$, a self-adjoint operator with a continuous spectrum represented in Eq.(6.75).
As usual wit continuous spectra the Dirac delta function is used for normalization. Also called Delta-function normalization, Eq.(6.76).
Again, the Heaviside step function is used.
The probability density for the observable represented by $\hat{Q}$ is given in Eq.(6.81).
Then, Boccio summarized the topic of quantum dynamics and the action to be taken.
It is about time dependency.

## 6.4 Quantum Pictures

Three ways are presented to make expectation values dependent on time.
- The Schrödinger Picture: states depend on time, operators do not.
- Heisenberg Picture: operators depend on time, states do not.
- Interaction Picture: as indicated by the name a mixture of the foregoing two pictures for an important class of problems.

*All of these pictures must agree in the sense that they all give the same time dependence for* $\langle\hat{Q}(t)\rangle$**.** *There is after all, a unique world out there.*
Then Boccio summarized the fundamental dynamical variables: Position, linear momentum, angular momentum and energy.

## 6.5 Transformations of States and Observables. The Way it must be.

Laws of nature are invariant under certain space-time symmetry transformations.
Pure states are used to discus the subject matter.
In these transformations the eigenvalues are unchanged.
Similarly, probabilities are unchanged.

### 6.5.1 Antiunitary/Antilinear Operators

Eq. (6.87) defines the antilinear operator:
$\hat{T}(|\psi\rangle + |\phi\rangle) = \hat{T}|\psi\rangle + \hat{T}|\phi\rangle$ and $\hat{T}c|\psi\rangle = c^*\hat{T}|\psi\rangle$ .

### 6.5.2 Wigner's Theorem

The unitary and antiunitary operators are defined. Boccio showed these operators to be linear. To this end the example of a series of displacements are presented to illustrate this.
Eq.(6.92), with $|q'_n\rangle = \hat{U}|q_n\rangle$,
$\hat{Q}'|q'_n\rangle = \hat{Q}'\hat{U}|q_n\rangle \rightarrow q_n|q'_n\rangle = \hat{Q}'\hat{U}|q_n\rangle \rightarrow q_n\hat{U}|q_n\rangle = \hat{Q}'\hat{U}|q_n\rangle$ .
In Eq.(6.95), the corresponding transformation rule for linear operators is presented.

### 6.5.3 The Transformation Operator and its Generator

Let $t$ to be a continuous parameter. A family of unitary operators is presented in Eq.(6.96). Then, the Hamiltonian to be Hermitian is derived, Eq.(6.102). See also Susskind pages 99-101.
With Eq.(6.101), Eqs((6.104) and (6.105) are obtained.
Boccio summarized this section with: "*The generator $\hat{H}$ of the infinitesimal transformation, determines the operator*
$\hat{U}(t) = e^{-i\hat{H}t}$,
*for a finite transformation.*"

## 6.6 The Schrödinger Picture.

The question to be answered is: *How are the state vectors $|\psi(0)\rangle$ and $|\psi(t)\rangle$ related to each other?*
Fitzpatrick discussed the subject matter in The Graduate Course Chapter 3.
Then some 6 assumptions are summarized.
Wigner's theorem, Eq.(6.107): there exists a unitary, linear operator $\hat{U}(t)$ such that
$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$,
see also Susskind pages 97 and 98.
Then, Schrodinger's time dependent equation is derived, Eq.(6.113).
The important issue here is to derive the Hamiltonian operator. Well, a possibility to obtain the Hamiltonian from classical physics. Bring the Hamiltonian in operator form and see how it works out.
Next, Boccio presented an alternative approach to unitary translation operators.
In Figure 6.1, page 385, Boccio illustrates the meaning of translation in space.

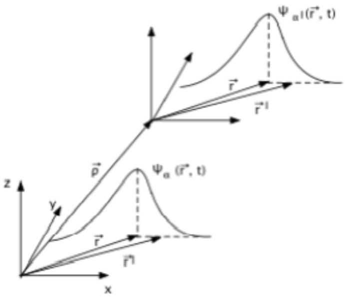



Figure 6.1: Space Translation

The spatial translation operator is given by Eq.(6.124).
It always interesting to read other courses on the subject matter, Fitzpatrick Graduate Course Chapter 2.
Then, time displacement is analysed, page 386.
Time dilation is presented by Eq.(6.125) and illustrated in Figure 6.2 Boccio.

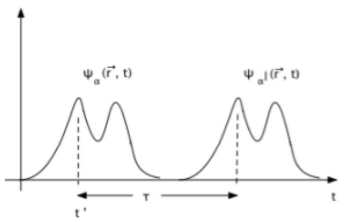


Figure 6.2: Time Translation

A unitary operator is introduced for this transformation, Eq.(6.126).

This unitary operator is presented by an exponential function using $\hat{E} = \hat{H} = i\hbar\frac{\partial}{\partial t}$.

To obtain Eq.(6.131), $t$ has been replaced by $t + \tau$ .

## 6.7 The Heisenberg Picture

*In the Heisenberg picture operators change with time and states are constant in time.*

Eq.(6.137) should read:

$$\hat{Q}(t) = e^{\frac{i\hat{H}t}{\hbar}}\hat{Q}(0)e^{\frac{-i\hat{H}t}{\hbar}} .$$

At the top of page 388, just below property number 4, "…*then the spectral decomposition of* $\hat{Q}(0)$….." should read "……then the spectral decomposition of $\hat{Q}(t)$…..".

## 6.8 Interaction Picture

Eq. (6.149) should read:

$$i\frac{d}{dt}|\psi_I(t)\rangle = \hat{V}_I(t)|\psi_I(t)\rangle \text{ ?}$$

*In the interaction picture both state vectors and the operators are dependent on time.*

## 6.9 Symmetries of Space-Time.

Velocities are considered to be small compared to the speed of light. This section deals with how to find $\hat{H}$? Symmetries play a key role.

Transformation are presented in Eq.(6.152).

Rotations are given by Eqs.(6.153)-(6.156), and illustrated in Figure 6.3 .

A group of transformations is defined on page 391, as well as a one-parameter subgroup. An example of a subgroup is rotation about a fixed axis as shown in Figure 6.3. The one-parameter is the angle of rotation $\phi$, Figure 6.3.

Boccio summarized the total group of transformation at the bottom of page 391 and top of page 392: 10 parameters:

- rotations,
- space translations,
- Galilean boosts or Lorentz boosts,
- time translations.

*The time evolution operator, discussed already in the foregoing sections, $\hat{U}(t)$, belongs to the time translation transformation.*

## 6.10 Generators of the Group Transformations.

In Eq.(6.160), the ten parameters are presented in a general way as a product.

*A ten-parameter group transformation is then defined by the product of ten one-parameter subgroup transformations*, top of page 392.

Boccio analysed Eq.(6.160) for all ten parameters to be infinitesimally small, Eq.(6.163).

In Eqs.(6.171)-(6.178), all four transformations are summarized.

## 6.11 Commutators and Identities

Boccio started by ignoring the identity operator in Eq.(6.179)≡(6.170).
By physical arguments for the commutators in Eq.(6.179), some commutators can be derived, Eqs. (6.180)-(6.185). In this way, the remaining unknown commutators are allocated, Eq.(6.186).
Then, a general procedure to find the latter commutators is presented on page 396.
11 commutators are obtained by this procedure, Eqs.(6.207)-(6.210).
So, there is one commutator left to be found.
Boccio showed that the identity operator can be neglected.
Then, this last commutator is presented in Eq.(6.223).

## 6.12 Identification of Operators with Observables.

The dynamics of a free particle is used to identify the operators representing the dynamical variables or observables for this free particle.
A position operator is defined in Eqs.(6.224) and (6.225).
The relation between the position operator and the velocity operator is given in Eq.(6.228).
Assuming this relation, Eq.(6.229) represents the result of Eq.(6.228) for a pure state.
The looks like the Schrödinger Picture. The displacement operator not to be time dependent.
Then Boccio rehearsed the time transformation for a ket vector: Eqs.(6.230)-(6.234). This results into an expression for the velocity operator as the commutator of the position operator and $\hat{H}$, where $\hat{H}$ is still unknown.
Finally, Boccio obtained *one of the most important results in the theory of quantum mechanics*: Eq.(6.252) → the commutator of position operators..
In Eq.(6.266) the commutators of the position operator $\hat{\boldsymbol{Q}}$ are presented.
Boccio reviewed some mathematical ideas, page 405, about sets of operators and subspaces.
Then some examples are given of Schur's Lemma.
- Example 1 Free Particle-no internal degrees of freedom.

A result of this example I Eq.(6.297):

$\hat{H} = \frac{\hat{P}^2}{2M}$,

and we arrive at the meaning of the operator $\hat{H}$ as summarized in Eq.(6.290).
- Example 2 Free Particle-with Spin.

The spin operator $\hat{\boldsymbol{S}}$ *is defined to be an internal contribution to the total angular momentum of the system,* Eq. (6.296).
- Example 3 A Particle Interacting with External Fields.

In this example Boccio considers only spinless particles.
We see, due to the external field the occurrence of the vector potential and the scalar potential.

## 6.13 Multiparticle Systems

In this section the single particle results are generalized to a system with more than one particle.
Boccio analysed the multiparticle system with a two particle system. A two particle system without any interaction with each other.
The properties of the two particles can be measured independently.
In Eq.(6.326) the systems of the two particles are presented by their state vector, observable and eigenvalue. The two state vector is represented by a direct product, i.e., a

tensor product. Sometimes denoted as a product state(product vector), Eq.(6.328).
In Eq.(6.329) it is shown how the operator for particle 1 works on the product state.
Furthermore, the action of the operator on particle two is given. (See, e.g., Susskind Lecture 6).
On page 414, Boccio presented an example for two operators and two basis vectors $|+\rangle$ and $|-\rangle$. The operators are represented by $2 \times 2$ matrices, Eq.(6.333).
The product space is 4-dimensional, with the 4 product states given in Eq.(6.334).
The general operator, a $4 \times 4$, matrix is given by Eq.(6.335). Here, Boccio gave the example $\hat{Q}_{12} = \beta_1{}^{(1)} \otimes \hat{I}^{(2)}$, the matrix elements,
where
$\beta_1{}^{(1)} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, the operator acting on particle (1), and $\hat{I}^{(2)}$, the unit operator for particle (1).
So, with tensor multiplication,

$$\hat{Q}_{12} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} a & 0 & b & 0 \\ 0 & a & 0 & b \\ c & 0 & d & 0 \\ 0 & c & 0 & d \end{pmatrix}, \text{ Eq.(6.335).}$$

Boccio presented the general operator in more detail, using the state vectors in Eq.(6.334). (See also Susskind Lecture 7).
The result for particle (2) is presented in Eq.(6.336).
The combined operator is given in Eq.(6.337).
Then, Boccio translated the results for the Pauli spin operators.
In Eqs.(6.340)-(6.342), the three tensor product for the spin operators are presented.
It is not clear to me which matrix product is given in Eq.(6.343). I think $\hat{\sigma}_1{}^1$is a $2 \times 2$ spin operator acting on particle 1. Furthermore, I think the product $\hat{\sigma}_1{}^1 \cdot \hat{\sigma}_2{}^2$, is just matrix multiplication. Then, the latter product is a $2 \times 2$ matrix:
$\hat{\sigma}_1{}^1 \cdot \hat{\sigma}_2{}^2 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$.
So, to me there remains a question mark:?.
I have a similar problem with Eq.(6.344).There appears the term $a\hat{I}$. I think the unit operator is a $2 \times 2$ matrix.
**Remark:** Just above Eq.(6.348), page 417, Boccio mentioned the outer product. I denoted the operator $\otimes$ to be tensor product.
I thought outer product to be matrix multiplication.
**Extending This Idea**
*An internal degree of freedom is one which is independent of the center of mass degrees of freedom.* The independence is defined by commutators.
Boccio discussed the results of the various commutators on page 417.
The result of this: Single particle states can be written as direct products, Eqs.(6.349)-(6.356).
Then, the condition for statistical independence is used, Eq.(6.357).

## 6.14 Equations of Motion Revisited and Finished, Page 419

In this section, time dependence and time evolution are discussed from a more general point of view.
Boccio starts with the time dependent Schrödinger equation, Eq.(6.361).
In Eq.(6.364) use has been made of $\hat{H}(t)$ to be Hermitian.
Just below Eq.(6.365) is written: *"If $\hat{H}$ is Hermitian……."*. I think, use has already been made

of $\hat{H}$ being Hermitian in deriving Eq.(6.364) from Eq.(6.363).
On page 420, Boccio derived the equation of motion for the density operator, Eq.(6.370). A pure state is used for simplicity.
In Eqs.(6.375) and (6.376), the expectation value of the general operator $\hat{Q}$, Eq.(6.375) is presented. The expectation value is time dependent due to the time dependent density operator. The Schrodinger picture.
In Eq.(6.377) , the Heisenberg Picture is presented.
In Eqs.(6.380) and (6.381) the time derivatives of the expectation value of a general operator is presented in both pictures.

### 6.15 Symmetries, Conservation Laws and Stationary States, Page 422.

A continuous unitary transformation with a Hermitian generator is presented. Boccio presented the condition for another observable to be invariant under this transformation, Eqs.(6.384) and (6.385). The commutator condition for invariance is given, Eq.(6.387).
On page 424 and 425 some examples are discussed: invariance under space displacement, invariance under rotation and invariance under time translation.
The time evolution of the state vector is given in Eq. (6.393).
The stationary state is defined: *In a stationary state the expectation values and probabilities of all observables are independent of time.*
Finally, quantum numbers are defined.

### 6.16. The Collapse or Reduction Postulate, page 425.

How a measurement system and a quantum system evolve based on unitary time evolution is given in Eq.(6.396), the initial and the final system, a superposition of a quantum system and a measurement system.(See also Lecture 7.8, *The Process of Measurement*, Susskind).
On page 426 and 427, Boccio interprets the state vector for two models. The collapse of the state vector is explained. Then, Boccio mentioned the reduction process/collapse has never been observed in the laboratory. *"… it is hard to understand in what sense it can be thought of as areal physical process."*
On page 428, Boccio presented some proposed mechanisms for the collapse/reduction.
Conclusion: *it works for doing calculations*.
Boccio: *We should not stop worrying about the interpretation of the wavefunction,* page 429.
On pages 429-431, an experiment with electrons in a box with a hole in it and a stern-Gerlach device is discussed.

### 6.17 Putting Some of These Ideas Together, page 431

#### 6.17.1 Composite Quantum systems; Tensor Product, page 431

A composite system, an entangled state, is analysed.
Now, a system is describes where all the particle are interacting quantum mechanically.
The vector describing a quantum system is presented in Eq.(6.420).

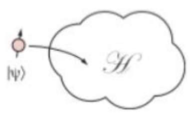



Figure 6.4: Quantum systems are described by vectors in own Hilbert space

The projectors are given as the outer products of the different basis vectors, e.g., Eqs(6.423)-(6.424).

**Two-Level Systems**
The discussion about the subject matter is about a quantum system in a 2-dimensinal Hilbert space. The system has two eigenstates, up and down. The relevant equations are Eqs.(6.427)-(6.431).
**Hilbert space for Composite Systems**
Boccio starts with building Hilbert space for two distinct particles, illustrated in Figure 6.5, page 434.

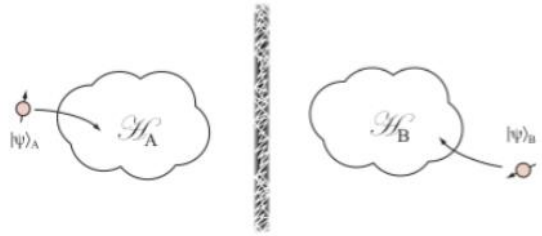



Figure 6.5: Hilbert space for 2 quantum systems independent of one another

So, Boccio defined two different Hilbert spaces, with their own projectors, Eqs(6.432)-(6.433).
**Tensor Product of Hilbert Spaces**
Now the particles are brought together. *A suitable composite Hilbert space must be assembled.*

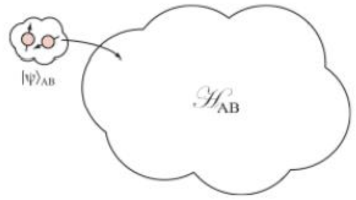



Figure 6.6: Hilbert space for 2 quantum systems independent of one another

New basis vectors are defined, Eqs.(6.437)-(6.440). To obtain these vectors the tensor product is used. The projectors, outer products are given in Eqs.(6442)-(6.443).
**Tensor Product of Matrices (a rehearsal).**
As an example , let choose one of the expressions of Eq.(6.444):
$\hat{P}^{AB}_{\uparrow\uparrow}$

with $|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix} \to \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$.

Then, with Eq.(6.443)

$$\hat{P}^{AB}_{\uparrow\uparrow} = |\uparrow\uparrow\rangle\langle\uparrow\uparrow| = |\uparrow\uparrow\rangle_{AB}\langle\uparrow\uparrow| = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}(1\ \ 0\ \ 0\ \ 0) = \begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}.$$

For Eq.(6.444), the procedure for the tensor product is summarized in Eq.(6.448).
Of which I showed one example: $\hat{P}^{AB}_{\uparrow\uparrow}$.

### 6.17.2 Quantum Entanglement and the EPR Paradox, page 438

EPR: Einstein, Podolsky and Rosen.

The operators $\hat{P}_{\uparrow}^{A}$ and $\hat{P}_{\uparrow}^{B}$ are given in matrix representation, Eq.(6.449). These operators are the projection operators derived in section 6.17.1 Eq.(6.431). Boccio explained how to use the operators.

**States in the Tensor Product Hilbert Space**

Properties of composite quantum systems are discussed in this subsection.
Such a composite system is given in Eqs. (6.452) and (6.453).

**Quantum Entanglement**

Here Boccio discussed the question: Can every state in the general form Eq.(6.454) be written as a product state eq.(6.453)?
A similar question is raised by Susskind: Can a singlet state be written in the form of a product state? The answer is : no.

**Consequences of Entanglement**

The consequences are discussed with the combined state as presented on page 440.
The concept of partial projectors is introduced at the bottom of page 440.

### 6.17.3 Entanglement and Communication, page 440

**To Communicate Superluminally, or Not**

It is about propagating of information faster than the speed of light.
Boccio discussed the subject matter.

$$|\psi\rangle_{AB} = \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle_{AB} + \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle_{AB} = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix}$$

Here are presented Eq. (6.454): the joint state of Alice and Bob, the usual suspects.
In Eq.(6.464) the shared state is denominated by:
$|\psi_{+}\rangle_{AB}$.
Boccio discussed two measurement procedures: measuring the observables along the $z$-direction and along the $x$-direction.
Boccio conclude: when Alice obtains results in the $x$-direction, Bob also measured in the $x$-direction. Both for the up and down directions.

**Using this for a Communication System**

Here the probabilities of communication are explained.

### 6.17.4 Nonlocality and Tests of Quantum Entanglement, page 444

Remember, a state like $|\psi_{+}\rangle_{AB}$, Eq.(6.473) cannot be written as a product state, eq.(6.474).
Next, Boccio discussed the question whether or not it would be possible to mimic a anything that behaves like quantum entanglement using classical physics.
The following classical assumptions are expected to be true.

- Objective Reality,
- Local determinism.

**Bell Inequalities**

Bell suggested an experiment to test whether the aforementioned classical assumptions are true. The results of this experiment are summarized in Table 6.1, page 445.

**Internal Information**

Under the classical assumptions, each particle carries the information as given in Eq.(6.475).

**Violations of Bell's Inequality**

Bell's inequality is presented in Eq.(6.478).
Boccio demonstrated the violation of Bell's inequality with a graph of a simple quantum mechanical case, Eq(6.497) and Figure 6.7.

## 6.18 Expanding on the Density Operator and the Statistical Description of Quantum Systems, page 447

In this section Boccio summarizes the knowledge acquired so far about density operators.
In classical mechanics the probability density function is used to describe the system statistically.
in quantum mechanics the state is characterized by the state vector.
Problem: how to describe the quantum mechanical state with incomplete information?
Incompleteness can be described in two ways. One will be investigated later. The other is by use of the reduced density operator method. This method will be described later too.

### 6.18.1 Statistical Description of Quantum Systems and the Nonexistence of an Averaged Quantum System, page 448

A mixed ensemble of similar systems of which information is limited to the probability distributions over some specified state vectors of this mixed ensemble.
In Eq.(6.486) an accessible state of the system is presented. Furthermore, the probability distribution for the accessible state, eq. (6.485) is uniform. Consequently, the average quantum state is zero, Eq.(6.489). Such a system cannot be described by a state vector. To be able to evaluate the system an ensemble average, density matrix, is introduced, Eq.(6.490). The average of which does not vanish, shown by Boccio, page 490.
Note, at the top of page 490 eq.(6.485) should read Eq.(6.486). This difference in the numbers of equations does not go away. At the top of page 451, Eq.(6) is mentioned. I assume this should read Eq.(6.487).
Eq.(6.498) represents the well known expression for the expectation value of an operator expressed in the trace of the matrix product of the density matrix and the operator in matrix representation.
Boccio concluded this section with the comparison of the density operator in quantum mechanics with the probability distribution in the statistical description of classical physics.

### 6.18.2 Open Quantum Systems and the Reduced density Operator, page 451

This section is about the interaction of a system with its environment.
Note: alas, the difference in equation numbers continue in this new section.
The reduced density operator is defined in Eq.(6.508).
To conclude: the density operator and the reduced density operators are the instruments to describe systems of which the information is incomplete.

## 6.19 Problems, Boccio-1 Page 91

### 6.19.1 Can it be written?

Show that a density matrix $\hat{\rho}$ represents a state vector ( i.e. can be written as $|\psi\rangle\langle\psi|$ for some normalized vector $|\psi\rangle$) if and only if,
$\hat{\rho}^2 = \hat{\rho}$ .
First we assume $\hat{\rho}$ to be a linear operator with eigenvector( "represent a state vector") $|\psi\rangle$
$\Longrightarrow \hat{\rho} = \hat{P}_{|\psi\rangle} = |\psi\rangle\langle\psi|$.
Hence
$\hat{\rho}^2 = (|\psi\rangle\langle\psi|)^2 = |\psi\rangle\langle\psi||\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \hat{\rho}$.
Any vector $|\phi\rangle$ orthogonal to $|\psi\rangle$ is an eigenvector of $|\psi\rangle\langle\psi|$ with eigenvalue zero:

$\Longrightarrow |\psi\rangle\langle\psi|\,|\phi\rangle = |\psi\rangle\,\langle\phi|\psi\rangle = 0|\psi\rangle$.
So, the eigenvalues of $|\psi\rangle\langle\psi|$ are 0 or 1.
There is only one eigenvector with eigenvalue 1: $|\psi\rangle$.

Next, we assume for the density operator
$\hat{\rho}^2 = \hat{\rho}$.
Then Boccio proved this not to lead to a contradiction by writing $\hat{\rho}$ as a sum of projection operators
$\hat{\rho} = \sum_{d=1}^{D} w_d\, \hat{P}_{|\psi_d\rangle}$ ,
for a orthonormal set of states $\{|\psi_1\rangle, \dots \dots, |\psi_D\rangle\}$ and the set of real numbers $\{w_1, \dots \dots, w_D\}$.
Consequently,
$\hat{P}_{|\psi_c\rangle}\hat{P}_{|\psi_d\rangle} = \delta_{cd}\hat{P}_{|\psi_d\rangle}$.
Remark: this basically reflects what is written above:
$|\psi\rangle\langle\psi|\,|\phi\rangle = |\psi\rangle\,\langle\phi|\psi\rangle = 0|\psi\rangle$.
I illustrate the proof by Boccio with
$\hat{\rho} = w_1|\psi\rangle\langle\psi| + w_2|\phi\rangle\langle\phi|$,
where
$0 < \{w_1, w_2\} \leq 1$ , and $w_1 + w_2 = 1$.
Note: think of $\{w_1, w_2\}$ to be probabilities.
$\hat{\rho}^2 = w_1^2(|\psi\rangle\langle\psi|)^2 + w_2^2(|\phi\rangle\langle\phi|)^2 + w_1 w_2|\psi\rangle\langle\psi||\phi\rangle\langle\phi| + w_2 w_1|\phi\rangle\langle\phi||\psi\rangle\langle\psi| =$
$= w_1^2(|\psi\rangle\langle\psi|)^2 + w_2^2(|\phi\rangle\langle\phi|)^2 = w_1^2|\psi\rangle\langle\psi| + w_2^2|\phi\rangle\langle\phi|$,
where use has been made of $\langle\psi|\phi\rangle = 0$.
We assumed:
$\hat{\rho}^2 = \hat{\rho}$ .
Hence,
$w_1^2|\psi\rangle\langle\psi| + w_2^2|\phi\rangle\langle\phi| = w_1|\psi\rangle\langle\psi| + w_2|\phi\rangle\langle\phi|$.
Multiply the preceding expression with $|\psi\rangle\langle\psi|$.
The resulting expression is:
$(w_1^2 - w_1)|\psi\rangle\langle\psi| = 0$.
So,
$w_1 = 0$, or $w_1 = 1$.
Since $w_1 > 0 \Longrightarrow w_1 = 1$.
Consequently
$\hat{\rho} = w_1|\psi\rangle\langle\psi| + w_2|\phi\rangle\langle\phi| \Longrightarrow \hat{\rho} = |\psi\rangle\langle\psi|$.
$\hat{\rho}$ represents a state vector(pure state) for $\hat{\rho}^2 = \hat{\rho}$.
Note: obviously we could have multiplied
$w_1^2|\psi\rangle\langle\psi| + w_2^2|\phi\rangle\langle\phi| = w_1|\psi\rangle\langle\psi| + w_2|\phi\rangle\langle\phi|$
with
$|\phi\rangle\langle\phi|$, for that matter.

### 6.19.2 Pure and Nonpure states

Consider a observable $\sigma$ that can only take on two values $+1$ or $-1$ . The eigenvectors of the operator are denoted by $|+\rangle$ and $|-\rangle$. Consider the following states:
**a)** The one-parameter family of pure states that are represented by the vectors
$|\theta\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{e^{i\varphi}}{\sqrt{2}}|-\rangle$ ,
for arbitrary phase $\varphi$ .

**b)** The density matrix of the nonpure state
$\rho = \frac{1}{2}| +\rangle\langle +| + \frac{1}{2}| -\rangle\langle -|$ .
The expectation value of $\langle\sigma\rangle = Tr\hat{\rho}\hat{\sigma}$.
**First the pure state:**
The density matrix:
$\hat{\rho}_\theta = |\theta\rangle\langle\theta| = \frac{1}{2}\left[| +\rangle + e^{i\varphi}| -\rangle\right]\left[\langle +| + e^{-i\varphi}\langle -|\right] =$
$= \frac{1}{2}(| +\rangle\langle +| + | -\rangle\langle -|) + \frac{1}{2}e^{i\varphi}| -\rangle\langle +| + \frac{1}{2}e^{-i\varphi}| +\rangle\langle -|$.
Presenting this density matrix as a matrix by using $| +\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and $| -\rangle = \begin{pmatrix}0\\1\end{pmatrix}$, it appears $| -\rangle\langle +|$ and $| +\rangle\langle -|$ does not contribute to the Trace:
$\frac{1}{2}e^{i\varphi}| -\rangle\langle +| + \frac{1}{2}e^{-i\varphi}| +\rangle\langle -| = \frac{1}{2}\begin{pmatrix}0 & e^{-i\varphi}\\ e^{i\varphi} & 0\end{pmatrix}$.
Furthermore,
$\frac{1}{2}(| +\rangle\langle +| + | -\rangle\langle -|) = \frac{1}{2}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$.
Consequently
$\hat{\rho}_\theta = \frac{1}{2}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix} + \frac{1}{2}\begin{pmatrix}0 & e^{-i\varphi}\\ e^{i\varphi} & 0\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & e^{-i\varphi}\\ e^{i\varphi} & 1\end{pmatrix}$
With the given eigenvalues and eigenvectors of $\sigma$, we have
$\hat{\sigma} = | +\rangle\langle +| - | -\rangle\langle -|$, i.e., the sum of the projection operators times the respective eigenvalues.
Or on matrix representation
$\hat{\sigma} = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$
So
$\hat{\rho}_\theta\hat{\sigma} = \frac{1}{2}(| +\rangle\langle +| + | -\rangle\langle -| + e^{i\varphi}| -\rangle\langle +| + e^{-i\varphi}| +\rangle\langle -|)(| +\rangle\langle +| - | -\rangle\langle -|)$.
In matrix representation
$\hat{\rho}_\theta\hat{\sigma} = \frac{1}{2}\begin{pmatrix}1 & -e^{-i\varphi}\\ e^{i\varphi} & -1\end{pmatrix}$.
Hence
$\langle\sigma\rangle_\theta = \frac{1}{2}Tr(| +\rangle\langle +| - | -\rangle\langle -|) = \frac{1}{2}(1-1) = 0$.
**Note:**
Thinking of the eigenvectors as representing spin, $\hat{\sigma} = \sigma_z$.

**Next, the nonpure state:**
$\hat{\rho}\hat{\sigma} = \frac{1}{2}\left[| +\rangle\langle +| + \frac{1}{2}| -\rangle\langle -|\right][| +\rangle\langle +| - | -\rangle\langle -|]$.
We again obtain
$\langle\sigma\rangle = \frac{1}{2}Tr(| +\rangle\langle +| - | -\rangle\langle -|) = \frac{1}{2}Tr\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} = 0$.

The question to be answered is:
In both cases $\langle\sigma\rangle = 0$. What if any, are the physical differences between these two states, and how could they be measured?
Boccio analysed this question for the spin operator $\sigma_x = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$.

We obtained already:

$\hat{\rho}_\theta = \frac{1}{2}\begin{pmatrix} 1 & e^{-i\varphi} \\ e^{i\varphi} & 1 \end{pmatrix}$, for the pure state.

Given for the nonpure state

$\hat{\rho} = \frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-| = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

So, we find

$\hat{\rho}_\theta \sigma_x = \frac{1}{2}\begin{pmatrix} e^{-i\varphi} & 1 \\ 1 & e^{i\varphi} \end{pmatrix}$, and $\hat{\rho}\sigma_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.

Hence

$\langle\sigma_x\rangle_\theta = Tr\hat{\rho}_\theta\sigma_x = \frac{1}{2}\left(e^{-i\varphi} + e^{i\varphi}\right) = \cos\varphi$, pure state,

and

$\langle\sigma_x\rangle = Tr\hat{\rho}\sigma_x = 0$, nonpure state(or mixed state).

Consequently, there exists a value for $\varphi = 0$, resulting into $\langle\sigma_x\rangle_\theta = 1$.

Whereas, for $\hat{\rho}$, any expectation value of an observable is equal to 0.

### 6.19.3 Probabilities

Suppose the operator

$M = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$,

represents an observable.

In problem 4.22.14 *Spectral Decomposition* the eigenvalues and eigenvectors have been calculated, I present the analysis here again:

The eigenvalues:

$$\begin{vmatrix} -q & 1 & 0 \\ 1 & -q & 1 \\ 0 & 1 & 0-q \end{vmatrix} = 0,$$

with the general expression for the $3 \times 3$ determinant(Chisholm and Morris, page 423) the resulting cubic equation is:

$-q^3 + 2q = 0 \Longrightarrow q_i = 0, \pm\sqrt{2}$.

Then with:

$M|q_i\rangle = q_i|q_i\rangle$, the vectors can be obtained.

$$q_1 = 0 \Longrightarrow |q_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = |0\rangle$$

I reproduce the result for $|q_2\rangle$, Boccio,

$$|q_2\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = |\sqrt{2}\rangle.$$

I present the $|q_3\rangle$, where I represent the ket in column representation $\begin{pmatrix} a \\ b \\ c \end{pmatrix}$:

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = -\sqrt{2}\begin{pmatrix} a \\ b \\ c \end{pmatrix}.$$

Then,

$b = -a\sqrt{2}$,

$a + c = -b\sqrt{2}$,
$b = -c\sqrt{2}$.
Normalization,
$a^2 + b^2 + c^2 = 1 \Longrightarrow \frac{b^2}{2} + b^2 + \frac{b^2}{2} = 1 \Longrightarrow b = \pm\frac{1}{2}\sqrt{2}$.
I choose $b = \frac{1}{2}\sqrt{2}$.
Hence
$$|q_3\rangle = \frac{1}{2}\begin{pmatrix} -1 \\ \sqrt{2} \\ -1 \end{pmatrix} = |-\sqrt{2}\rangle.$$
Apparently, Boccio choose $b = -\frac{1}{2}\sqrt{2}$. A phase difference of $e^{i\pi}$.
Calculate the probability $Prob(M = 0|\rho)$ for the state operator:
**a)** $\rho_a = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{pmatrix}$.
Note: Caveat notation, $\rho$ is not the density matrix!
**Question**: meaning of $Prob(M = 0|\rho)$?
Page 373: $Prob\left(Q = q\middle|\widehat{W}\right)$ = probability that the observable represented by $\hat{Q}$ will have the discrete value $q$ in the ensemble characterized by $\widehat{W}$.
Eqs.(6.61)-(6.64): $Prob\left(Q = q\middle|\widehat{W}\right) = Tr[\widehat{W}\hat{P}(q)]$.

Now $Prob(M = 0|\rho)$
$\langle\rho_a\rangle = Tr\hat{P}_0\hat{\rho}_a = \langle 0|\hat{\rho}_a|0\rangle$.
$$\hat{P}_0 = |0\rangle\langle 0| = \frac{1}{2}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}(1 \ \ 0 \ \ 1) = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$
Plug into $\langle 0|\hat{\rho}_a|0\rangle$ the eigenvector $|0\rangle$ and the operator $\rho_a$.
Then,
$\langle\rho_a\rangle = \frac{3}{8}$,
or
$$Tr\hat{P}_0\hat{\rho}_a = Tr\begin{pmatrix} \frac{1}{4} & 0 & -\frac{1}{8} \\ 0 & 0 & 0 \\ -\frac{1}{4} & 0 & \frac{1}{8} \end{pmatrix} = \frac{3}{8}.$$
**b)** $\rho_b = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$.
$\langle\rho_b\rangle = Tr\hat{P}_0\hat{\rho}_b = \langle 0|\hat{\rho}_b|0\rangle$.
Plug into $\langle 0|\hat{\rho}_b|0\rangle$ the eigenvector $|0\rangle$ and the operator $\rho_b$.
Then,
$\langle\rho_b\rangle = 0$ .

**c)** $\rho_c = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix}$.

$\langle \rho_c \rangle = Tr\hat{P}_0\hat{\rho}_c = \langle 0|\hat{\rho}_c|0\rangle$.

Plug into $\langle 0|\hat{\rho}_c|0\rangle$ the eigenvector $|0\rangle$ and the operator $\rho_c$.

Then,

$\langle \rho_c \rangle = \frac{1}{2}$.

Boccio proposed another way to find out about the expectation value of the state operators. To this end, the analysis of $\rho_a$ has been chosen.

$$\rho_a = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{pmatrix}.$$

The eigen values are obtained from the polynomial

$$\left(\frac{1}{2} - \lambda\right)\left(\frac{1}{4} - \lambda\right)^2 = 0.$$

The eigen vectors are obtained from:

$$\begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \\ c \end{pmatrix}.$$

With normalization and orthogonality, the three eigenvectors are:

$|\frac{1}{2}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, denoted by $|1\rangle$ ,

$|\frac{1}{4}\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, denoted by $|0\rangle$, caveat this notation is also used for the eigenvector of $M$,

and

$|\frac{1}{4}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$, denoted by $|-1\rangle$.

Then the spectral decomposition of $\rho_a$ with projection operators and eigenvalues:

$$\hat{\rho}_a = \frac{1}{2}|1\rangle\langle 1| + \frac{1}{4}|0\rangle\langle 0| + \frac{1}{4}|-1\rangle\langle -1|.$$

In matrix representation

$$\hat{\rho}_a = +\frac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Next Boccio expanded the three eigenvectors of the operator $\hat{\rho}_a$ into the eigenvectors of the operator $M$. I denote the eigen vector $|0\rangle$ by $|0'\rangle$.

Then

$$|0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\left[\frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}\right] = \frac{1}{\sqrt{2}}(|\sqrt{2}\rangle - |-\sqrt{2}\rangle).$$

$$|1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix} = \frac{1}{2}[\frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix} + \frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix}] + \frac{1}{2}\begin{pmatrix}1\\0\\-1\end{pmatrix} = \frac{1}{2}\left[|\sqrt{2}\rangle + |-\sqrt{2}\rangle\right] + \frac{1}{\sqrt{2}}|0'\rangle,$$

and

$$|-1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix} = \frac{1}{2}[\frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix} + \frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix}] + \frac{1}{2}\begin{pmatrix}1\\0\\-1\end{pmatrix} = \frac{1}{2}\left[|\sqrt{2}\rangle + |-\sqrt{2}\rangle\right] - \frac{1}{\sqrt{2}}|0'\rangle.$$

Plug these three expressions for $|0\rangle$, $|1\rangle$ and $|-1\rangle$, into spectral decomposition $\hat{\rho}_a = \frac{1}{2}|1\rangle\langle 1| + \frac{1}{4}|0\rangle\langle 0| + \frac{1}{4}|-1\rangle\langle -1|$, the result of which is again $\langle\ \hat{\rho}_a\rangle = \frac{3}{8}$.

### 6.19.4 Acceptable Density Operators

Which of the following are acceptable as state operators?

- $\rho_1 = \begin{pmatrix}\frac{1}{4} & \frac{3}{4}\\ \frac{3}{4} & \frac{3}{4}\end{pmatrix}$, $\rho_2 = \begin{pmatrix}\frac{9}{25} & \frac{12}{25}\\ \frac{12}{25} & \frac{16}{25}\end{pmatrix}$, $\rho_3 = \begin{pmatrix}\frac{1}{2} & 0 & \frac{1}{4}\\ 0 & \frac{1}{2} & 0\\ \frac{1}{4} & 0 & 0\end{pmatrix}$, $\rho_4 = \begin{pmatrix}\frac{1}{2} & 0 & \frac{1}{4}\\ 0 & \frac{1}{4} & 0\\ \frac{1}{4} & 0 & \frac{1}{4}\end{pmatrix}$,

and

$\rho_5 = \frac{1}{3}|u\rangle\langle u| + \frac{2}{3}|v\rangle\langle v| + \frac{\sqrt{2}}{3}|u\rangle\langle v| + \frac{\sqrt{2}}{3}|v\rangle\langle u|.$

In addition: $\langle u|u\rangle = \langle v|v\rangle = 1$, and $\langle u|v\rangle = 0$ .

The test whether these operators are state operators is:

$\rho^2 = \rho$, and $Tr(\rho^2) = 1$.

So,

$$\rho_1 = \begin{pmatrix}\frac{1}{4} & \frac{3}{4}\\ \frac{3}{4} & \frac{3}{4}\end{pmatrix} \to \rho_1^2 = \begin{pmatrix}\frac{5}{8} & \frac{3}{4}\\ \frac{3}{4} & \frac{9}{8}\end{pmatrix} \to Tr(\rho_1^2) = \frac{7}{4}\text{, a mixed state.}$$

$$\rho_2 = \begin{pmatrix}\frac{9}{25} & \frac{12}{25}\\ \frac{12}{25} & \frac{16}{25}\end{pmatrix} \to \rho_2^2 = \begin{pmatrix}\frac{13}{25} & \frac{12}{25}\\ \frac{12}{25} & \frac{12}{25}\end{pmatrix} \to Tr(\rho_2^2) = 1\text{, a pure state.}$$

$$\rho_3 = \begin{pmatrix}\frac{1}{2} & 0 & \frac{1}{4}\\ 0 & \frac{1}{2} & 0\\ \frac{1}{4} & 0 & 0\end{pmatrix} \to \rho_3^2 = \begin{pmatrix}\frac{5}{16} & 0 & \frac{1}{8}\\ 0 & \frac{4}{16} & 0\\ \frac{1}{8} & 0 & \frac{1}{16}\end{pmatrix} \to\ Tr(\rho_3^2) = \frac{5}{8}\text{, a mixed state.}$$

$$\rho_4 = \begin{pmatrix}\frac{1}{2} & 0 & \frac{1}{4}\\ 0 & \frac{1}{4} & 0\\ \frac{1}{4} & 0 & \frac{1}{4}\end{pmatrix} \to \rho_4^2 = \begin{pmatrix}\frac{5}{16} & \frac{1}{16} & \frac{3}{16}\\ 0 & \frac{1}{16} & 0\\ \frac{3}{16} & 0 & \frac{2}{16}\end{pmatrix} \to\ Tr(\rho_4^2) = \frac{1}{2}\text{, a mixed state.}$$

$$\rho_5 = \frac{1}{3}|u\rangle\langle u| + \frac{2}{3}|v\rangle\langle v| + \frac{\sqrt{2}}{3}|u\rangle\langle v| + \frac{\sqrt{2}}{3}|v\rangle\langle u| \to$$

$$\to \rho_5^2 = (\frac{1}{3}|u\rangle\langle u| + \frac{2}{3}|v\rangle\langle v| + \frac{\sqrt{2}}{3}|u\rangle\langle v| + \frac{\sqrt{2}}{3}|v\rangle\langle u|)^2 =$$

$= \frac{1}{3}|u\rangle\langle u| + \frac{2}{3}|v\rangle\langle v| + \frac{\sqrt{2}}{3}|u\rangle\langle v| + \frac{\sqrt{2}}{3}|v\rangle\langle u| \rightarrow \rho_5 \rightarrow Tr(\rho_5^2) = Tr(\rho_5)$, a pure state.
Hence, we have two pure states: $\rho_2$ and $\rho_5$.
Next, the state vectors for the pure states.

- $\rho_2 = \begin{pmatrix} \frac{9}{25} & \frac{12}{25} \\ \frac{12}{25} & \frac{16}{25} \end{pmatrix}$.

The eigenvalues

$$\begin{vmatrix} \frac{9}{25} - \lambda & \frac{12}{25} \\ \frac{12}{25} & \frac{16}{15} - \lambda \end{vmatrix} = 0 \rightarrow \lambda_1 = 0 \text{, and } \lambda_2 = 1 .$$

The eigenvector:

$$|\lambda\rangle = \frac{1}{5}\begin{pmatrix} 3 \\ 4 \end{pmatrix} .$$

- $\rho_5 = \frac{1}{3}|u\rangle\langle u| + \frac{2}{3}|v\rangle\langle v| + \frac{\sqrt{2}}{3}|u\rangle\langle v| + \frac{\sqrt{2}}{3}|v\rangle\langle u|$ , a pure state $\rightarrow |\psi_5\rangle\langle\psi_5|$.

Hence

$$|\psi_5\rangle = \alpha_u|u\rangle + \alpha_v|v\rangle.$$

Then equating

$$|\psi_5\rangle\langle\psi_5| = (\alpha_u|u\rangle + \alpha_v|v\rangle)(\alpha_u^*\langle u|) + \alpha_v^*\langle v|) = \rho_5,$$

we obtain

$$\alpha_u\alpha_u^* = \frac{1}{3} \text{, and } \alpha_v\alpha_v^* = \frac{2}{3} .$$

Consequently

$$|\psi_5\rangle = \alpha_u|u\rangle + \alpha_v|v\rangle = \frac{1}{\sqrt{3}}|u\rangle + \sqrt{\frac{2}{3}}|v\rangle.$$

Obviously, e.g.,

$\alpha_u\alpha_v^*|u\rangle\langle v| = \frac{\sqrt{2}}{3}|u\rangle\langle v|$, as it should be.

### 6.9.5 Is it a Density Matrix?

Let $\hat{\rho}_1$ and $\hat{\rho}_2$ be a pair of density matrices. Show that

$$\hat{\rho} = r\hat{\rho}_1 + (1-r)\hat{\rho}_2$$

is a density matrix for all real numbers $r$, and $0 \le r \le 1$.
Since $\hat{\rho}_1$ and $\hat{\rho}_2$ are density matrices$\Longrightarrow \langle\psi|\hat{\rho}_1|\psi\rangle \ge 0 \;\; , \langle\psi|\hat{\rho}_2|\psi\rangle \ge 0$ .
Furthermore

$$0 \le r \le 1 \Longrightarrow 0 \le (1-r) \le 1.$$

Hence, for the expectation value of $\hat{\rho}$:

$$\langle\psi|\hat{\rho}|\psi\rangle = r\langle\psi|\hat{\rho}_1|\psi\rangle + (1-r)\langle\psi|\hat{\rho}_2|\psi\rangle.$$

Consequently

$$\langle\psi|\hat{\rho}|\psi\rangle \ge 0 .$$

To determine the Trace of $\hat{\rho}$, we use linearity and the Trace of a density matrix is equal 1:

$$Tr\hat{\rho} = r \cdot Tr\hat{\rho}_1 + (1-r) \cdot Tr\hat{\rho}_2 = r + (1-r) = 1.$$

Then,

$$\hat{\rho} = r\hat{\rho}_1 + (1-r)\hat{\rho}_2,$$

represents a density matrix.

### 6.19.6 Unitary Operators

An important class of operators are unitary, defined as those that preserve inner products:
$|\tilde{\psi}\rangle = \hat{U}|\psi\rangle$, and $|\tilde{\varphi}\rangle = \hat{U}|\varphi\rangle \longrightarrow \langle\tilde{\varphi}|\tilde{\psi}\rangle = \langle\tilde{\varphi}|\hat{U}^\dagger\hat{U}|\psi\rangle = \langle\varphi|\psi\rangle$.

**a)** Show that unitary operators satisfy $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = I$, i.e., the adjoint is the inverse.
With
$\langle\tilde{\varphi}|\tilde{\psi}\rangle = \langle\tilde{\varphi}|\hat{U}^\dagger\hat{U}|\psi\rangle = \langle\varphi|\psi\rangle = \langle\varphi|I|\psi\rangle \Longrightarrow \hat{U}^\dagger\hat{U} = I.$
So, with $\hat{U}^\dagger\hat{U} = I$, and multiply both sides with $\hat{U}$,
$\hat{U}\hat{U}^\dagger\hat{U} = \hat{U}I = \hat{U} \Longrightarrow \hat{U}\hat{U}^\dagger = I.$
Hence
$\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = I.$

**b)** Consider $\hat{U} = e^{i\hat{A}}$, where $\hat{A}$ is a Hermitian operator. Show that $\hat{U}^\dagger = e^{-i\hat{A}}$ and thus $\hat{U}$ is unitary.
We use expansion of the exponential, and $\hat{A}$ is a Hermitian operator
$\hat{U} = e^{i\hat{A}} = \sum_{n=0}^{\infty}\frac{1}{n!}\left(i\hat{A}\right)^n \Longrightarrow \hat{U}^\dagger = \sum_{n=0}^{\infty}\frac{1}{n!}\left(-i\hat{A}^\dagger\right)^n = \sum_{n=0}^{\infty}\frac{1}{n!}\left(-i\hat{A}\right)^n = e^{-i\hat{A}}.$
Now, plug these results into
$\hat{U}^\dagger\hat{U} \Longrightarrow e^{i\hat{A}}e^{-i\hat{A}} = I.$
$\hat{U}$ is unitary.

**c)** Let $\hat{U}(t) = e^{-\frac{i\hat{H}t}{\hbar}}$, where $t$ is time and $\hat{H}$ is the Hamiltonian.
Let $|\psi(0)\rangle$ be the state at $t = 0$. Show that $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = e^{-\frac{i\hat{H}t}{\hbar}}|\psi(0)\rangle$ is a solution of the time-dependent Schrödinger equation, i.e., the state evolves according to a unitary map.
We have
$\frac{\partial\psi}{\partial t} = \frac{\partial\hat{U}}{\partial t}|\psi(0)\rangle = -\frac{i\hat{H}}{\hbar}e^{-\frac{i\hat{H}t}{\hbar}}|\psi(0)\rangle = -\frac{i\hat{H}}{\hbar}\hat{U}(t)|\psi(0)\rangle = -\frac{i\hat{H}}{\hbar}|\psi(t)\rangle.$
Hence,
$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle \longrightarrow$ the time-dependent Schrödinger equation.
At time $t = 0$, $\langle\psi(0)|\psi(0)\rangle = 1 \longrightarrow$ the conservation of distinction (Susskind). At later time, $t > 0$ the probability must be conserved.
$\langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|\psi(0)\rangle = 1 \rightarrow$ time evolution is unitary:
$\hat{U}^\dagger(t)\hat{U}(t) = I$ .

**d)** Let $\{|u_n\rangle\}$ be a complete set of eigenfunctions of the Hamiltonian operator:
$\hat{H}|u_n\rangle = E_n|u_n\rangle,$
where $E_n$ are the eigenvalues.
We learned, from the projection operators of the complete set $\{|u_n\rangle\}$:
$\sum_n|u_n\rangle\langle u_n| = I$ .
We use $\hat{U}(t) = e^{-\frac{i\hat{H}t}{\hbar}}$.
So,
$\hat{U}(t) = \hat{U}(t)I = \hat{U}(t)\sum_n|u_n\rangle\langle u_n| = \sum_n e^{-\frac{i\hat{H}t}{\hbar}}|u_n\rangle\langle u_n|.$
With the expansion of the exponential in the preceding expression, we use $\hat{H}|u_n\rangle = E_n|u_n\rangle$, and we obtain:

$\widehat{U}(t) = \sum_n e^{-\frac{iE_n t}{\hbar}} |u_n\rangle\langle u_n|.$
Furthermore,

$|\psi(t)\rangle = \widehat{U}(t)|\psi(0)\rangle = \sum_n e^{-\frac{iE_n t}{\hbar}} |u_n\rangle\langle u_n|\psi(0)\rangle.$
Then, the preceding expression can be written:

$|\psi(t)\rangle = \sum_n c_n e^{-\frac{iE_n t}{\hbar}} |u_n\rangle,$
where $c_n = \langle u_n|\psi(0)\rangle$.

### 6.19.7 More Density Operators

Suppose we have a system with total angular momentum 1. Pick a basis to the three eigenvectors of the $z$-component of the angular momentum, $J_z$, with eigenvalues $+1, 0, -1$, respectively. An ensemble of such systems is described by te density matrix

$$\rho = \frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}.$$

**a)** Is $\rho$ a density matrix?
- Density matrices are Hermitian. The matrix is Hermitian
- Trace of the density matrix is 1. The Trace of the matrix is 1.
- The eigenvalues of the density matrix lie between 0 and 1.

The eigenvalues $\lambda_i$?

$$\begin{vmatrix} 2-\lambda & 1 & 1 \\ 1 & 1-\lambda & 0 \\ 1 & 0 & 1-\lambda \end{vmatrix} = 0 \longrightarrow (2-\lambda)(1-\lambda)(1-\lambda) - 2(1-\lambda) = 0 \longrightarrow$$
$$(1-\lambda)\lambda(\lambda-3) = 0.$$

To be a bit more precise: the eigenvalue equation reads

$$\left(\frac{1}{4} - \lambda\right)\lambda\left(\lambda - \frac{3}{4}\right) = 0$$

Hence, the eigenvalues are non-negative and $< 1$: $\lambda_i = 0, \frac{1}{4}, \frac{3}{4}$ .

$\sum_i \lambda_i = 1$ .

Consequently, $\rho$ is a valid density matrix.

Now, $\rho^2$:

$$Tr(\rho^2) = Tr\frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \cdot \frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} = Tr\frac{1}{16}\begin{pmatrix} 6 & 3 & 3 \\ 3 & 2 & 1 \\ 3 & 1 & 2 \end{pmatrix} = \frac{10}{16}.$$

$Tr(\rho^2) < 1$, a mixed state.

**b)** Given $\rho$, what is the average value of $J_z$?

The matrix representation of $J_z$

$$J_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The average value of $J_z$ is found from

$$\langle J_z\rangle = Tr(\rho J_z) = Tr\frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} = Tr\frac{1}{4}\begin{pmatrix} 2 & 0 & -1 \\ 1 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix} = \frac{1}{4}.$$

**c)** What is the standard deviation in the measured values of $J_z$?

The standard deviation:

$\Delta J_z = \sqrt{\langle J_z^2\rangle - \langle J_z\rangle^2}$ .

$$\langle J_z^2\rangle = Tr\frac{1}{4}\begin{pmatrix}2 & 1 & 1\\ 1 & 1 & 0\\ 1 & 0 & 1\end{pmatrix}\cdot\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}\cdot\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix} = Tr\frac{1}{4}\begin{pmatrix}2 & 0 & 1\\ 1 & 0 & 0\\ 1 & 0 & 1\end{pmatrix} = \frac{3}{4}.$$

$\Delta J_z = \sqrt{\frac{3}{4} - \frac{1}{16}} = \sqrt{\frac{11}{16}}$.

### 6.19.8 Scale Transformation

Space is invariant under the scale transformation

$x \to x' = e^c x$ ,

where $c$ is a parameter.

The corresponding unitary operator may be written as

$\hat{U} = e^{-ic\hat{D}}$,

where $\hat{D}$ is the dilation generator(See also Fitzpatrick Graduate Course chapter 2)

Determine $[\hat{D}, \hat{x}]$ and $[\hat{D}, \hat{p}_x]$.

Then,

$|x'\rangle = \hat{U}|x\rangle \Longrightarrow U^{-1}|x'\rangle = |x\rangle$

The eigenvector and eigenvalue equation is

$\hat{x}|x\rangle = x|x\rangle$.

Using $U^{-1}|x'\rangle = |x\rangle$ in the preceding expression

$\hat{x}U^{-1}|x'\rangle = xU^{-1}|x'\rangle$.

With $x$ a number, the preceding expression can be written as

$\hat{x}U^{-1}|x'\rangle = U^{-1}x|x'\rangle$.

Then multiply the preceding expression with $\hat{U}$ to the left:

$\hat{U}\hat{x}U^{-1}|x'\rangle = \hat{U}U^{-1}x|x'\rangle = x|x'\rangle$.

So,

$\hat{U}\hat{x}U^{-1}|x'\rangle = x|x'\rangle = e^{-c}e^{c}x|x'\rangle = e^{-c}x'|x'\rangle$.

With $\hat{x}|x'\rangle = x'|x'\rangle$

$\hat{U}\hat{x}U^{-1}|x'\rangle = e^{-c}\hat{x}|x'\rangle \Longrightarrow \hat{U}\hat{x}U^{-1} = e^{-c}\hat{x}$.

Consequently

$e^c\hat{x} = U^{-1}\hat{x}\hat{U}$.

**Note:**

Let us have a closer look into $U^{-1}\hat{x}\hat{U} = e^c\hat{x}$.

Then,

$U^{-1}\hat{x}\hat{U}|x\rangle = e^c\hat{x}|x\rangle \to U^{-1}\hat{x}|x'\rangle = e^c x|x\rangle \to U^{-1}x'|x'\rangle = x'|x\rangle \to U^{-1}|x'\rangle = |x\rangle$.

As it should be.

$e^c\hat{x} = U^{-1}\hat{x}\hat{U} = e^{ic\hat{D}}\hat{x}e^{-ic\hat{D}}$.

Boccio introduced an identity to be derived in Problem 6.19.11(See also Eq. (6.249)).

Then, $e^{ic\hat{D}}\hat{x}e^{-ic\hat{D}}$ can be written as

$e^{ic\hat{D}}\hat{x}e^{-ic\hat{D}} = \hat{x} + c[i\hat{D}, \hat{x}] + \frac{1}{2}c^2\left[i\hat{D}, [i\hat{D}, \hat{x}]\right] + \cdots$..

In addition, we have the expansion

$$e^c\hat{x} = \hat{x}(1 + c + \frac{1}{2}c^2 + \cdots \dots).$$

Consequently, compare the coefficients of $c^k$ in both expansions term by term, we have $\left[i\widehat{D},\hat{x}\right] = \hat{x}$ .

Now we make use of the Jacobi identity(Eq.6.212):

$$[[\widehat{D},\hat{p}_x],\hat{x}] + \left[[\hat{p}_x,\hat{x}],\widehat{D}\right] + \left[[\ \hat{x},\widehat{D}],\hat{p}_x\right] = 0.$$

We have already

- $\left[i\widehat{D},\hat{x}\right] = \hat{x} \Longrightarrow \left[\hat{x},\widehat{D}\right] = i\hat{x}$,
- $[\hat{p}_x,\hat{x}] = -i\hbar$.

Then, with the Jacobi identity and $\left[-i\hbar,\widehat{D}\right] = 0$:

$$\left[[\widehat{D},\hat{p}_x],\hat{x}\right] = \hbar.$$

Use $[i\hat{p}_x,\hat{x}] = \hbar$ in the preceding expression.

Then,

$$\left[\widehat{D},\hat{p}_x\right] = i\hat{p}_x.$$

From the latter expression it follows:

$$\widehat{D} = \frac{1}{\hbar}(\hat{x}\hat{p}_x + \hat{p}_x\hat{x}).$$

Plug the preceding expression into $\left[\widehat{D},\hat{p}_x\right] = i\hat{p}_x$:

$$(\hat{x}\hat{p}_x + \hat{p}_x\hat{x})\,\hat{p}_x - \hat{p}_x(\hat{x}\hat{p}_x + \hat{p}_x\hat{x}) = i\hbar\hat{p}_x \Longrightarrow \hat{x}\hat{p}_x\hat{p}_x - \hat{p}_x\hat{p}_x\hat{x} = i\hbar\hat{p}_x \Longrightarrow$$

$$\Longrightarrow (\hat{x}\hat{p}_x - \hat{p}_x\hat{x})\hat{p}_x = i\hbar\hat{p}_x \Longrightarrow [\hat{x},\hat{p}_x]\hat{p}_x = i\hbar\hat{p}_x,$$ QED.

What about $\widehat{D}$?

$$\widehat{D}^\dagger = \frac{1}{\hbar}\{(\hat{x}\hat{p}_x)^\dagger + (\hat{p}_x\hat{x})^\dagger\} = \frac{1}{\hbar}\left\{\hat{p}_x{}^\dagger\hat{x}^\dagger + \hat{x}^\dagger\hat{p}_x{}^\dagger\right\} = \frac{1}{\hbar}(\hat{p}_x\hat{x} + \hat{x}\hat{p}_x).$$

Hence:

$\widehat{D} = \widehat{D}^\dagger \Longrightarrow \widehat{D}$ is Hermitian.

### 6.19.9 Operator Properties

**a)** Prove that if $\widehat{H}$ is a Hermitian operator, $\widehat{U} = e^{i\widehat{H}}$ is a unitary operator[3].

With

$$\widehat{U} = e^{i\widehat{H}} \rightarrow \widehat{U}^\dagger = e^{-i\widehat{H}} \Longrightarrow \widehat{U}\widehat{U}^\dagger = 1.$$

Then,

$\widehat{U} = e^{i\widehat{H}}$ is a unitary operator.

**b)** Show that $\det\widehat{U} = e^{iTr\widehat{H}}$.

Boccio used the following theorem:

*An Hermitian matrix $H$ can be diagonalized by a transformation $U^\dagger HU = D$, where $U$ is a unitary matrix, $\widehat{U}\widehat{U}^\dagger = 1$, whose columns are the normalized eigenvectors of $U$. The trace of $H$ is invariant under this transformation $\Longrightarrow TrD = TrH$ .*

Boccio expanded $e^{i\widehat{H}}$, by using

$$U^\dagger H^n U = U^\dagger HU \dots \dots . . U^\dagger HU = D^n.$$

Consequently,

$$U^\dagger e^{iH} U = U^\dagger e^{iD} U.$$

[3] $\widehat{U}$ and $U$ are used alternately.

Boccio presented the matrix representation of $e^{iD}$, a diagonalized matrix as it should be. Furthermore, use is made of $\hat{U}\hat{U}^{\dagger} = 1 \Longrightarrow \hat{U}^{\dagger}\hat{U} = 1$:

$\det(e^{i\hat{H}}) = \det\left(e^{i\hat{H}}\hat{U}\hat{U}^{\dagger}\right) = \det\left(\hat{U}\hat{U}\hat{U}^{\dagger}\right) = \det\left(\hat{U}\hat{U}^{\dagger}\hat{U}\right) = \det\left(\hat{U}^{\dagger}\hat{U}\hat{U}\right) =$

$= \det\left(\hat{U}^{\dagger}e^{i\hat{H}}\hat{U}\right) = \det\left(U^{\dagger}e^{iD}U\right) = \det(e^{iD})$.

With the diagonal elements of $D$:

$\det\left(e^{iD}\right) = e^{iTrD}$.

We know now

$Tr(U^{\dagger}HU) = TrH = TrD.$

Then, using

$\det(e^{i\hat{H}}) = e^{iTrD} \Longrightarrow \det(U) = e^{iTrH}$.

### 6.19.10 An Instantaneous Boost.

The unitary operator

$\hat{U}(\vec{v}) = e^{i\vec{v}\cdot\hat{\vec{G}}}$,

describes the instantaneous $(t = 0)$ effect of a transformation to a frame of reference moving at velocity $\vec{v}$ with respect to the original reference frame.

Its effects on the velocity operator, $\hat{\vec{V}}$ , and position operator, $\hat{\vec{Q}}$ , are:

$\hat{U}\hat{\vec{V}}\hat{U}^{-1} = \hat{\vec{V}} - \hat{v}\hat{I}$ , $\hat{U}\hat{\vec{Q}}\hat{U}^{-1} = \hat{\vec{Q}}$.

Find an operator $\hat{G}_t$ such that the unitary operator

$\hat{U}(\vec{v}, t) = e^{i\vec{v}\cdot\hat{\vec{G}}_t}$

will yield the full Galilean transformation

$\hat{U}\hat{\vec{V}}\hat{U}^{-1} = \hat{\vec{V}} - \hat{v}\hat{I}$ , and $\hat{U}\hat{\vec{Q}}\hat{U}^{-1} = \hat{\vec{Q}} - \hat{v}t\hat{I}$.

The restricted Galilean transformation is given by the unitary operator

$\hat{U}(\vec{v}) = e^{i\vec{v}\cdot\hat{\vec{G}}}$,

and its effect is described above. This transformation is instantaneous and causes no change in position:

$\hat{U}\hat{\vec{Q}}\hat{U}^{-1} = \hat{\vec{Q}}$.

Boccio presented two methods:

**Method 1:**

$\hat{U}\hat{\vec{Q}}\hat{U}^{-1} = e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{\vec{Q}}e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{\vec{Q}} - \hat{v}t\hat{I}$ .

We also have, not proved [4],

$e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{\vec{Q}}e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{\vec{Q}} + i\left[\vec{v}\cdot\hat{G}_t, \hat{\vec{Q}}\right] + \cdots = \hat{\vec{Q}} - \hat{v}t\hat{I}$.

Plug $\hat{\vec{G}}_t = -\frac{\hat{\vec{P}}}{\hbar}t + \frac{1}{\hbar}\hat{\vec{Q}}$ , into the preceding expression to obtain

$i\left[\vec{v}\cdot\hat{G}_t, \hat{\vec{Q}}\right] = -\hat{v}t\hat{I}$,

where use has been made of $\left[\hat{\vec{P}}, \hat{\vec{Q}}\right] = -i\hbar$ and $\frac{i}{\hbar}\left(\vec{v}\cdot\hat{\vec{Q}}\hat{\vec{Q}} - \hat{\vec{Q}}\vec{v}\cdot\hat{\vec{Q}}\right) = 0$.

**Method 2:**

[4] Problem 6.19.11(See also Eq. (6.249)).

The desired transformation $\hat{U}(\vec{v},t) = e^{i\vec{v}\cdot\hat{\vec{G}}_t}$ is a combination of an instantaneous Galilean transformation, which effects the velocity operator, but not the position operator, and a space displacement through the distance $\vec{v}t$.
So, we try
$\hat{\vec{G}}_t = M\hat{\vec{Q}} - t\hat{\vec{P}}$ → instantaneous boost and space translation. $M$ equals mass.
To reduce the work a bit $\hbar$ is set equal 1.
With $e^{ic\hat{D}}\hat{x}e^{-ic\hat{D}} = \hat{x} + c[i\hat{D},\hat{x}] + \frac{1}{2}c^2\left[i\hat{D},[i\hat{D},\hat{x}]\right] + \cdots$ .. problem 6.19.11,
Apply the preceding expression for $\hat{\vec{G}}_t = M\hat{\vec{Q}} - t\hat{\vec{P}}$ , first for $\hat{\vec{Q}} = \{\hat{Q}_\alpha\}$,
$e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{Q}_\alpha e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{Q}_\alpha + \left[i\vec{v}\cdot\hat{\vec{G}}_t,\hat{Q}_\alpha\right]$ +higher order terms.
Then with $\hat{\vec{G}}_t = M\hat{\vec{Q}} - t\hat{\vec{P}}$,
$\left[i\vec{v}\cdot\hat{\vec{G}}_t,\hat{Q}_\alpha\right] = \left[i\vec{v}\cdot\left(M\hat{Q}_\alpha - t\hat{\vec{P}}\right),\hat{Q}_\alpha\right] = [i\vec{v}\cdot M\hat{Q}_\alpha,\hat{Q}_\alpha] - \left[i\vec{v}\cdot t\hat{\vec{P}},\hat{Q}_\alpha\right] = -v_\alpha t\hat{I}$,
where use has been made of $[\hat{Q}_\alpha,\hat{Q}_\alpha] = 0$, and $\left[\hat{\vec{P}},\hat{\vec{Q}}\right] = -i\hbar = -i$.
Hence,
$e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{Q}_\alpha e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{Q}_\alpha - v_\alpha t\hat{I}$,
or
$\hat{U}\hat{\vec{Q}}\hat{U}^{-1} = e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{\vec{Q}}e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{\vec{Q}} - \hat{v}t\hat{I}$.
The higher order terms in the above expansion are all zero being multiples of $[\hat{I},\hat{I}]$.
Next, as mentioned by Boccio, in a similar way,
$e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{P}_\alpha e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{P}_\alpha + \left[i\vec{v}\cdot\hat{\vec{G}}_t,\hat{P}_\alpha\right]$ + higher order terms.
Then with $\hat{\vec{G}}_t = M\hat{\vec{Q}} - t\hat{\vec{P}}$,
$\left[i\vec{v}\cdot\hat{\vec{G}}_t,\hat{P}_\alpha\right] = [i\vec{v}\cdot(M\hat{Q}_\alpha - t\hat{P}_\alpha),\hat{P}_\alpha] = [i\vec{v}\cdot M\hat{Q}_\alpha,\hat{P}_\alpha] - [i\vec{v}\cdot t\hat{P}_\alpha,\hat{P}_\alpha] = -Mv_\alpha\hat{I}$,
where use has been made of $[\hat{P}_\alpha,\hat{P}_\alpha] = 0$, and $\left[\hat{\vec{P}},\hat{\vec{Q}}\right] = -i\hbar = -i$.
Again, the higher order terms in the above expansion are all zero being multiples of $[\hat{I},\hat{I}]$.
Hence
$e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{P}_\alpha e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{P}_\alpha - Mv_\alpha\hat{I}$.
Divide the preceding expression by $M$
$e^{i\vec{v}\cdot\hat{\vec{G}}_t}\frac{\hat{P}_\alpha}{M}e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \frac{\hat{P}_\alpha}{M} - v_\alpha\hat{I} \Longrightarrow e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{V}_\alpha e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{V}_\alpha - v_\alpha\hat{I}$, the transformation of the velocity operator.
So, $\hat{U}\hat{\vec{V}}\hat{U}^{-1} = e^{i\vec{v}\cdot\hat{\vec{G}}_t}\hat{V}_\alpha e^{-i\vec{v}\cdot\hat{\vec{G}}_t} = \hat{V}_\alpha - v_\alpha\hat{I} = \hat{\vec{V}} - \hat{v}\hat{I}$

**Commutation**

Verify that $\hat{G}_t$ satisfies the same commutation relation with $\vec{P},\vec{J}$ and $\vec{H}$ as does $\vec{G}$.
Boccio writes: "*Consider $\hat{G}_{t1}$ with $\hat{H}$ …….*" $\hat{G}_{t1}$? I suppose the index 1 is the 1-direction. Then, the analysis of section 6.11 *Commutators and Identities* can be used.
In section 6.10 *Generators of the Group Transformations,* $\vec{P},\vec{J}$ and $\vec{H}$ are generators.
However, the commutation problem is discussed in section 6.11, see for example Eq.(6.187).
This is about $\hat{G}_1$ and $\hat{H}$.
So, for $\hat{G}_{t1}$ with $\hat{H}$:

$$e^{i\epsilon\hat{H}}e^{i\epsilon\hat{G}_{t1}}e^{-i\epsilon\hat{H}}e^{-i\epsilon\hat{G}_{t1}} = (\hat{I} + i\epsilon\hat{H})(\hat{I} + i\epsilon\hat{G}_{t1})(\hat{I} - i\epsilon\hat{H})(\hat{I} - i\epsilon\hat{G}_{t1}) =$$
$$= \hat{I} + \epsilon^2[\hat{G}_{t1}, \hat{H}] + O(\epsilon^3) = e^{-i(-\epsilon^2)\hat{P}_1} = \hat{I} + i\epsilon^2\hat{P}_1,$$
and
$$[\hat{G}_{t1}, \hat{H}] = i\hat{P}_1.$$
Boccio: *"This is unchanged from results in the text with $\hat{G}_1$ and so this commutator does not change and similarly for all others."*

### 6.9.11 A very Useful Identity.

Now the identity used in the foregoing problems is proven.
It is about the following identity, in which $\hat{A}$ and $\hat{B}$ are operators and $x$ is a parameter,
$$e^{x\hat{A}}\hat{B}e^{-x\hat{A}} = \hat{B} + [\hat{A}, \hat{B}]x + [\hat{A}, [\hat{A}, \hat{B}]]\frac{x^2}{2!} + [\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]\frac{x^3}{3!} + \cdots \ldots ..$$
It is about the *Baker-Hausdorff lemma.* See also Fitzpatrick, the Graduate Course, Chapter 5.
Here we use to the proof the lemma Taylor expansion and regroup the expansion in powers of $x$ to construct the commutator expansion.
$$e^{x\hat{A}}\hat{B}e^{-x\hat{A}} = \left\{\sum_n \frac{(x\hat{A})^n}{n!}\right\}\hat{B}\{\sum_n \frac{(-x\hat{A})^n}{n!}\} =$$
$$= \left(1 + x\hat{A} + \frac{(x\hat{A})^2}{2!} + \cdots\right)\hat{B}\left(1 - x\hat{A} + \frac{(x\hat{A})^2}{2!} - \cdots\right) =$$
$$= \hat{B} + [\hat{A}, \hat{B}]x + \left\{-\hat{A}\hat{B}\hat{A} + \frac{1}{2}(\hat{A}^2\hat{B} - \hat{B}\hat{A}^2)\right\}x^2 + \cdots . =$$
$$= \hat{B} + [\hat{A}, \hat{B}]x + \{\hat{A}(\hat{A}\hat{B} - \hat{B}\hat{A}) - (\hat{A}\hat{B} - \hat{B}\hat{A})\hat{A}\}\frac{x^2}{2!} + \cdots . =$$
$$= \hat{B} + [\hat{A}, \hat{B}]x + [\hat{A}, [\hat{A}, \hat{B}]]\frac{x^2}{2!} + \cdots .$$
As you notice, to find out about the commutator factors of $\frac{x^3}{3!}$ is already a lot of work.

### 6.9.12 A Very Useful Identity with some help [5].

The operator $U(a) = e^{ipa/\hbar}$ is a unitary translation operator in space One dimension is considered.
Note: $U(a)U(a)^\dagger = 1$.
We need to prove
$$e^A B e^{-A} = \sum_0^\infty \frac{1}{n!}([A, A, \ldots [A)_n, B(] \ldots ]])_n =$$
$$= B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \cdots$$
**a)** Consider $B(t) = e^{tA}Be^{-tA}$, where $t$ is a real parameter.
Now,
$$\frac{d}{dt}B(t) = e^{tA}ABe^{-tA} - e^{tA}BAe^{-tA} = e^{tA}[A, B]e^{-tA} .$$
**b)** With $B(t) = e^{tA}Be^{-tA} \to B(0) = B$ and $B(1) = e^A B e^{-A}$.
Then,
$$B(1) - B(0) = \int_0^1 dt \, \frac{d}{dt}B(t) \to B(1) = B(0) + \int_0^1 dt \, \frac{d}{dt}B(t).$$
Use the power series $B(t) = \sum_{n=0}^\infty t^n B_n$, where $B(0) \equiv B_0$.
We have found

[5] See 5.4 *Intermezzo. A proof of Baker-Hausdorff Lemma* in *Quantum Mechanics in Texas* ,my notes on Quantum Mechanics Graduate Course, Fitzpatrick, www.leennoordzij.me

$\frac{d}{dt}B(t) = e^{tA}[A,B]e^{-tA} = e^{tA}(AB - BA)e^{-tA} = e^{tA}ABe^{-tA} - e^{tA}BAe^{-tA} =$
$e^{tA}Ae^{-tA}e^{tA}Be^{-tA} - e^{tA}Be^{-tA}e^{tA}Ae^{-tA} = e^{tA}Ae^{-tA}B(t) - B(t)e^{tA}Ae^{-tA}$ .
Then, Boccio presented $e^{tA}Ae^{-tA}B(t) - B(t)e^{tA}Ae^{-tA} = [A, B(t)]$.
Meaning: $e^{tA}Ae^{-tA} = A$. Well, it looks like use has been made of the "Very Useful Identity".
However, I thought this identity to be proved here.
Consequently,
$B(1) = B_0 + \int_0^1 dt\ \ [A, B(t)]$ .
We need an expression for $B(1)$, with $B(t) = \sum_{n=0}^{\infty} t^n B_n$,
$B(1) = B + \int_0^1 dt\ \frac{d}{dt}B(t) = B + \int_0^1 dt \sum_{n=0}^{\infty} nt^{n-1} B_n = B + \sum_{n=0}^{\infty} B_n \int_0^1 nt^{n-1}\, dt =$
$= B + \sum_{n=1}^{\infty} B_n = B(0) + \sum_{n=1}^{\infty} B_n = B_0 + \sum_{n=1}^{\infty} B_n = \sum_{n=0}^{\infty} B_n$.
Then,
$B(1) = B_0 + \int_0^1 dt\ \ [A, B(t)] \rightarrow\ \sum_{n=0}^{\infty} B_n = B_0 + \sum_{n=0}^{\infty}[A, B_n] \int_0^1 t^n\, dt = B_0 + \sum_{n=0}^{\infty} \frac{[A,B_n]}{n+1}$.

Hence,
$\sum_{n=1}^{\infty} B_n = \sum_{k=0}^{\infty} \frac{[A,B_k]}{k+1}$ .
So , with $k = n - 1 \rightarrow\ \sum_{n=1}^{\infty} B_n = \sum_{n=1}^{\infty} \frac{[A,B_{n-1}]}{n} \Longrightarrow B_n = \frac{1}{n}[A, B_{n-1}]$.
The next step is to show by induction
$B_n = \frac{1}{n!}([A, [A, \dots [A, )_n B(] \dots ]])_n$ .
We make use of
$B_{n-1} = \frac{1}{n-1}[A, B_{n-2}]$.
Then Boccio

$$\begin{aligned} B_n &= \frac{1}{n}[A, B_{n-1}] = \frac{1}{n}\left[A, \frac{1}{n-1}[A, B_{n-2}]\right] \\ &= \frac{1}{n(n-1)}[A,[A,B_{n-2}]] = \dots\dots\dots = \frac{1}{n(n-1)\dots.(n-n+1)}[A, \dots\dots.[A, B_{n-n}]] \\ &= \frac{1}{n!}[A,[A,\dots..[A,B]\dots.]] \quad \text{(with n nested commutators)} \end{aligned}$$

We have already shown
$e^A B e^A = B(1) = \sum_{n=0}^{\infty} B_n$.
Hence,
$e^A B e^A = B(1) = \sum_{n=0}^{\infty} B_n = \sum_{n=0}^{\infty} \frac{1}{n!}([A, [A, \dots [A, )_n B(] \dots ]])_n$ .
The last step to prove the operator
$U(a) = e^{ipa/\hbar}$
is a translation operator.
Now $A = e^{ipa/\hbar}$ .
So we have:
$e^{ipa/\hbar} x e^{-ipa/\hbar} = \sum_{n=0}^{\infty} \frac{a^n}{n!} (\frac{i}{\hbar})^n [p, p, \dots [p, x] \dots ]]$.
Let us demonstrate what will happen by looking at the first three terms:
$x + \frac{ia}{\hbar}[p, x] + \frac{(ia)^2}{2!}[p, [p, x]] + \cdots = x + \frac{ia}{\hbar}(-i\hbar) + \frac{(ia)^2}{2!}[p, -i\hbar] + \cdots = x + a + 0 + \cdots =$
$= x + a$.

**Alternative Method**

This method closely resembles the method I derived in:

5.4 *Intermezzo. A proof of Baker-Hausdorff Lemma* in *Quantum Mechanics in Texas* ,my notes on Quantum Mechanics Graduate Course, Fitzpatrick, www.leennoordzij.me .
I present this Intermezzo here:

5.4 *Intermezzo*. A proof of Baker-Hausdorff lemma

$e^{\lambda G} A e^{-\lambda G} = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} ([G,)^k A(])^k$ .

To this end I define, with $\{k \in \mathbb{N}\}$:

$k = 0$: $([G,)^k A(])^k = A$ , $2^k$ terms,

$k = 1$: $([G,)^k A(])^k = [G, A]$ , $2^k$ terms,

$k = 2$: $([G,)^k A(])^k = [G, [G, A]]$ , $2^k$ terms, ………

*The Proof:*

I use Taylor's series expansion:

$f(\lambda) = \sum_{k=0}^{\infty} \frac{a_k}{k!} \lambda^k$,

where $a_k = \frac{d^k f}{d(\lambda)^k}$ , at $\lambda = 0$,

and

$f(\lambda) \stackrel{\text{def}}{=} e^{\lambda G} A e^{-\lambda G}$.

With (C.5.4.18) , (C.5.4.19), and (C.5.4.20)

$a_o = A$,

$a_1 = \frac{df}{d\lambda}|_{\lambda=0} = GA - AG = [G, A]$,

$a_2 = \frac{d^2 f}{d(\lambda)^2}|_{\lambda=0} = \frac{d}{d\lambda}\frac{df}{d\lambda}|_{i\lambda=0} = \frac{d}{d\lambda}[G, f]|_{\lambda=0} = ([G,)^2 A(])^2$,

$a_3 = \frac{d^3 f}{d(\lambda)^3}|_{\lambda=0} = \frac{d}{d\lambda}[G[G, f] - [G, f]G]|_{\lambda=0} = ([G,)^3 A(])^3$, etc.

So for induction I assume

$a_k = \frac{d^k f}{d(\lambda)^k}|_{\lambda=0} = \frac{d}{d\lambda}([G,)^{k-1} f(])^{k-1} = ([G,)^k A(])^k$.

Then, with $a_k = ([G,)^k A(])^k$,

we have for $k + 1$

$a_{k+1} = \frac{d^{k+1} f}{d(\lambda)^{k+1}}|_{\lambda=0} = \frac{d}{d\lambda}([G,)^k f(])^k|_{\lambda=0} = ([G,)^{k+1} A(])^{k+1}$.

*End of Proof*

*End of intermezzo.*

Now Boccio's alternative method.

Let $\hat{f}(x) = e^{x\hat{A}} \hat{B} e^{-x\hat{A}}$.

The Taylor expansion is used(see Intermezzo above):

$\hat{f}(x) = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{d^k \hat{f}(x)}{dx^k}|_{x=0} x^k$.

For the first two derivatives:

$\frac{d\hat{f}(x)}{dx}|_{x=0} = \hat{A} e^{x\hat{A}} \hat{B} e^{-x\hat{A}} - e^{x\hat{A}} \hat{B} e^{-x\hat{A}} \hat{A} = [\hat{A}, \hat{f}(0)] = [\hat{A}, \hat{B}]$.

Knowing this, the Taylor expansion is helpful.

$\frac{d^2 \hat{f}(x)}{dx^2}|_{x=0} = \frac{d}{dx}[\hat{A}, \hat{f}(x)] = \left[\hat{A}, \frac{d\hat{f}(x)}{dx}\right] = \left[\hat{A}, [\hat{A}, \hat{f}(0)]\right] = \left[\hat{A}, [\hat{A}, \hat{B}\ ]\right]$, etc.

Hence

$e^{x\hat{A}} \hat{B} e^{-x\hat{A}} = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{d^k \hat{f}(x)}{dx^k}|_{x=0} x^k = \hat{B} + [\hat{A}, \hat{B}]x + \left[\hat{A}, [\hat{A}, \hat{B}\ ]\right] \frac{x^2}{2!} + \cdots$ .

In the Intermezzo above I used induction to make '… ' meaningful.

At the end of this problem Boccio made a remark about the Taylor series expansion and the solution of the first order ODE. I do not understand that remark. The Taylor series expansion is an expansion at $x = 0$.

### 6.19.13 Another Very Useful Identity

Prove that

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\frac{1}{2}[\hat{A},\hat{B}]},$$

provided that the operators $\hat{A}$ and $\hat{B}$ satisfy

$$\left[\hat{A},[\hat{A},\hat{B}]\right] = \left[\hat{B},[\hat{A},\hat{B}]\right] = 0 \, .$$

Define $\hat{f}(x) = e^{x\hat{A}}e^{x\hat{B}}$. A bit different from $\hat{f}(x) = e^{x\hat{A}}\hat{B}e^{-x\hat{A}}$ in problem 6.19.12.

Then, Boccio,

$$\frac{d\hat{f}(x)}{dx} = \hat{A}e^{x\hat{A}}e^{x\hat{B}} + e^{x\hat{A}}\hat{B}e^{x\hat{B}} = \hat{A}e^{x\hat{A}}e^{x\hat{B}} + e^{x\hat{A}}\hat{B}e^{-x\hat{A}}e^{x\hat{A}}e^{x\hat{B}}$$
$$= \left(\hat{A} + e^{x\hat{A}}\hat{B}e^{-x\hat{A}}\right)e^{x\hat{A}}e^{x\hat{B}} = \left(\hat{A} + e^{x\hat{A}}\hat{B}e^{-x\hat{A}}\right)\hat{f}(x)$$

With

$$\left[\hat{A},[\hat{A},\hat{B}]\right] = 0,$$

we have

$$e^{x\hat{A}}\hat{B}e^{-x\hat{A}} = \hat{B} + [\hat{A},\hat{B}]x.$$

Consequently,

$$\frac{d\hat{f}(x)}{dx} = \left(\hat{A} + e^{x\hat{A}}\hat{B}e^{-x\hat{A}}\right)\hat{f}(x) = \left(\hat{A} + \hat{B} + \left[\hat{A},\hat{B}\right]x\right)\hat{f}(x)$$

So , the non-homogeneous first ODE has the solution (textbook or WolframAlpha):

$$\hat{f}(x) = e^{x\hat{A}}e^{x\hat{B}} = e^{(\hat{A}+\hat{B})x + [\hat{A},\hat{B}]x^2/2}.$$

Boccio: $x = 1$ in the preceding expression

$$e^{\hat{A}}e^{\hat{B}} = e^{(\hat{A}+\hat{B}) + \frac{1}{2}[\hat{A},\hat{B}]}.$$

Then,

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\frac{1}{2}[\hat{A},\hat{B}]}.$$

Note

$$\left[\hat{A},[\hat{A},\hat{B}]\right] = \left[\hat{B},[\hat{A},\hat{B}]\right] = 0.$$

Proving

$$e^{A}Be^{-A} = B + [A,B],$$

we need $\left[\hat{A},[\hat{A},\hat{B}]\right] = 0$ .

Where does

$\left[\hat{A},[\hat{A},\hat{B}]\right] = \left[\hat{B},[\hat{A},\hat{B}]\right] = 0$ comes into play?

$$\hat{A}[\hat{A},\hat{B}] - [\hat{A},\hat{B}]\hat{A} = \hat{B}[\hat{A},\hat{B}] - [\hat{A},\hat{B}]\hat{B} \rightarrow (\hat{A}-\hat{B})[\hat{A},\hat{B}] = [\hat{A},\hat{B}](\hat{A}-\hat{B}) \rightarrow$$

$\rightarrow \left[(\hat{A}-\hat{B}),[\hat{A},\hat{B}]\right] = 0$ . Meaning?

### 6.19.14 Pure to Nonpure?

Use the equation of motion for the density operator $\hat{\rho}$ to show that a pure state cannot evolve into a nonpure state and vice versa.

The time dependent equation for the density operator:

$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H}(t), \hat{\rho}(t)]$.
For a pure state
- $Tr\hat{\rho}^2 = 1$,
- $\hat{\rho}^2 = \hat{\rho}$,
and
$\hat{\rho} = |\psi\rangle\langle\psi|$.
Then,
$\frac{d}{dt}Tr\hat{\rho}^2 = Tr2\hat{\rho}\frac{d\hat{\rho}}{dt} = -\frac{2i}{\hbar}Tr\left(\hat{\rho}\left[\hat{H}(t), \hat{\rho}(t)\right]\right) = -\frac{2i}{\hbar}Tr(\hat{\rho}\hat{H}\hat{\rho} - \hat{\rho}\hat{\rho}\hat{H})$.
We know
$TrAB = TrBA \longrightarrow Tr\hat{\rho}\hat{H}\hat{\rho} = Tr\hat{\rho}\hat{\rho}\hat{H}$.
So,
$\frac{d}{dt}Tr\hat{\rho}^2 = -\frac{2i}{\hbar}Tr\left(\hat{\rho}\hat{H}\hat{\rho} - \hat{\rho}\hat{\rho}\hat{H}\right) = -\frac{2i}{\hbar}Tr\left(\hat{\rho}\hat{\rho}\hat{H} - \hat{\rho}\hat{\rho}\hat{H}\right) = 0$.
Consequently
$\frac{d}{dt}Tr\hat{\rho}^2 = constant = 1$, independent of time → a pure state cannot change in a mixed state.
Boccio presented also an alternative approach with unitary operators leading to the same result.

### 6.19.15 Schur's Lemma

Let $G$ be the space of complex differentiable test functions, $g(x)$, where $x$ is real.
It is convenient to extend $G$ to encompass all functions, $\tilde{g}(x)$, such that
$\tilde{g}(x) = g(x) + c$,
$c$ is any constant.
The extended space is $\tilde{G}$.
Let $\hat{q}$ and $\hat{p}$ be linear operators on $\tilde{G}$
$\hat{q}g(x) = xg(x)$, a position operator.
And
$\hat{p}g(x) = -i\frac{d}{dx}g(x) = -ig'(x)$ , a momentum operator.
**1)** Show that $\hat{q}$ and $\hat{p}$ are Hermitian on space $\tilde{G}$.
Space $\tilde{G}$ is equipped with the scalar product
$S(f, g) = \int_{-\infty}^{\infty} dx\, f^*(x)g(x)$,
for any $f$ and $g$ in $\tilde{G}$.
Then with $\hat{q}g(x) = xg(x)$
$S(f, \hat{q}g) = \int_{-\infty}^{\infty} dx\, f^*(x)xg(x) = \int_{-\infty}^{\infty} dx\, f^*(x)xg(x)$
Now
$S(f, \hat{q}^\dagger g) = \int_{-\infty}^{\infty} dx\, xf^*(x)g(x) = S(\hat{q}f, g) = S(f, \hat{q}g)$
Hence
$\hat{q} = \hat{q}^\dagger$.
**Note**, with Dirac Algebra:
$S(f, g) = \langle f|g\rangle$ .
$S(f, \hat{q}g) = \langle f|\hat{q}g\rangle = x\langle f|g\rangle = \langle f\hat{q}|g\rangle = \left\langle f\middle|\hat{q}^\dagger g\right\rangle \Longrightarrow\ \hat{q} = \hat{q}^\dagger$.
Hence,
$\hat{q}$ is Hermitian on space $\tilde{G}$.
For the operator $\hat{p}$. Again with Dirac Algebra.
$S(f, g) = \langle f|g\rangle$.

$S(f,\hat{p}g) = \langle f|\hat{p}g\rangle = -i\left\langle f\middle|\frac{d}{dx}g\right\rangle = -i\left\langle f\frac{d}{dx}\middle|g\right\rangle = \langle f\hat{p}|g\rangle = \left\langle f\middle|\hat{p}^{\dagger}g\right\rangle \Longrightarrow \hat{p} = \hat{p}^{\dagger}$.
Hence,
$\hat{p}$ is Hermitian on space $\tilde{G}$.
**2)** Suppose $\widehat{M}$ is a linear operator on $\tilde{G}$ that commutes with $\hat{q}$ and $\hat{p}$.
Show that $\widehat{M}$ is a constant multiplier of the identity operator.
So, we have
$[\widehat{M},\hat{q}] = 0$ .
Then,
multiply the $\widehat{M}\hat{q} - \hat{q}\widehat{M} = 0$ to the left with $\hat{q}$ and add to the left hand side and the right hand side of the equality sign $\widehat{M}\hat{q}^2$, we have
$\hat{q}\widehat{M}\hat{q} - \hat{q}^2\widehat{M} + \widehat{M}\hat{q}^2 = \widehat{M}\hat{q}^2$ or
$\hat{q}\widehat{M}\hat{q} - \widehat{M}\hat{q}^2 - \hat{q}^2\widehat{M} + \widehat{M}\hat{q}^2 = 0$
$(\hat{q}\widehat{M} - \widehat{M}\hat{q})\hat{q} - \hat{q}^2\widehat{M} + \widehat{M}\hat{q}^2 = 0 \rightarrow \hat{q}^2\widehat{M} - \widehat{M}\hat{q}^2 = 0$,
so, $[\hat{q}^2,\widehat{M}] = 0$, etc., $[\hat{q}^n,\widehat{M}] = 0$, $n = 1,2,3,\ldots$.
In this way we have the expansion of the exponential:
$[\widehat{M}, e^{it\hat{q}}] = 0$.
From this toy may conclude:
any function of the operator $\hat{q}$ with the Fourier transform $f(\hat{q}) = \int_{-\infty}^{\infty} dt\,\tilde{f}(t)e^{it\hat{q}}$, we have
$[\widehat{M}, f(\hat{q})] = 0$.
Hence,
$\widehat{M}f(\hat{q})g(x) = f(\hat{q})\widehat{M}g(x)$.
Since $\hat{q}$ is the position operator $\Longrightarrow \hat{q}g(x) = xg(x) \Longrightarrow \hat{q}^n g(x) = x^n g(x) \Longrightarrow$
$\Longrightarrow e^{it\hat{q}}g(x) = e^{itx}g(x)$.
Consequently, any function with a Fourier transform given above satisfies
$f(\hat{q})g(x) = f(x)g(x)$.
So, with $\widehat{M}f(\hat{q})g(x) = f(\hat{q})\widehat{M}g(x)$
$\widehat{M}f(x)g(x) = f(\hat{q})\widehat{M}g(x)$.
Then, Boccio set $g(x) = 1$ and when $g(x) = 1$, $\widehat{M}g(x) = m(x)$. Furthermore,
$\widehat{M}f(x) = f(\hat{q})\widehat{M}g(x) = f(\hat{q})m(x) = f(x)m(x)$.
In the preceding expression we can replace $f(x)$ by $g(x)$ or $\frac{d}{dx}g(x)$:
$\widehat{M}g(x) = g(x)m(x)$, and $\widehat{M}\frac{d}{dx}g(x) = m(x)\frac{d}{dx}g(x)$.
Next, $\widehat{M}$ commutes with $\hat{p}$.
Meaning, with $\widehat{M}\frac{d}{dx}g(x) = m(x)\frac{d}{dx}g(x)$,
$\hat{p}\widehat{M}g(x) = \widehat{M}\hat{p}g(x) = -i\widehat{M}\frac{d}{dx}g(x) = -i\frac{d}{dx}g(x)m(x) = -ig'(x)m(x)$.
To prevent confusion, I used $\frac{d}{dx}g(x) = g'(x)$.
And with $\widehat{M}g(x) = g(x)m(x)$,
$\hat{p}\widehat{M}g(x) = \hat{p}g(x)m(x) = -i\frac{d}{dx}[g(x)m(x)]$.
So with
$\hat{p}\widehat{M}g(x) = -ig'(x)m(x)$ , and $\hat{p}\widehat{M}g(x) = -i\frac{d}{dx}[g(x)m(x)]$,
$\frac{d}{dx}[g(x)m(x)] = g'(x)m(x)$.
From the product rule of differentiation we learn:

$\frac{d}{dx}m(x) = 0 \Longrightarrow m(x) = \kappa$, a constant.
Hence,
$\widehat{M}g(x) = g(x)m(x) \Longrightarrow \widehat{M}g(x) = \kappa g(x)$.
So, we finally obtain
$\widehat{M} = \kappa\hat{I}$.

### 6.19.16 More About the Density Operator

Here attention is paid to the connections of the density operator formalism and information or entropy. A two state system is considered. $\rho$ is any general density matrix operating on the two-dimensional Hilbert space of the system.

**a)** Calculate the entropy,
$s = -Tr(\rho \ln \rho)$.
The density matrix $\rho$ is Hermitian.
A simple representation does proof this:
$\rho = prob1|\phi_1\rangle\langle\phi_1| + prob2|\phi_2\rangle\langle\phi_2| + prob3|\phi_3\rangle\langle\phi_3|$.
Hence,
$\rho = \rho^\dagger$.
Then
$\rho = \begin{pmatrix} a_{11} & a_{12} \\ a_{12}^\dagger & a_{22} \end{pmatrix}$.
A Hermitian matrix $\rho$ can be diagonalized by a transformation $P^\dagger\rho P$, where $P$ is a unitary matrix whose columns are eigenvectors of $\rho$.
So,
$\rho = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$.
The trace of this density matrix is 1: $a + b = 1 \Longrightarrow b = 1 - a \Longrightarrow \rho = \begin{pmatrix} a & 0 \\ 0 & 1-a \end{pmatrix}$
The eigenvalues of $\rho$ are:
$\rho_1 = a$, and $\rho_2 = 1 - a$ .
The corresponding eigenvectors $(0 < a < 1)$
$\rho_1 = a$ , $|\rho_1\rangle = \frac{1}{2a}\begin{pmatrix} \sqrt{4a^2 - 1} \\ 1 \end{pmatrix}$,
and
$\rho_2 = 1 - a$ , $|\rho_2\rangle = \frac{1}{2a}\begin{pmatrix} 1 \\ \sqrt{4a^2 - 1} \end{pmatrix}$.
Hence,
$\rho = \rho_1|\rho_1\rangle\langle\rho_1| + \rho_2|\rho_2\rangle\langle\rho_2|$.
A pure state is obtained with $Tr\rho^2 = 1$.
So,
$\begin{pmatrix} a & 0 \\ 0 & 1-a \end{pmatrix}\begin{pmatrix} a & 0 \\ 0 & 1-a \end{pmatrix} = \begin{pmatrix} a^2 & 0 \\ 0 & (1-a)^2 \end{pmatrix}$.
Then
$a^2 + (1-a)^2 = 1 - 2a + 2a^2 \Longrightarrow 1 - 2a + 2a^2 = 1 \Longrightarrow a(1-a) = 0$.
Hence, for $a = 1$, or $a = 0$, we have a pure state.
- $a = 0$.
$\rho = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ of which the eigenvalue is 1 and the eigen vector is $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$.
- $a = 1$.

$\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ of which the eigenvalue is 1 and the eigen vector is $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$.
Now with $0 < a < 1$ and $s = -Tr(\rho \ln \rho)$, see section 5.4 *Principle of Maximum Entropy,*
$s = -\sum_i prob_i \ln prob_i = -\rho_1 \ln \rho_1 - \rho_2 \ln \rho_2 = -a \ln a - (1-a)\ln(1-a)$.
Boccio used $\theta$ instead of $a$ .
**b)** A graph of the entropy as a function of $\theta$.

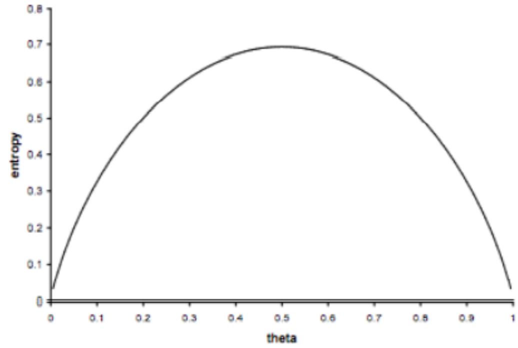



Figure 6.1: The entropy as a function of $\theta$

As follows from the analysis under a)**,** the entropy of a pure state with $\theta = 1$ or $\theta = 0$:
$s = -\sum_i prob_i \ln prob_i \Longrightarrow s = 0$.
Reminder: $\lim_{x\to 0} x \ln x = \lim_{x\to 0} \frac{\ln x}{1/x} \Longrightarrow \lim_{x\to 0} \frac{\frac{d}{dx}\ln x}{\frac{d}{dx}(\frac{1}{x})} = \lim_{x\to 0} \frac{\frac{1}{x}}{-\frac{1}{x^2}} = \lim_{x\to 0} -x = 0$.
The entropy increases until $\theta = \frac{1}{2}$, meaning minimal knowledge of the state.
**c)** Consider a system with ensemble $\rho$ to be a mixture of two ensembles $\rho_1$and $\rho_2$:
$\rho = \theta\rho_1 + (1-\theta)\rho_2$,
with $0 \le \theta \le 1$.
As an example, suppose
$\rho_1 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, and $\rho_2 = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$,
in some basis.
Prove for the entropy of the combined ensemble
$s(\rho) \ge \theta s(\rho_1) + (1-\theta)s(\rho_2)$.
With equality if $\theta = 0$, or $\theta = 1$.
The entropy of ensemble 1 is, the probabilities both $\frac{1}{2}$:
$s(\rho_1) = -\sum_i prob_i \ln prob_i = -\frac{1}{2}\ln\frac{1}{2} - \frac{1}{2}\ln\frac{1}{2} = \ln 2$.
Furthermore $Tr\rho_1^2 = \frac{1}{4}$.
For the ensemble 2 we find $Tr\rho_2^2 = 1$.
Consequently, ensemble 2 represents a pure state. Hence, $s(\rho_2) = 0$.
The eigenvalues of ensemble 2 are 0 and 1,
$s(\rho_2) = -\sum_i prob_i \ln prob_i = -0\ln 0 - 1\ln 1 = 0$.
Now, the entropy of the combined ensemble.
The density matrix of the combined ensemble
$\rho = \theta\rho_1 + (1-\theta)\rho_2 = \theta\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + (1-\theta)\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1-\theta \\ 1-\theta & 1 \end{pmatrix}$.
The eigenvalues of the combined ensemble

$$\begin{vmatrix} \frac{1}{2}-\lambda & \frac{1-\theta}{2} \\ \frac{1-\theta}{2} & \frac{1}{2}-\lambda \end{vmatrix} = 0 \Longrightarrow \left(\frac{1}{2}-\lambda\right) = \pm\left(\frac{1}{2}-\frac{\theta}{2}\right) \Longrightarrow \lambda_{1,2} = \frac{\theta}{2}, 1-\frac{\theta}{2}.$$

With these eigenvalues, probabilities, the entropy of the combined ensemble

$s(\rho) = -\sum_i prob_i \ln prob_i = -(1-\frac{\theta}{2})\ln\left(1-\frac{\theta}{2}\right) - \frac{\theta}{2}\ln\frac{\theta}{2}$.

$s(\rho)$ in the preceding expression

for $\theta = 1$, $s(\rho) = \ln 2$, and for $\theta = 0$, $s(\rho) = 0$.

We compare these results with the following expression

$s(\rho) \geq \theta s(\rho_1) + (1-\theta)s(\rho_2) = \theta \ln 2$ .

So for $\theta = 1$, $s(\rho) = s(\rho_1) = \ln 2$, and for $\theta = 0$, $s(\rho) = s(\rho_1) = 0$.

Next we must prove the inequality.

We take the difference: $s(\rho) - \theta s(\rho_1) + (1-\theta)s(\rho_2)$

$$-\left(1-\frac{\theta}{2}\right)\ln\left(1-\frac{\theta}{2}\right) - \frac{\theta}{2}\ln\frac{\theta}{2} - \theta\ln 2 = -\ln[\left(1-\frac{\theta}{2}\right)^{\left(1-\frac{\theta}{2}\right)} \cdot \frac{\theta^{\frac{\theta}{2}}}{2} \cdot 2^{\theta}] .$$

This must result in a number larger than zero. Consequently

$$\ln[\left(1-\frac{\theta}{2}\right)^{\left(1-\frac{\theta}{2}\right)} \cdot \frac{\theta^{\frac{\theta}{2}}}{2} \cdot 2^{\theta}] < 1.$$

For convenience , we rewrite $\left(1-\frac{\theta}{2}\right)^{\left(1-\frac{\theta}{2}\right)} \cdot \frac{\theta^{\frac{\theta}{2}}}{2} \cdot 2^{\theta} \to \left(1-\frac{\theta}{2}\right)^{\left(1-\frac{\theta}{2}\right)} (2\theta)^{\frac{\theta}{2}}$.

So,

$$\ln[\left(1-\frac{\theta}{2}\right)^{\left(1-\frac{\theta}{2}\right)} \cdot \frac{\theta^{\frac{\theta}{2}}}{2} \cdot 2^{\theta}] = \ln\left[\left(1-\frac{\theta}{2}\right)^{\left(1-\frac{\theta}{2}\right)} (2\theta)^{\frac{\theta}{2}}\right] = \left(1-\frac{\theta}{2}\right)\ln\left(1-\frac{\theta}{2}\right) + \frac{\theta}{2}\ln 2\theta.$$

Then,

$$\left(1-\frac{\theta}{2}\right)\ln\left(1-\frac{\theta}{2}\right) + \frac{\theta}{2}\ln 2\theta < 1?$$

To find out about this inequality let us look for the maximum of

$$\left(1-\frac{\theta}{2}\right)\ln\left(1-\frac{\theta}{2}\right) + \frac{\theta}{2}\ln 2\theta \Longrightarrow \frac{d}{d\theta}\left[\left(1-\frac{\theta}{2}\right)\ln\left(1-\frac{\theta}{2}\right) + \frac{\theta}{2}\ln 2\theta\right] = 0 \to$$

$$\to \ln 2\theta - \ln\left(1-\frac{\theta}{2}\right) = 0 \Longrightarrow \ln\frac{2\theta}{1-\frac{\theta}{2}} = 0 \Longrightarrow \theta = \frac{2}{5}.$$

Consequently,

$$s(\rho) = -\left(1-\frac{\theta}{2}\right)\ln\left(1-\frac{\theta}{2}\right) - \frac{\theta}{2}\ln\frac{\theta}{2} = 0.500,$$

and

$$\theta s(\rho_1) + (1-\theta)s(\rho_2) = \theta\ln 2 = 0.277.$$

The theorem is not contradicted.

### 6.19.17 Entanglement and the Purity of a Reduced Density Operator

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$, and $\{|0_B\rangle, |1_B\rangle\}$. Let $|\Psi_{AB}\rangle$ be the state

$|\Psi_{AB}\rangle = \cos\theta\,|0_A\rangle \otimes |0_B\rangle + \sin\theta|1_A\rangle \otimes |1_B\rangle$ .

With $0 < \theta < \frac{\pi}{2}$ , $|\Psi_{AB}\rangle$ is an entangled state.

The purity $\varsigma$ of the reduced density operator

$\tilde{\rho}_A = Tr_B|\Psi_{AB}\rangle\langle\Psi_{AB}|$,

is given by

$\varsigma = Tr|\tilde{\rho}_A^2|$.

This is a good measure of the entanglement of states in $\mathcal{H}_{AB}$.

For pure states of the above form, find extrema of $\varsigma$ with respect to $\theta$. Determine $\varsigma$ for entangled states.

- Density operator $\rho$ corresponding to $|\Psi_{AB}\rangle$. It is about two-dimensional spaces.

So, we could choose

$|0_{A,B}\rangle$ to be $\begin{pmatrix}0\\1\end{pmatrix}_{A,B}$ and $|1_{A,B}\rangle$ to be $\begin{pmatrix}1\\0\end{pmatrix}_{A,B}$. However, Boccio used a short hand notation:

$|\Psi_{00}\rangle = |0_A\rangle \otimes |0_B\rangle$, $\langle\Psi_{00}| = \langle 0_A| \otimes \langle 0_B|$, etc.

Then,

$\rho = |\Psi_{AB}\rangle\langle\Psi_{AB}| = \cos^2\theta\,|\Psi_{00}\rangle\langle\Psi_{00}| + \cos\theta\sin\theta\,|\Psi_{00}\rangle\langle\Psi_{11}| + \cos\theta\sin\theta\,|\Psi_{11}\rangle\langle\Psi_{00}| +$
$+\sin^2\theta\,|\Psi_{11}\rangle\langle\Psi_{11}|$.

Back to column vector representation:

$$|\Psi_{00}\rangle\langle\Psi_{00}| = |0_A\rangle \otimes |0_B\rangle\langle 0_A| \otimes \langle 0_B| = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}(0\;0\;0\;1) = \begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&1\end{pmatrix}.$$

$$|\Psi_{00}\rangle\langle\Psi_{11}| = |0_A\rangle \otimes |0_B\rangle\langle 1_A| \otimes \langle 1_B| = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}(1\;0\;0\;0) = \begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\1&0&0&0\end{pmatrix}.$$

$$|\Psi_{11}\rangle\langle\Psi_{00}| = |1_A\rangle \otimes |1_B\rangle\langle 0_A| \otimes \langle 0_B| = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}(0\;0\;0\;1) = \begin{pmatrix}0&0&0&1\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}.$$

$$|\Psi_{11}\rangle\langle\Psi_{11}| = |1_A\rangle \otimes |1_B\rangle\langle 1_A| \otimes \langle 1_B| = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}(1\;0\;0\;0) = \begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}.$$

Then

$$\rho = |\Psi_{AB}\rangle\langle\Psi_{AB}| = \begin{pmatrix}\sin^2\theta&0&0&\cos\theta\sin\theta\\0&0&0&0\\0&0&0&0\\\cos\theta\sin\theta&0&0&\cos^2\theta\end{pmatrix}.$$

Now, the reduced density operator:

$\tilde{\rho}_A = Tr_B|\Psi_{AB}\rangle\langle\Psi_{AB}|$.

**Note**: $Tr_B$ means: the system $B$ is traced out to obtain the reduced density matrix on $A$, https://en.wikipedia.org/wiki/Quantum entanglement. Then, the summation of the trace is over the base states of the Hilbert space $\mathcal{H}_B$. Caveat, this is about a 2-dimensional base, whereas $|\Psi_{AB}\rangle\langle\Psi_{AB}|$ is about a $4 \times 4$ matrix.

Consequently,

$\tilde{\rho}_A = Tr_B|\Psi_{AB}\rangle\langle\Psi_{AB}| = (I_A \otimes \langle 0_B|)|\Psi_{AB}\rangle\langle\Psi_{AB}|((I_A \otimes |0_B\rangle) +$
$+(I_A \otimes \langle 1_B|)|\Psi_{AB}\rangle\langle\Psi_{AB}|((I_A \otimes |1_B\rangle)$.

$\tilde{\rho}_A = Tr_B|\Psi_{AB}\rangle\langle\Psi_{AB}| = \langle 0_B|\Psi_{AB}\rangle\langle\Psi_{AB}|0_B\rangle + \langle 1_B|\Psi_{AB}\rangle\langle\Psi_{AB}|1_B\rangle =$
$= \cos^2\theta\,(\langle 0_B|\Psi_{00}\rangle\langle\Psi_{00}|0_B\rangle + \langle 1_B|\Psi_{00}\rangle\langle\Psi_{00}|1_B\rangle) +$
$+\cos\theta\sin\theta\,(\langle 0_B|\Psi_{00}\rangle\langle\Psi_{11}|0_B\rangle + \langle 1_B|\Psi_{00}\rangle\langle\Psi_{11}|1_B\rangle) +$
$+\cos\theta\sin\theta\,(\langle 0_B|\Psi_{11}\rangle\langle\Psi_{00}|0_B\rangle + \langle 1_B|\Psi_{11}\rangle\langle\Psi_{00}|1_B\rangle) +$
$+\sin^2\theta\,(\langle 0_B|\Psi_{11}\rangle\langle\Psi_{11}|0_B\rangle + \langle 1_B|\Psi_{11}\rangle\langle\Psi_{11}|1_B\rangle)$.

Now

$\cos^2\theta\,(\langle 0_B|\Psi_{00}\rangle\langle\Psi_{00}|0_B\rangle + \langle 1_B|\Psi_{00}\rangle\langle\Psi_{00}|1_B\rangle) =$
$\cos^2\theta\,(\langle 0_B|0_A\rangle \otimes |0_B\rangle\langle 0_A| \otimes \langle 0_B|0_B\rangle + \langle 1_B|0_A\rangle \otimes |0_B\rangle\langle 0_A| \otimes \langle 0_B|1_B\rangle) =$
$= \cos^2\theta\,(\langle 0_B|0_B\rangle \otimes |0_A\rangle\langle 0_A| \otimes \langle 0_B|0_B\rangle + \langle 1_B|0_A\rangle \otimes |0_B\rangle\langle 0_A| \otimes \langle 0_B|1_B\rangle) =$
$= \cos^2\theta\,|0_A\rangle\langle 0_A|,$
and $\langle 1_B|0_A\rangle \otimes |0_B\rangle\langle 0_A| \otimes \langle 0_B|1_B\rangle = 0$, since $\langle 0_B|1_B\rangle = 0$.
Note $|0_A\rangle$ and $|0_B\rangle$ are independent:
$\langle 0_B|0_A\rangle \otimes |0_B\rangle\langle 0_A| \otimes \langle 0_B|0_B\rangle = \langle 0_B|0_B\rangle \otimes |0_A\rangle\langle 0_A| \otimes \langle 0_B|0_B\rangle = |0_A\rangle\langle 0_A|$ .
So, we have one term of $\tilde{\rho}_A$: $\cos^2\theta\,|0_A\rangle\langle 0_A|$.
I leave out further details and the other term of $\tilde{\rho}_A$ appears to be: $\sin^2\theta\,|1_A\rangle\langle 1_A|$.
Hence,
$\tilde{\rho}_A = \cos^2\theta\,|0_A\rangle\langle 0_A| + \sin^2\theta\,|1_A\rangle\langle 1_A|$.
So,
$\tilde{\rho}_A^2 = \cos^4\theta\,|0_A\rangle\langle 0_A| + \sin^4\theta\,|1_A\rangle\langle 1_A| = \begin{pmatrix}\sin^4\theta & 0\\ 0 & \cos^4\theta\end{pmatrix}$.
Consequently
$\varsigma = Tr|\tilde{\rho}_A^2| = \cos^4\theta + \sin^4\theta$.
The extreme of $\varsigma$
$\frac{d\varsigma}{d\theta} = -4\cos^3\theta\sin\theta + 4\sin^3\theta\cos\theta = 0 \Longrightarrow \cos^3\theta\sin\theta = \sin^3\theta\cos\theta \Longrightarrow$
$\Longrightarrow \cos\theta\,(1-\sin^2\theta)\sin\theta = \sin\theta\,(1-\cos^2\theta)\cos\theta \Longrightarrow \cos^2\theta = \sin^2\theta \Longrightarrow \tan\theta = 1$
Then $\theta = \frac{\pi}{4}$.
$\cos^2\theta = \sin^2\theta = \frac{1}{2} \Longrightarrow\ \varsigma = \frac{1}{2}$.
Furthermore for $\theta = \frac{\pi}{4}$
$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|0_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |1_B\rangle)$, a highly entangled state.
For $\theta = 0$
$|\Psi_{AB}\rangle = |0_A\rangle \otimes |0_B\rangle$, a pure state,
and
$\varsigma = 1$ .

### 6.19.18 The Controlled-Not Operator

Again let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$, and $\{|0_B\rangle, |1_B\rangle\}$. Consider the controlled-not operator on $\mathcal{H}_{AB}$ :
$U_{AB} = P_0^A \otimes I^B + P_1^A \otimes \sigma_x^B$,
where
$P_0^A = |0_A\rangle\langle 0_A|$ , $P_1^A = |1_A\rangle\langle 1_A|$ ,
and
$\sigma_x^B = |0_B\rangle\langle 1_B| + |1_B\rangle\langle 0_B|$.

Note: in the preceding expression Boccio presented the second term to be $|1_B\rangle\langle 0_0|$.
A typo I suppose.

-Write a matrix representation for $U_{AB}$ with respect to the following (ordered) basis of $\mathcal{H}_{AB}$
$|0_A\rangle\otimes|0_B\rangle$ , $|0_A\rangle\otimes|1_B\rangle$, $|1_A\rangle\otimes|0_B\rangle$, $|1_A\rangle\otimes|1_B\rangle$ .
- Find the eigenvectors of $U_{AB}$ and
- Do these eigenvectors correspond to entangled states?
The matrix representation of $U_{AB} = P_0^A \otimes I^B + P_1^A \otimes \sigma_x^B$.
When I assume the column representation of $|0_A\rangle$ to be $\begin{pmatrix}0\\1\end{pmatrix}$, etc, like I did in the foregoing

problem, I find for $U_{AB}$

$$U_{AB} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Next, for the column presentation I choose $|0_A\rangle$ to be $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, etc, and with some more detail I construct the matrix representation of $U_{AB}$.

$$P_0^A = |0_A\rangle\langle 0_A| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}(1\ \ 0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

$$P_0^A \otimes I^B = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

$$P_1^A = |1_A\rangle\langle 1_A| = \begin{pmatrix} 0 \\ 1 \end{pmatrix}(0\ \ 1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

$$\sigma_x^B = |0_B\rangle\langle 1_B| + |1_B\rangle\langle 0_B| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}(0\ \ 1) + \begin{pmatrix} 0 \\ 1 \end{pmatrix}(1\ \ 0) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Then

$$P_1^A \otimes \sigma_x^B = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

$$U_{AB} = P_0^A \otimes I^B + P_1^A \otimes \sigma_x^B = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

This $U_{AB}$ differs from the earlier found $U_{AB}$. Does it matter?

With $U_{AB} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$, the eigenvectors are, by inspection,

$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$, and $\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$.

These two eigenstates can be obtained by the tensor products:

$$|0_A\rangle \otimes |0_B\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix},$$

and

$$|0_A\rangle \otimes |1_B\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}.$$

The two eigenstates are not entangled.

Note: Let us choose the first obtained matrix of $U_{AB}$, the eigenvectors are

$|1_A\rangle \otimes |0_B\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$, and $|1_A\rangle \otimes |1_B\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$.

The two remaining eigenstates are found by orthogonality, normalization and simplicity. These are

$$\frac{1}{\sqrt{2}}\begin{pmatrix}0\\0\\1\\1\end{pmatrix}=\frac{1}{\sqrt{2}}\left[\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\right]=\frac{1}{\sqrt{2}}(|1_A\rangle\otimes|0_B\rangle+|1_A\rangle\otimes|1_B\rangle)=$$

$$=\frac{1}{\sqrt{2}}|1_A\rangle\otimes(|0_B\rangle+|1_B\rangle)$$, not entangled,

and,

$$\frac{1}{\sqrt{2}}\begin{pmatrix}0\\0\\1\\-1\end{pmatrix}=\frac{1}{\sqrt{2}}\left[\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}-\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\right]=\frac{1}{\sqrt{2}}(|1_A\rangle\otimes|0_B\rangle-|1_A\rangle\otimes|1_B\rangle)=$$

$$=\frac{1}{\sqrt{2}}|1_A\rangle\otimes(|0_B\rangle-|1_B\rangle)$$, not entangled.

I conclude it does not matter whether

$$U_{AB}=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}, \text{ or } U_{AB}=\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},$$

is chosen.

### 6.19.19 Creating Entanglement via Unitary Evolution

Working with the same system as in Problems 6.19.17 and 6.19.18, find a factorizable input state

$|\Psi_{AB}^{in}\rangle=|\Psi_A\rangle\otimes|\Psi_B\rangle,$

such that the output state

$|\Psi_{AB}^{out}\rangle=U_{AB}|\Psi_{AB}^{in}\rangle,$

is maximally entangled.

That is, find any factorizable $|\Psi_{AB}^{in}\rangle$ such that $Tr[\tilde{\rho}_A^2]=\frac{1}{2}$,

where the reduced density matrix is

$\tilde{\rho}_A=Tr_B[|\Psi_{AB}^{out}\rangle\langle\Psi_{AB}^{out}|.$

Again let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle,|1_A\rangle\}$, and $\{|0_B\rangle,|1_B\rangle\}$.

With these base vectors a general factorizable input state has the form

$|\Psi_{AB}^{in}\rangle=(a_0|0_A\rangle+a_1|1_A\rangle)\otimes(b_0|0_B\rangle+b_1|1_B\rangle)=$

$=a_0b_0|0_A\rangle\otimes|0_B\rangle+a_0b_1|0_A\rangle\otimes|1_B\rangle+a_1b_0|1_A\rangle\otimes|0_B\rangle+a_1b_1|1_A\rangle\otimes|1_B\rangle$,

where, with normalization

$|a_0|^2+|a_1|^2=1,$

and

$|b_0|^2+|b_1|^2=1.$

We have, with $|\Psi_{AB}^{in}\rangle$, a product state. The main feature of which(Susskind) is *that each subsystem behaves independently of each other*.

Now, apply the unitary operator

$|\Psi_{AB}^{out}\rangle=U_{AB}|\Psi_{AB}^{in}\rangle=$

$=a_0b_0|0_A\rangle\otimes|0_B\rangle+a_0b_1|0_A\rangle\otimes|1_B\rangle+a_1b_0|1_A\rangle\otimes|0_B\rangle+a_1b_1|1_A\rangle\otimes|1_B\rangle.$

So, $|\Psi_{AB}^{out}\rangle$ is determined by $|\Psi_{AB}^{in}\rangle$. Since, Susskind, *we have the conservation of distinction* this is what we requires from $U_{AB}$. So, how on earth can we obtain entanglement after

operating $U_{AB}$? Let us find out.
We use a simple method to find out about a maximally entangled output state by choosing the following amplitudes to be:
$a_0 = a_1 = \frac{1}{\sqrt{2}}$,
and
$b_0 = 1$, or $b_1 = 1$.
With
$a_0 = a_1 = \frac{1}{\sqrt{2}}$, and $b_0 = 1$:
$|\Psi_{AB}^{out}\rangle = \frac{1}{\sqrt{2}}(b_0|0_A\rangle \otimes |0_B\rangle + b_0|1_A\rangle \otimes |0_B\rangle)$.
With
$a_0 = a_1 = \frac{1}{\sqrt{2}}$, and $b_1 = 1$:
$|\Psi_{AB}^{out}\rangle = \frac{1}{\sqrt{2}}(b_1|0_A\rangle \otimes |1_B\rangle + b_1|1_A\rangle \otimes |1_B\rangle)$.
Next we determine the reduced matrix, with $b_0 = 1$:
$\tilde{\rho}_A = Tr_B[|\Psi_{AB}^{out}\rangle\langle\Psi_{AB}^{out}| = \langle 0_B|\Psi_{AB}^{out}\rangle\langle\Psi_{AB}^{out}|0_B\rangle + \langle 1_B|\Psi_{AB}^{out}\rangle\langle\Psi_{AB}^{out}|1_B\rangle =$
$= \frac{1}{2}[\langle 0_B(|0_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |0_B\rangle)(\langle 0_A| \otimes \langle 0_B| + \langle 1_A| \otimes \langle 0_B|)0_B\rangle +$
$+\langle 1_B(|0_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |0_B\rangle)(\langle 0_A| \otimes \langle 0_B| + \langle 1_A| \otimes \langle 0_B|)1_B\rangle] =$
$= \frac{1}{2}(|0_A\rangle + |1_A\rangle)(\langle 0_A| + \langle 1_A|)$.
With $|0_A\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, and $|1_A\rangle = \begin{pmatrix}0\\1\end{pmatrix}$:
$\tilde{\rho}_A = \frac{1}{2}(|0_A\rangle + |1_A\rangle)(\langle 0_A| + \langle 1_A|) = \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}$.
Hence
$Tr\tilde{\rho}_A = 1$, and $Tr[\tilde{\rho}_A^2] = 1$, in stead of $Tr[\tilde{\rho}_A^2] = \frac{1}{2}$.
Now, we determine the reduced matrix, with $b_1 = 1$:
$|\Psi_{AB}^{out}\rangle = \frac{1}{\sqrt{2}}(|0_A\rangle \otimes |1_B\rangle + |1_A\rangle \otimes |1_B\rangle)$.
$\tilde{\rho}_A = Tr_B[|\Psi_{AB}^{out}\rangle\langle\Psi_{AB}^{out}| = \langle 0_B|\Psi_{AB}^{out}\rangle\langle\Psi_{AB}^{out}|0_B\rangle + \langle 1_B|\Psi_{AB}^{out}\rangle\langle\Psi_{AB}^{out}|1_B\rangle =$
$= \frac{1}{2}[\langle 0_B(|0_A\rangle \otimes |1_B\rangle + |1_A\rangle \otimes |1_B\rangle)(\langle 0_A| \otimes \langle 1_B| + \langle 1_A| \otimes \langle 1_B|)0_B\rangle +$
$+\langle 1_B(|0_A\rangle \otimes |1_B\rangle + |1_A\rangle \otimes |1_B\rangle)(\langle 0_A| \otimes \langle 1_B| + \langle 1_A| \otimes \langle 1_B|)1_B\rangle] =$
$= \frac{1}{2}(|0_A\rangle + |1_A\rangle)(\langle 0_A| + \langle 1_A|)$.
With $|0_A\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, and $|1_A\rangle = \begin{pmatrix}0\\1\end{pmatrix}$:
$\tilde{\rho}_A = \frac{1}{2}(|0_A\rangle + |1_A\rangle)(\langle 0_A| + \langle 1_A|) = \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}$.
Hence
$Tr\tilde{\rho}_A = 1$, and $Tr[\tilde{\rho}_A^2] = 1$, in stead of $Tr[\tilde{\rho}_A^2] = \frac{1}{2}$.
Hence, I conclude: no entanglement.
Let us find out about $\tilde{\rho}_A^{in}$ for $a_0 = a_1 = \frac{1}{\sqrt{2}}$, and $b_1 = 1$,
$\tilde{\rho}_A^{in} = Tr_B[|\Psi_{AB}^{in}\rangle\langle\Psi_{AB}^{in}| = \langle 0_B|\Psi_{AB}^{in}\rangle\langle\Psi_{AB}^{in}|0_B\rangle + \langle 1_B|\Psi_{AB}^{in}\rangle\langle\Psi_{AB}^{in}|1_B\rangle =$
$= \frac{1}{2}[\langle 0_B(|0_A\rangle \otimes |1_B\rangle + |1_A\rangle \otimes |1_B\rangle)(\langle 0_A| \otimes \langle 1_B| + \langle 1_A| \otimes \langle 1_B|)0_B\rangle +$
$+\langle 1_B(|0_A\rangle \otimes |1_B\rangle + |1_A\rangle \otimes |1_B\rangle)(\langle 0_A| \otimes \langle 1_B| + \langle 1_A| \otimes \langle 1_B|)1_B\rangle] =$
$= \frac{1}{2}(|0_A\rangle + |1_A\rangle)(\langle 0_A| + \langle 1_A|)$.
With $|0_A\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, and $|1_A\rangle = \begin{pmatrix}0\\1\end{pmatrix}$:

$\tilde{\rho}_A^{in} = \frac{1}{2}(|0_A\rangle + |1_A\rangle)(\langle 0_A| + \langle 1_A|) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$.

Hence

$Tr\, \tilde{\rho}_A^{in} = 1$, and $Tr(\, \tilde{\rho}_A^{in})^2 = 1$.

Entanglement?

### 6.19.20 Tensor-Product Bases

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$, and $\{|0_B\rangle, |1_B\rangle\}$. Consider the following entangled state in the joint Hilbert space:

$\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$,

$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|0_A 1_B\rangle + |1_A 0_B\rangle)$,

where $|0_A 1_B\rangle \equiv |0_A\rangle \otimes |1_B\rangle$ and $|1_A 0_B\rangle \equiv |1_A\rangle \otimes |0_B\rangle$ and so on.

Rewrite $|\Psi_{AB}\rangle$ in terms of a new basis

$\{|\tilde{0}_A \tilde{0}_B\rangle, |\tilde{0}_A \tilde{1}_B\rangle, |\tilde{1}_A \tilde{0}_B\rangle, |\tilde{1}_A \tilde{1}_B\rangle\}$,

where

$|\tilde{0}_A\rangle = \cos\frac{\phi}{2}|0_A\rangle + \sin\frac{\phi}{2}|1_A\rangle$,

$|\tilde{1}_A\rangle = -\sin\frac{\phi}{2}|0_A\rangle + \cos\frac{\phi}{2}|1_A\rangle$,

and similarly for the set $\{\, |\tilde{0}_B\rangle,\ |\tilde{1}_B\rangle\}$:

$|\tilde{0}_B\rangle = \cos\frac{\phi}{2}|0_B\rangle + \sin\frac{\phi}{2}|1_B\rangle$,

$|\tilde{1}_B\rangle = -\sin\frac{\phi}{2}|0_B\rangle + \cos\frac{\phi}{2}|1_B\rangle$

Keep in mind: $|\tilde{0}_A \tilde{0}_B\rangle \equiv |\tilde{0}_A\rangle \otimes |\tilde{0}_B\rangle$, etc.

Is $|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|0_A 1_B\rangle + |1_A 0_B\rangle)$ a special choice?

With some algebra, we have

$|0_A\rangle = \cos\frac{\phi}{2}|\tilde{0}_A\rangle - \sin\frac{\phi}{2}|\tilde{1}_A\rangle$,

$|1_A\rangle = \sin\frac{\phi}{2}|\tilde{0}_A\rangle + \cos\frac{\phi}{2}|\tilde{1}_A\rangle$ .

Furthermore

$|0_B\rangle = \cos\frac{\phi}{2}|\tilde{0}_B\rangle - \sin\frac{\phi}{2}|\tilde{1}_B\rangle$,

$|1_B\rangle = \sin\frac{\phi}{2}|\tilde{0}_B\rangle + \cos\frac{\phi}{2}|\tilde{1}_B\rangle$

To rewrite $|\Psi_{AB}\rangle$ in the new basis, we have to express $|0_A 1_B\rangle$ and $|1_A 0_B\rangle$ in the new basis.

$|0_A 1_B\rangle = |0_A\rangle \otimes |1_B\rangle = (\cos\frac{\phi}{2}|\tilde{0}_A\rangle - \sin\frac{\phi}{2}|\tilde{1}_A\rangle) \otimes \left(\sin\frac{\phi}{2}|\tilde{0}_B\rangle + \cos\frac{\phi}{2}|\tilde{1}_B\rangle\right) =$

$= \cos\frac{\phi}{2}\sin\frac{\phi}{2}|\tilde{0}_A \tilde{0}_B\rangle + \cos^2\frac{\phi}{2}|\tilde{0}_A \tilde{1}_B\rangle - \sin^2\frac{\phi}{2}|\tilde{1}_A \tilde{0}_B\rangle - \sin\frac{\phi}{2}\cos\frac{\phi}{2}|\tilde{1}_A \tilde{1}_B\rangle$,

and

$|1_A 0_B\rangle = |1_A\rangle \otimes |0_B\rangle = (\sin\frac{\phi}{2}|\tilde{0}_A\rangle + \cos\frac{\phi}{2}|\tilde{1}_A\rangle) \otimes (\,\cos\frac{\phi}{2}|\tilde{0}_B\rangle - \sin\frac{\phi}{2}|\tilde{1}_B\rangle) =$

$= \sin\frac{\phi}{2}\cos\frac{\phi}{2}|\tilde{0}_A \tilde{0}_B\rangle - \sin^2\frac{\phi}{2}|\tilde{0}_A \tilde{1}_B\rangle + \cos^2\frac{\phi}{2}|\tilde{1}_A \tilde{0}_B\rangle - \cos\frac{\phi}{2}\sin\frac{\phi}{2}|\tilde{1}_A \tilde{1}_B\rangle$.

With these results, in the new basis

$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|0_A 1_B\rangle + |1_A 0_B\rangle) = \frac{1}{\sqrt{2}}[\sin\phi\left(|\tilde{0}_A \tilde{0}_B\rangle - |\tilde{1}_A \tilde{1}_B\rangle\right) + \cos\phi\left(|\tilde{0}_A \tilde{1}_B\rangle + |\tilde{1}_A \tilde{0}_B\rangle\right)]$.

The choice of

$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|0_A 1_B\rangle + |1_A 0_B\rangle)$,

is not considered special.

Suppose Boccio meant

$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|0_A 1_B\rangle - |1_A 0_B\rangle)$?

Well, in that case:

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|0_A 1_B\rangle - |1_A 0_B\rangle) = \frac{1}{\sqrt{2}}(|\tilde{0}_A \tilde{1}_B\rangle - |\tilde{1}_A \tilde{0}_B\rangle).$$

Now the state has the same coefficients in the old and in the new basis. Boccio considered this to be unusual.

Let us look at the column representation of

$$|0_A 1_B\rangle = |0_A\rangle \otimes |1_B\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}.$$

$$|\tilde{0}_A\rangle = \cos\frac{\phi}{2}|0_A\rangle + \sin\frac{\phi}{2}|1_A\rangle,$$

and

$$|\tilde{1}_B\rangle = -\sin\frac{\phi}{2}|0_B\rangle + \cos\frac{\phi}{2}|1_B\rangle.$$

$$|\tilde{0}_A \tilde{1}_B\rangle = |\tilde{0}_A\rangle \otimes |\tilde{1}_B\rangle = \left(\cos\frac{\phi}{2}|0_A\rangle + \sin\frac{\phi}{2}|1_A\rangle\right) \otimes \left(-\sin\frac{\phi}{2}|0_B\rangle + \cos\frac{\phi}{2}|1_B\rangle\right) =$$

$$= \begin{pmatrix} \cos\frac{\phi}{2} \\ \sin\frac{\phi}{2} \end{pmatrix} \otimes \begin{pmatrix} -\sin\frac{\phi}{2} \\ \cos\frac{\phi}{2} \end{pmatrix} = \begin{pmatrix} -\sin\frac{\phi}{2}\cos\frac{\phi}{2} \\ \cos^2\frac{\phi}{2} \\ -\sin^2\frac{\phi}{2} \\ \sin\frac{\phi}{2}\cos\frac{\phi}{2} \end{pmatrix}.$$

This example illustrates the differences in coefficients.

### 6.19.21 Matrix Representations

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$, and $\{|0_B\rangle, |1_B\rangle\}$.

Furthermore

$|0_A 0_B\rangle \equiv |0_A\rangle \otimes |0_B\rangle$, etc.

These tensor products of the basis kets can be represented in column vector representation

$$|0_A 0_B\rangle \equiv |0_A\rangle \otimes |0_B\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

Then,

$$|0_A 1_B\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |1_A 0_B\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \text{ and } |1_A 1_B\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

In the following we will use the density operator:

$$\rho_{AB} = \frac{3}{8}|0_A\rangle\langle 0_A| \otimes \frac{1}{2}(|0_B\rangle + |1_B\rangle)(\langle 0_B| + \langle 1_B|) +$$
$$+ \frac{5}{8}|1_A\rangle\langle 1_A| \otimes \frac{1}{2}(|0_B\rangle - |1_B\rangle)(\langle 0_B| - \langle 1_B|).$$

**a)** The matrix representation of $\rho_{AB}$.

Rewrite the expression in column vector representation.

$$\rho_{AB} = \frac{3}{8}|0_A\rangle\langle 0_A| \otimes \frac{1}{2}(|0_B\rangle\langle 0_B| + |0_B\rangle\langle 1_B| + |1_B\rangle\langle 0_B| + |1_B\rangle\langle 1_B|) +$$
$$+ \frac{5}{8}|1_A\rangle\langle 1_A| \otimes \frac{1}{2}(|0_B\rangle\langle 0_B| - |0_B\rangle\langle 1_B| - |1_B\rangle\langle 0_B| + |1_B\rangle\langle 1_B|) =$$

$$= \frac{3}{16}\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} \otimes \left[\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} + \begin{pmatrix}0 & 1\\0 & 0\end{pmatrix} + \begin{pmatrix}0 & 0\\1 & 0\end{pmatrix} + \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}\right] +$$
$$+ \frac{5}{16}\begin{pmatrix}0 & 0\\0 & 1\end{pmatrix} \otimes [\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} - \begin{pmatrix}0 & 1\\0 & 0\end{pmatrix} - \begin{pmatrix}0 & 0\\1 & 0\end{pmatrix} + \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix} =$$
$$= \frac{3}{16}\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} \otimes \begin{pmatrix}1 & 1\\1 & 1\end{pmatrix} + \frac{5}{16}\begin{pmatrix}0 & 0\\0 & 1\end{pmatrix} \otimes \begin{pmatrix}1 & -1\\-1 & 1\end{pmatrix} = \frac{3}{16}\begin{pmatrix}1 & 1 & 0 & 0\\1 & 1 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\end{pmatrix} +$$
$$+ \frac{5}{16}\begin{pmatrix}0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 1 & -1\\0 & 0 & -1 & 0\end{pmatrix} = \frac{1}{16}\begin{pmatrix}3 & 3 & 0 & 0\\3 & 3 & 0 & 0\\0 & 0 & 5 & -5\\0 & 0 & -5 & 5\end{pmatrix}.$$

**b)** About partial projectors Problem 6.19.18:
$P_0^A = |0_A\rangle\langle 0_A|$ , $P_1^A = |1_A\rangle\langle 1_A|$ .
Here we have $P_0^B$, and $P_1^B$.
Find the matrix representation of
$I^A \otimes P_0^B$, and $I^A \otimes P_1^B$.
With column representation:
$$P_0^B = |0_B\rangle\langle 0_B| = \begin{pmatrix}1\\0\end{pmatrix}(1 \;\; 0) = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix},$$
and
$$P_1^B = |1_B\rangle\langle 1_B| = \begin{pmatrix}0\\1\end{pmatrix}(0 \;\; 1) = \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}.$$
Then
$$I^A \otimes P_0^B = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix} \otimes \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} = \begin{pmatrix}1 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & 0\end{pmatrix}.$$
$$I^A \otimes P_1^B = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix} \otimes \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix} = \begin{pmatrix}0 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 1\end{pmatrix}.$$
Now the matrix representation of:
- $I^A \otimes P_0^B \; \rho_{AB} \; I^A \otimes P_0^B$

All the ingredients are there:
$$\begin{pmatrix}1 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & 0\end{pmatrix} \frac{1}{16}\begin{pmatrix}3 & 3 & 0 & 0\\3 & 3 & 0 & 0\\0 & 0 & 5 & -5\\0 & 0 & -5 & 5\end{pmatrix}\begin{pmatrix}1 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & 0\end{pmatrix} = \frac{1}{16}\begin{pmatrix}3 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 5 & 0\\0 & 0 & 0 & 0\end{pmatrix}.$$
- $I^A \otimes P_1^B \; \rho_{AB} \; I^A \otimes P_1^B$
$$\begin{pmatrix}0 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 1\end{pmatrix} \frac{1}{16}\begin{pmatrix}3 & 3 & 0 & 0\\3 & 3 & 0 & 0\\0 & 0 & 5 & -5\\0 & 0 & -5 & 5\end{pmatrix}\begin{pmatrix}0 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 1\end{pmatrix} = \frac{1}{16}\begin{pmatrix}0 & 0 & 0 & 0\\0 & 3 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 0 & 5\end{pmatrix}.$$
Then
$$I^A \otimes P_0^B \; \rho_{AB} \; I^A \otimes P_0^B + I^A \otimes P_1^B \; \rho_{AB} \; I^A \otimes P_1^B = \frac{1}{16}\begin{pmatrix}3 & 0 & 0 & 0\\0 & 3 & 0 & 0\\0 & 0 & 5 & 0\\0 & 0 & 0 & 5\end{pmatrix}.$$
**c)** The matrix representation of reduced density operator
$\tilde{\rho}_A = Tr_B \rho_{AB}$.
So in bras and kets, the density operator

$\rho_{AB} = \frac{3}{8}|0_A\rangle\langle 0_A|\otimes\frac{1}{2}(|0_B\rangle + |1_B\rangle)(\langle 0_B| + \langle 1_B|) +$
$+\frac{5}{8}|1_A\rangle\langle 1_A|\otimes\frac{1}{2}(|0_B\rangle - |1_B\rangle)(\langle 0_B| - \langle 1_B|) =$
$= \frac{3}{8}|0_A\rangle\langle 0_A|\otimes\frac{1}{2}(|0_B\rangle\langle 0_B| + |0_B\rangle\langle 1_B| + |1_B\rangle\langle 0_B| + |1_B\rangle\langle 1_B|) +$
$+\frac{5}{8}|1_A\rangle\langle 1_A|\otimes\frac{1}{2}(|0_B\rangle\langle 0_B| - |0_B\rangle\langle 1_B| - |1_B\rangle\langle 0_B| + |1_B\rangle\langle 1_B|) =$
$= \frac{3}{16}(|0_A 0_B\rangle\langle 0_A 0_B| + |0_A 1_B\rangle\langle 0_A 0_B| + |0_A 0_B\rangle\langle 0_A 1_B| + |0_A 1_B\rangle\langle 0_A 1_B|) +$
$+\frac{5}{16}(|1_A 0_B\rangle\langle 1_A 0_B| - |1_A 0_B\rangle\langle 1_A 1_B| - |1_A 1_B\rangle\langle 1_A 0_B| + |1_A 1_B\rangle\langle 1_A 1_B|.$
Then,
$\tilde{\rho}_A = Tr_B\rho_{AB} = \langle 0_B|\rho_{AB}|0_B\rangle + \langle 1_B|\rho_{AB}|1_B\rangle.$
For example:
$\frac{3}{16}\langle 0_B|0_A 0_B\rangle\langle 0_A 0_B|0_B\rangle = \frac{3}{16}|0_A\rangle\langle 0_A|,$
$\langle 0_B|0_A 1_B\rangle\langle 0_A 0_B|0_B\rangle = 0$, since $\langle 0_B|1_B\rangle = 0,$
$\frac{5}{16}\langle 0_B|1_A 0_B\rangle\langle 1_A 0_B|0_B\rangle = \frac{5}{16}|1_A\rangle\langle 1_A|,$
$\frac{3}{16}\langle 1_B|0_A 1_B\rangle\langle 0_A 1_B|1_B\rangle = \frac{3}{16}|0_A\rangle\langle 0_A|,$
and
$\frac{5}{16}\langle 1_B|1_A 1_B\rangle\langle 1_A 1_B|1_B\rangle = \frac{5}{16}|1_A\rangle\langle 1_A|.$
So,
$\tilde{\rho}_A = Tr_B\rho_{AB} = \langle 0_B|\rho_{AB}|0_B\rangle + \langle 1_B|\rho_{AB}|1_B\rangle = \frac{3}{8}|0_A\rangle\langle 0_A| + \frac{5}{8}|1_A\rangle\langle 1_A|.$
Finally, $\tilde{\rho}_A$ in matrix representation
$\tilde{\rho}_A = \frac{3}{8}\begin{pmatrix}1\\0\end{pmatrix}(1\ \ 0) + \frac{5}{8}\begin{pmatrix}0\\1\end{pmatrix}(0\ \ 1) = \frac{3}{8}\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} + \frac{5}{8}\begin{pmatrix}0 & 0\\0 & 1\end{pmatrix} = \frac{1}{8}\begin{pmatrix}3 & 0\\0 & 5\end{pmatrix}.$

### 6.19.22 Practice with Dirac Language for Joint Systems

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$, and $\{|0_B\rangle, |1_B\rangle\}$.
Furthermore
$|0_A 0_B\rangle \equiv |0_A\rangle\otimes|0_B\rangle$, etc.
Consider the joint state
$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|0_A 0_B\rangle + |1_A 1_B\rangle).$
**a)** For this particular joint state, find the most general form of an observable $O^A$ acting only on the $A$ subsystem such that
$\langle\Psi_{AB}|O^A\otimes I^B|\Psi_{AB}\rangle = \langle\Psi_{AB}|(I^A\otimes P_0^B)O^A\otimes I^B(I^A\otimes P_0^B)|\Psi_{AB}\rangle,$
where
$P_0^B = |0_B\rangle\langle 0_B|.$
Note: here I used the usual notation for the basis vectors to prevent confusion with the operator $O^A$. Boccio used $0^B$ for the base vector in the projection operator.
$\langle\Psi_{AB}|O^A\otimes I^B|\Psi_{AB}\rangle = \langle\Psi_{AB}|(I^A\otimes P_0^B)O^A\otimes I^B(I^A\otimes P_0^B)|\Psi_{AB}\rangle =$
$= \langle\Psi_{AB}|I^A O^A I^A\otimes P_0^B I^B P_0^B|\Psi_{AB}\rangle = \langle\Psi_{AB}|O^A\otimes P_0^B P_0^B|\Psi_{AB}\rangle = \langle\Psi_{AB}|O^A\otimes P_0^B|\Psi_{AB}\rangle.$
Plug into this expression the ket and bra representation of $|\Psi_{AB}\rangle$:
$\langle\Psi_{AB}|O^A\otimes P_0^B|\Psi_{AB}\rangle = \frac{1}{2}(\langle 0_A 0_B| + \langle 1_A 1_B|)O^A\otimes P_0^B(|0_A 0_B\rangle + |1_A 1_B\rangle).$
Plug $P_0^B = |0_B\rangle\langle 0_B|$ into the preceding expression:
$\langle\Psi_{AB}|O^A\otimes P_0^B|\Psi_{AB}\rangle = \frac{1}{2}(\langle 0_A 0_B| + \langle 1_A 1_B|)O^A\otimes|0_B\rangle\langle 0_B|(|0_A 0_B\rangle + |1_A 1_B\rangle).$
Hence,

$\langle\Psi_{AB}|O^A \otimes I^B|\Psi_{AB}\rangle = \langle\Psi_{AB}|O^A \otimes P_0^B|\Psi_{AB}\rangle = \frac{1}{2}\langle 0_A|O^A|0_A\rangle$.

On the other hand we know:

$\langle\Psi_{AB}|O^A \otimes I^B|\Psi_{AB}\rangle = \frac{1}{2}(\langle 0_A 0_B| + \langle 1_A 1_B|)O^A \otimes I^B(|0_A 0_B\rangle + |1_A 1_B\rangle) =$

$= \frac{1}{2}(\langle 0_A|O^A|0_A\rangle + \frac{1}{2}\langle 1_A|O^A|1_A\rangle$.

So, we are missing $\langle 1_A|O^A|1_A\rangle$.

Knowing this we can finally formulate the most general form of an observable $O^A$ acting only on the $A$ subsystem. In general the observable for system $A$ with all the projection operators and eigenvalues is:

$O^A = \lambda_1|0_A\rangle\langle 0_A| + \lambda_2|0_A\rangle\langle 1_A| + \lambda_3|1_A\rangle\langle 0_A| + \lambda_4|1_A\rangle\langle 1_A|$.

Here $\lambda_1$ and $\lambda_4$ are real and $\lambda_2 = \lambda_3^*$.

Having calculated the nonexistence of $\langle 1_A|O^A|1_A\rangle \Longrightarrow \lambda_4 = 0$.

Consequently

$O^A = a|0_A\rangle\langle 0_A| + (b + ic)|0_A\rangle\langle 1_A| + (b - ic)\,|1_A\rangle\langle 0_A|$,

with $a, b, c \in \mathbb{R}$ .

**b)** Consider the specific operator

$X^A = |0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|$,

which satisfies the general form $O^A$ found under **a)**.

Note: Note: here I used the usual notation for the basis vectors to prevent confusion with the operators superscript.

Find the most general state vector $|\Psi'_{AB}\rangle$ such that

$\langle\Psi'_{AB}|X^A \otimes I^B|\Psi'_{AB}\rangle \neq \langle\Psi_{AB}|(I^A \otimes P_0^B)X^A \otimes I^B(I^A \otimes P_0^B)|\Psi_{AB}\rangle$.

The general form of a joint state factor is

$|\Psi'_{AB}\rangle = c_{00}|0_A 0_B\rangle + c_{01}|0_A 1_B\rangle + c_{10}|1_A 0_B\rangle + c_{11}|1_A 1_B\rangle$ .

Then

$X^A \otimes I^B\ |\Psi'_{AB}\rangle = c_{00}(|0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|)|0_A 0_B\rangle + c_{01}(|0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|)|0_A 1_B\rangle +$
$+ c_{10}(|0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|)|1_A 0_B\rangle + c_{11}(|0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|)|1_A 1_B\rangle$.

The term with $c_{00}$:

$c_{00}(|0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|)|0_A 0_B\rangle = c_{00}(|0_A\rangle\langle 1_A|0_A\rangle \otimes |0_B\rangle + |1_A\rangle\langle 0_A|0_A\rangle \otimes |0_B\rangle) =$
$= c_{00}|1_A\rangle \otimes |0_B\rangle = c_{00}|1_A 0_B\rangle$.

The term with $c_{01}$:

$c_{01}(|0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|)|0_A 1_B\rangle = c_{01}(|0_A\rangle\langle 1_A|0_A\rangle \otimes |1_B\rangle + |1_A\rangle\langle 0_A|0_A\rangle \otimes |1_B\rangle) =$
$= c_{01}|1_A\rangle \otimes |1_B\rangle = c_{01}|1_A 1_B\rangle$.

The term with $c_{10}$:

$c_{10}(|0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|)|1_A 0_B\rangle = c_{10}(|0_A\rangle\langle 1_A|1_A\rangle \otimes |0_B\rangle + |1_A\rangle\langle 0_A|1_A\rangle \otimes |0_B\rangle) =$
$= c_{10}|0_A\rangle \otimes |0_B\rangle = c_{10}|0_A 0_B\rangle$.

The term with $c_{11}$:

$c_{11}(|0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|)|1_A 1_B\rangle = c_{11}(|0_A\rangle\langle 1_A|1_A\rangle \otimes |1_B\rangle + |1_A\rangle\langle 0_A|1_A\rangle \otimes |1_B\rangle) =$
$c_{11}|0_A\rangle \otimes |0_B\rangle = c_{11}|0_A 1_B\rangle$.

Collecting all the terms

$X^A \otimes I^B\ |\Psi'_{AB}\rangle = c_{00}|1_A 0_B\rangle + c_{01}|1_A 1_B\rangle + c_{10}|0_A 0_B\rangle + c_{11}|0_A 1_B\rangle$.

Hence,

$\langle\Psi'_{AB}|X^A \otimes I^B|\Psi'_{AB}\rangle = (c_{00}^*\langle 0_A 0_B| + c_{01}^*\langle 0_A 1_B| + c_{10}^*\langle 1_A 0_B| + c_{11}^*\langle 1_A 1_B|)\cdot$
$\cdot (c_{00}|1_A 0_B\rangle + c_{01}|1_A 1_B\rangle + c_{10}|0_A 0_B\rangle + c_{11}|0_A 1_B\rangle)$.

A combination of inner products and tensor products. For example:

$c_{00}^* c_{00}\langle 0_A 0_B|1_A 0_B\rangle = c_{00}^* c_{00}\langle 0_A| \otimes \langle 0_B|1_A\rangle \otimes |0_B\rangle = c_{00}^* c_{00} \cdot 0 = 0$,

since $\langle 0_A|1_A\rangle = 0$, or using the double Kronecker delta symbol $\langle ab|cd\rangle = \delta_{ac}\delta_{bd}$.

Consequently
$\langle\Psi'_{AB}|X^A\otimes I^B|\Psi'_{AB}\rangle = c^*_{00}c_{10}\langle 0_A0_B|0_A0_B\rangle + c^*_{01}c_{11}\langle 0_A1_B|0_A1_B\rangle + c^*_{10}c_{00}\langle 1_A0_B|1_A0_B\rangle +$
$+c^*_{11}c_{01}\langle 1_A1_B|1_A1_B\rangle = c^*_{00}c_{10} + c^*_{01}c_{11} + c^*_{10}c_{00} + c^*_{11}c_{01}$.
By representing the complex coefficients $c^*_ic_j$ as complex numbers with a real and a imaginary part, it follows
$\langle\Psi'_{AB}|X^A\otimes I^B|\Psi'_{AB}\rangle = 2Re[c^*_{00}c_{10} + c^*_{01}c_{11}]$.
Now, let us calculated the projected form, with $P^B_0 = |0_B\rangle\langle 0_B|$,
$(I^A\otimes P^B_0)|\Psi'_{AB}\rangle = I^A\otimes|0_B\rangle\langle 0_B|(c_{00}|0_A0_B\rangle + c_{01}|0_A1_B\rangle + c_{10}|1_A0_B\rangle + c_{11}|1_A1_B\rangle) =$
$= c_{00}|0_A0_B\rangle + c_{10}|0_B1_A\rangle$.
Then, with $X^A = |0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|$,
$X^A\otimes I^B\ (I^A\otimes P^B_0)|\Psi'_{AB}\rangle = c_{00}(|0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|)|0_A0_B\rangle +$
$+c_{10}(|0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A|)|0_B1_A\rangle = c_{00}|1_A\rangle\otimes|0_B\rangle + c_{10}|0_A\rangle\otimes|0_B\rangle =$
$= (c_{00}|1_A\rangle + c_{10}|0_A\rangle)\otimes|0_B\rangle = c_{00}|1_A0_B\rangle + c_{10}|0_A0_B\rangle$.
So,
$\langle\Psi'_{AB}|X^A\otimes I^B\ (I^A\otimes P^B_0)|\Psi'_{AB}\rangle = (c^*_{00}\langle 0_A0_B| + c^*_{01}\langle 0_A1_B| + c^*_{10}\langle 1_A0_B| + c^*_{11}\langle 1_A1_B|)\cdot$
$\cdot(c_{00}|1_A0_B\rangle + c_{10}|0_A0_B\rangle)$.
Let us use $\langle ab|cd\rangle = \delta_{ac}\delta_{bd}$ for the preceding expression.
As an example:
$\langle 0_A0_B|1_A0_B\rangle = \delta_{ac}\delta_{bb} = 0$, etc.
This gives us:
$\langle\Psi'_{AB}|X^A\otimes I^B\ (I^A\otimes P^B_0)|\Psi'_{AB}\rangle = c^*_{00}c_{10} + c^*_{10}c_{00} = 2Rec^*_{00}c_{10}$.
Consequently
$\langle\Psi'_{AB}|X^A\otimes I^B|\Psi'_{AB}\rangle \neq \langle\Psi_{AB}|(I^A\otimes P^B_0)X^A\otimes I^B(I^A\otimes P^B_0)|\Psi_{AB}\rangle$.
**c)** Find an example of a reduced density matrix $\tilde{\rho}_A$ for the $A$ subsystem such that no joint state vector $|\Psi'_{AB}\rangle$ of the general form found under **b)** can satisfy:
$\tilde{\rho}_A = Tr_B(|\Psi'_{AB}\rangle\langle\Psi'_{AB}|)$.
The general form of a joint state factor is
$|\Psi'_{AB}\rangle = c_{00}|0_A0_B\rangle + c_{01}|0_A1_B\rangle + c_{10}|1_A0_B\rangle + c_{11}|1_A1_B\rangle$ .
$\langle\Psi'_{AB}| = c^*_{00}\langle 0_A0_B| + c^*_{01}\langle 0_A1_B| + c^*_{10}\langle 1_A0_B| + c^*_{11}\langle 1_A1_B|$ .
Under **b)** we obtained $2Rec^*_{00}c_{10} \neq 0$.
So,
$|\Psi'_{AB}\rangle\langle\Psi'_{AB}| = c_{00}|0_A0_B\rangle(c^*_{00}\langle 0_A0_B| + c^*_{01}\langle 0_A1_B| + c^*_{10}\langle 1_A0_B| + c^*_{11}\langle 1_A1_B|) +$
$+c_{01}|0_A1_B\rangle(c^*_{00}\langle 0_A0_B| + c^*_{01}\langle 0_A1_B| + c^*_{10}\langle 1_A0_B| + c^*_{11}\langle 1_A1_B|) +$
$+c_{10}|1_A0_B\rangle(c^*_{00}\langle 0_A0_B| + c^*_{01}\langle 0_A1_B| + c^*_{10}\langle 1_A0_B| + c^*_{11}\langle 1_A1_B|) +$
$+c_{11}|1_A1_B\rangle(c^*_{00}\langle 0_A0_B| + c^*_{01}\langle 0_A1_B| + c^*_{10}\langle 1_A0_B| + c^*_{11}\langle 1_A1_B|)$.
Reminder
$\tilde{\rho}_A = Tr_B(|\Psi'_{AB}\rangle\langle\Psi'_{AB}|) = \langle 0_B|\Psi'_{AB}\rangle\langle\Psi'_{AB}|0_B\rangle + \langle 1_B|\Psi'_{AB}\rangle\langle\Psi'_{AB}|1_B\rangle$.
Then to demonstrate this:
$\langle 0_B|c_{00}|0_A0_B\rangle c^*_{00}\langle 0_A0_B|0_B\rangle = c_{00}|0_A\rangle c^*_{00}\langle 0_A|$,
and
$\langle 1_B|c_{00}|0_A0_B\rangle c^*_{00}\langle 0_A0_B|1_B\rangle = 0$.
So, keeping in mind orthogonality and tensor product:
$\tilde{\rho}_A = Tr_B(|\Psi'_{AB}\rangle\langle\Psi'_{AB}|) = \langle 0_B|\Psi'_{AB}\rangle\langle\Psi'_{AB}|0_B\rangle + \langle 1_B|\Psi'_{AB}\rangle\langle\Psi'_{AB}|1_B\rangle =$
$= c_{00}|0_A\rangle(c^*_{00}\langle 0_A| + c^*_{10}\langle 1_A|) + c_{01}|0_A\rangle(c^*_{01}\langle 0_A| + c^*_{11}\langle 1_A|) +$
$+c_{10}|1_A\rangle(c^*_{00}\langle 0_A| + c^*_{10}\langle 1_A|) + c_{11}|1_A\rangle(c^*_{01}\langle 0_A| + c^*_{11}\langle 1_A|) =$
$= (|c_{00}|^2 + |c_{01}|^2)|0_A\rangle\langle 0_A| + (c_{00}c^*_{10} + c_{01}c^*_{11})|0_A\rangle\langle 1_A| +$
$+(c_{10}c^*_{00} + c_{11}c^*_{01})|1_A\rangle\langle 0_A| + (|c_{10}|^2 + |c_{11}|^2)|1_A\rangle\langle 1_A|$.

We have, with $\langle\Psi'_{AB}|\Psi'_{AB}\rangle = 1$,
$|c_{00}|^2 + |c_{01}|^2 + |c_{10}|^2 + |c_{11}|^2 = 1.$
Now the question: *"Find an example of a reduced density matrix $\tilde{\rho}_A$ for the $A$ subsystem such that no joint state vector $|\Psi'_{AB}\rangle$ of the general form found under **b)** can satisfy:*
$\tilde{\rho}_A = Tr_B(|\Psi'_{AB}\rangle\langle\Psi'_{AB}|)$.*"*
Choose the reduced density matrix to be:
$\tilde{\rho}_A = |0_A\rangle\langle 0_A|.$
Then,
$\tilde{\rho}_A = (|c_{00}|^2 + |c_{01}|^2)|0_A\rangle\langle 0_A| + (c_{00}c_{10}^* + c_{01}c_{11}^*)|0_A\rangle\langle 1_A| +$
$+(c_{10}c_{00}^* + c_{11}c_{01}^*)|1_A\rangle\langle 0_A| + (|c_{10}|^2 + |c_{11}|^2)|1_A\rangle\langle 1_A| = |0_A\rangle\langle 0_A|.$
Hence
$|c_{00}|^2 + |c_{01}|^2 = 1.$
However, with the result of normalization and $2Re c_{00}^* c_{10} \neq 0$
$|c_{00}|^2 + |c_{01}|^2 = 1 - |c_{10}|^2 - |c_{11}|^2 \Rightarrow |c_{00}|^2 + |c_{01}|^2 \leq 1 - |c_{11}|^2.$

### 6.19.23 More Mixed States

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be a pair of two-dimensional Hilbert spaces with given orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$, and $\{|0_B\rangle, |1_B\rangle\}$.
Furthermore
$|0_A 0_B\rangle \equiv |0_A\rangle \otimes |0_B\rangle$, etc.
Consider the joint state
$|\Psi_{AB}^0\rangle = \frac{1}{\sqrt{2}}(|0_A 0_B\rangle + |1_A 1_B\rangle).$
**a)** Suppose the $A$ and $B$ systems prepared in the state $|\Psi_{AB}^0\rangle$ and give them to a person, who then performs the following procedure. A biased coin is flipped with probability $p$ for heads; if the result of the coin-flip is a head the result of the result of the procedure performed is the state
$|\Psi_{ABp}^{out}\rangle = \frac{1}{\sqrt{2}}(|0_A 0_B\rangle - |1_A 1_B\rangle).$
If the result of the coin flip is a tail, probability $1-p$, the result of the procedure performed is the state
$|\Psi_{AB(1-p)}^{out}\rangle = \frac{1}{\sqrt{2}}(|0_A 0_B\rangle + |1_A 1_B\rangle),$
i.e. nothing happened. After this procedure, what is the density operator to be used to represent the knowledge of the joint state?
The resulting density matrix/operator $\rho_{AB}$ reads:
$\rho_{AB} = \frac{p}{2}|\Psi_{ABp}^{out}\rangle\langle\Psi_{ABp}^{out}| + \frac{1-p}{2}|\Psi_{AB(1-p)}^{out}\rangle\langle\Psi_{AB(1-p)}^{out}| =$
$= \frac{p}{2}(|0_A 0_B\rangle - |1_A 1_B\rangle)(\langle 0_A 0_B| - \langle 1_A 1_B|) + \frac{1-p}{2}(|0_A 0_B\rangle + |1_A 1_B\rangle)(\langle 0_A 0_B| + \langle 1_A 1_B|) =$
$= \frac{p}{2}(|0_A 0_B\rangle\langle 0_A 0_B| - |0_A 0_B\rangle\langle 1_A 1_B| - |1_A 1_B\rangle\langle 0_A 0_B| + |1_A 1_B\rangle\langle 1_A 1_B|) +$
$+ \frac{1-p}{2}(|0_A 0_B\rangle\langle 0_A 0_B| + |0_A 0_B\rangle\langle 1_A 1_B| + |1_A 1_B\rangle\langle 0_A 0_B| + |1_A 1_B\rangle\langle 1_A 1_B|) =$
$= -p(|0_A 0_B\rangle\langle 1_A 1_B| + |1_A 1_B\rangle\langle 0_A 0_B|) +$
$+ \frac{1}{2}(|0_A 0_B\rangle\langle 0_A 0_B| + |1_A 1_B\rangle\langle 1_A 1_B| + |0_A 0_B\rangle\langle 1_A 1_B| + |1_A 1_B\rangle\langle 0_A 0_B|) =$
$= \frac{1}{2}(|0_A 0_B\rangle\langle 0_A 0_B| + |1_A 1_B\rangle\langle 1_A 1_B|) + \frac{1-2p}{2}(|0_A 0_B\rangle\langle 1_A 1_B| + |1_A 1_B\rangle\langle 0_A 0_B|).$
**b)** Take the $A$ and $B$ systems prepared in the state $|\Psi_{AB}^0\rangle$ and perform the alternate procedure.
A measurement is made of the observable

$O = I^A \otimes U_h$,
where $U_h = |0_B\rangle\langle 0_B| - |1_B\rangle\langle 1_B|$,
and the result of the measurement cannot be known.
After this procedure, what density operator should represent the joint state.
Assume the projection postulate(reduction) for state conditioning(preparation) can be used.
The spectral decomposition of $O$:
$O = (+1)I^A \otimes |0_B\rangle\langle 0_B| + (-1)I^A \otimes |1_B\rangle\langle 1_B|$.
For value $+1$,
$I^A \otimes |0_B\rangle\langle 0_B|\Psi_{AB}^0\rangle = I^A \otimes |0_B\rangle\langle 0_B|\frac{1}{\sqrt{2}}(|0_A 0_B\rangle + |1_A 1_B\rangle) = \frac{1}{\sqrt{2}}|0_A 0_B\rangle$.
For the projection postulate, we need
$\sqrt{\langle\Psi_{AB}^0|(I^A \otimes |0_B\rangle)|\Psi_{AB}^0\rangle}$ .
Then, with $(I^A \otimes |0_B\rangle\langle 0_B)|\Psi_{AB}^0\rangle = \frac{1}{\sqrt{2}}|0_A 0_B\rangle$,

$$\sqrt{\langle\Psi_{AB}^0|(I^A \otimes |0_B\rangle\langle 0_B)|\Psi_{AB}^0\rangle} = \sqrt{\frac{1}{\sqrt{2}}(\langle 0_A 0_B| + \langle 1_A 1_B|)\frac{1}{\sqrt{2}}|0_A 0_B\rangle} = \frac{1}{\sqrt{2}}.$$

Hence,

$$\frac{I^A \otimes |0_B\rangle\langle 0_B|\Psi_{AB}^0\rangle}{\sqrt{\langle\Psi_{AB}^0|(I^A \otimes |0_B\rangle\langle 0_B)|\Psi_{AB}^0\rangle}} = |0_A 0_B\rangle.$$

For the value $-1$,
$I^A \otimes |1_B\rangle\langle 1_B|\Psi_{AB}^0\rangle = I^A \otimes |1_B\rangle\langle 1_B|\frac{1}{\sqrt{2}}(|0_A 0_B\rangle + |1_A 1_B\rangle) = \frac{1}{\sqrt{2}}|1_A 1_B\rangle$.
Furthermore

$$\sqrt{\langle\Psi_{AB}^0|(I^A \otimes |1_B\rangle\langle 1_B)|\Psi_{AB}^0\rangle} = \sqrt{\frac{1}{\sqrt{2}}(\langle 0_A 0_B| + \langle 1_A 1_B|)\frac{1}{\sqrt{2}}|1_A 1_B\rangle} = \frac{1}{\sqrt{2}}.$$

Hence,

$$\frac{I^A \otimes |1_B\rangle\langle 1_B|\Psi_{AB}^0\rangle}{\sqrt{\langle\Psi_{AB}^0|(I^A \otimes |1_B\rangle\langle 1_B)|\Psi_{AB}^0\rangle}} = |1_A 1_B\rangle.$$

Consequently
$\rho_{AB} = \frac{1}{2}|0_A 0_B\rangle\langle 0_A 0_B| + \frac{1}{2}|1_A 1_B\rangle\langle 1_A 1_B|$ .

### 6.19.24 Complete Sets of Commuting Observables

Consider a three dimensional Hilbert space $\mathcal{H}_3$ and the following set of operators:

$$O_\alpha \leftrightarrow \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ O_\beta \leftrightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ O_\gamma \leftrightarrow \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Find all possible complete sets of commuting observables(CSCO).
So, determine whether or not each of the sets {}
$\{O_\alpha\}, \{O_\beta\}, \{O_\gamma\}, \{O_\alpha, O_\beta\}, \{O_\alpha, O_\gamma\}, \{O_\beta, O_\gamma\}, \{O_\alpha, O_\beta, O_\gamma\}$
constitutes a valid CSCO.
Note: do not confuse {} with Poisson brackets.
It is about commutation:

- $[O_\alpha, O_\beta] = O_\alpha O_\beta - O_\beta O_\alpha = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} =$

$$= \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0 ,$$

- $[O_\alpha, O_\gamma] = O_\alpha O_\gamma - O_\gamma O_\alpha = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} =$

$= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \neq 0\,,$

- $[O_\beta, O_\gamma] = O_\beta O_\gamma - O_\gamma O_\beta = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} =$

$= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0\,.$

The possible CSCO's are
$\{O_\alpha\}, \{O_\beta\}, \{O_\gamma\}, \{O_\alpha, O_\beta\}, \{O_\beta, O_\gamma\}$.
What about the eigenvalues of the operators?
- $O_\alpha$ .

$$\begin{vmatrix} 1-\lambda & 1 & 0 \\ 1 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{vmatrix} = 0 \Leftrightarrow -\lambda[-\lambda(1-\lambda) - 1] = \lambda[\lambda(1-\lambda) + 1] = 0.$$

Hence
$\lambda = 0$ , and $\lambda(1-\lambda) + 1 = 0$.
The roots of $\lambda(1-\lambda) + 1 = 0$ are
$\lambda = \frac{1}{2} \pm \frac{1}{2}\sqrt{5}$ .
$\{O_\alpha\}$ has three distinct roots: 0, $\frac{1}{2} + \frac{1}{2}\sqrt{5}$, $\frac{1}{2} - \frac{1}{2}\sqrt{5}$ .
Then, $\{O_\alpha\}$ is a valid CSCO.
So, $\{O_\alpha, O_\beta\}$ is a valid CSCO.
The eigenvalue equation of $O_\beta$ and $O_\gamma$ is:
$-\lambda(1-\lambda)^2 = 0 \Longrightarrow \lambda = 0{,}1 \Longrightarrow$ one nondegenerate eigenvalue, $\lambda = 0$, and two degenerate eigenvalues $\lambda = 1$.
So,
$\{O_\beta\}$ and $\{O_\gamma\}$ are no valid CSCO's.
The commutator $\{O_\beta, O_\gamma\}$ has the same eigenvalues: 0,1, in this case with $\lambda = 0$ of two fold degeneracy.
Consequently $\{O_\alpha, O_\beta\}$ and $\{O_\alpha, O_\gamma\}$ are valid CSCO's.
With the eigenvalues of $O_\beta$ and $O_\gamma$, we can construct a basis vectors, with normalization and orthogonality:
$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.
Consequently $\{O_\beta, O_\gamma\}$ is valid CSCO's.

## 6.19.25 Conserved Quantum Numbers

Determine which of the CSCO's in problem 6.19.24 are conserved by the Schrödinger equation with the Hamiltonian

$$H = \varepsilon_o \begin{pmatrix} 2 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \varepsilon_o(\{O_\alpha\} + \{O_\beta\}),$$

where

$O_\alpha \leftrightarrow \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$, and $O_\beta \leftrightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$.

In general we have

$\frac{d}{dt}\langle O\rangle = -\frac{i}{\hbar}\langle [O,H]\rangle$.

Hence, when $\langle O\rangle$ is conserved $\langle O\rangle$ commutes with the Hamiltonian: $\frac{d}{dt}\langle O\rangle = 0$.

Now we need to establish;

- $[O_\alpha, H] = \varepsilon_o[O_\alpha, O_\alpha + O_\beta] = \varepsilon_o(\begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 2 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 2 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} =$

$= \varepsilon_o\begin{pmatrix} 3 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 3 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0,$

or , with the results of problem 6.19.24,

$[O_\alpha, H] = \varepsilon_o[O_\alpha, O_\alpha + O_\beta] = \varepsilon_o(O_\alpha O_\alpha + O_\alpha O_\beta - O_\alpha O_\alpha - O_\beta O_\alpha) = 0.$

- $[O_\beta, H] = \varepsilon_o[O_\beta, O_\alpha + O_\beta] = \varepsilon_o(O_\beta O_\alpha + O_\beta O_\beta - O_\alpha O_\beta - O_\beta O_\beta) = 0.$

- $[O_\gamma, H]$, with the results of problem 6.19.24,

$[O_\gamma, H] = \varepsilon_o[O_\gamma, O_\alpha + O_\beta] = \varepsilon_o[O_\gamma, O_\alpha] + \varepsilon_o[O_\gamma, O_\beta] \neq 0.$

Hence $\langle O_\gamma\rangle$, is not conserved.

Conclusion, the sets

$\{O_\alpha\}, \{O_\beta\}$, and $\{O_\alpha, O_\beta\}$ are conserved.

# 7. How Does It really works: Photons, K-Mesons and Stern-Gerlach

## 7.1 Introduction

Polarization explained, classically, i.e., wavelike behaviour and quantum mechanically, i.e., wavelike and particle like behaviour.

Boccio analysed the particle behaviour of light(photon) with help of the polarization experiment.

Note page 466: $vecp \Longrightarrow \bar{p}$ .

Use is made of the quantized energy of light.

Boccio made a remark to be remembered on page 469:

> In order for any theory to make clear predictions about experiments, we will have to learn how to ask very precise questions. We must also remember that only questions about the results of experiments have a real significance in physics and it is only such questions that theoretical physics must consider.

The experimental result on a single photon and a Polaroid is: *A single photon passes through the Polaroid or it does not*.

With this experiment the probabilistic point of view is introduced, page 470.

**Remark**: Dirac discussed the subject matter in chapter 1: *The Principle of Superposition.*

### 7.1.1 Photon Interference, page 472

In this section Boccio started with the well known two-slit experiment to visualize the process of interference. It is about position and momentum of properties of photons.

In this experiment, the only language to describe the measurement is the language of probabilities. Conservation of energy is key.
Then, Boccio formulated some basic questions, pages 474-
- Is it really necessary to introduce the new concept of superposition and jump?
- Will this new theory give us a better model of the photon and of single photon processes?
- What about determinism?
The discussion on these questions presents some basic ideas about quantum mechanics. Boccio concluded this section with a remark on hidden variables and the incompleteness of quantum mechanics.

## 7.2 Photon Polarization, page 477.

In Eq. (7.14), the polarization states of the photon is presented as a ket vector in column representation. The state vector contains all the information about the state of polarization. At the bottom of page 477, Boccio presented four examples of polarization and the state vectors representing these examples.
In Eqs.(7.21) and (7.22) the two-dimensional vector space of polarization states are presented in the basis vectors of the preceding examples.
The superposition principle is also illustrated by Eqs.(7.23)-(7.26).

### 7.2.1 How Many Basis Sets?

The first example shown by Boccio is the set based on the cartesian frame rotated over an angle $\theta$, Figure 7.1.
Note: Eq. (7.32)≡Eq.(7.25).
**Remark:**
Eq. (7.35) should read, the matrix notation
$$\begin{pmatrix}\langle x'|\psi\rangle\\ \langle y'|\psi\rangle\end{pmatrix}=\begin{pmatrix}\langle x'|x\rangle & \langle x'|y\rangle\\ \langle y'|x\rangle & \langle y'|y\rangle\end{pmatrix}\begin{pmatrix}\langle x|\psi\rangle\\ \langle y|\psi\rangle\end{pmatrix},$$
a typo.
In the Eqs. (7.37)-(7.42) the transformation matrix of a rotation in the $x$-$y$ frame is derived.
To understand Eq.(7.53), I assume the following with Eq. (7.52)
- $\hat{j}_z \equiv \hat{J}_z$,
- $\frac{1}{3!}(\frac{i\hat{J}_z}{\hbar})^3\theta^3 = -\frac{i}{3!}(\theta Q)^3$.
- $\sin\theta\hbar\hat{J}_z$ should read $\sin\theta\frac{\hat{J}_z}{\hbar}$.

The second line in Eq.(7.53) with "$rac\theta^3 3!$" Is not clear to me. The final result in the third line is.
In Eq.(7.56), I assume $\frac{i}{\hbar}\sin\theta\,\hat{J}_z$, to be read as $\frac{i}{\hbar}\hat{J}_z\sin\theta$.
Eq. (7.60) is obtained by using Eq.(7.57) twice.
Eq.(7.67) is found using Eq.(7.62).
Then, on page 485, Boccio presented *the standard way to do things in quantum mechanics.* Here, the effect of phase is shown. Not just an arbitrary thing but something that has real physical meaning.
Are we allowed to conclude:
$+\langle R|\hat{J}_z|L\rangle\langle R|\psi\rangle^*\langle L|\psi\rangle+\langle L|\hat{J}_z|R\rangle\langle L|\psi\rangle^*\langle R|\psi\rangle$ in Eq.(7.74) to be zero?
I suppose so, see also the matrix representation of $\hat{J}_z$ in Eq.(7.76).
The Pauli matrix pops up: Eq.(7.77).

### 7.2.2 Projection Operators

The subject matter of this section is projection operators and density operators.
In Eq.(7.80) the outer product, the basis for the projection operator is presented.
In Eq. (7.81) there are just two projection operators and the other two are outer products.
The trace of a projection operator is 1.

### 7.2.3 Amplitudes and Probabilities

An important note by Boccio: *The probability interpretation we have been making follows from the concept of superposition.*
Then, Boccio stated the fact an $x$-polarized photon never passes through a $y$-polaroid and discussed the related problem: a contradiction.
On page 489 under 4. Boccio writes: "*A simple calculation* ........".
Well, I realized that the left hand side of (7.90) is zero:
$\langle x|y\rangle = 0 = \langle y|R\rangle\langle R|x\rangle + \langle y|L\rangle\langle L|x\rangle \Longrightarrow \langle y|R\rangle\langle R|x\rangle = -\langle y|L\rangle\langle L|x\rangle.$
Then, i.e., under 3 of page 489, take the expression
$\langle y|R\rangle^*\langle R|x\rangle^*\langle y|L\rangle\langle L|x\rangle,$
and use $\langle y|R\rangle\langle R|x\rangle = -\langle y|L\rangle\langle L|x\rangle.$
we find
$\langle y|R\rangle^*\langle R|x\rangle^*\langle y|L\rangle\langle L|x\rangle = -\langle y|R\rangle^*\langle R|x\rangle^*\langle y|R\rangle\langle R|x\rangle = -|\langle R|x\rangle|^2|\langle y|R\rangle|^2.$
Hence, using $\langle x|y\rangle = 0$,
the *probability* under 3 page 489 is zero.
**Remark:**
On page 490, Boccio calculated $\langle y|x\rangle$ and did not mention this inner product of two orthonormal states to be zero. Is it too trivial?

### 7.2.4 Pure States, Unpure States and Density operators, page 492

Boccio recapitulate the expression for the expectation value of an operator in terms of the trace of the product of the operator and the density operator, Eq. (7.96).
Boccio use the basic set $\{|x\rangle, |y\rangle\}$.
First, the photon is in state $|x\rangle$.
In this analysis use is made of:
$\hat{I} = |x\rangle\langle x| + |y\rangle\langle y|.$
With Eqs. (7.95)-(7.98), and the preceding expression for $\hat{I}$,
it is proved $|x\rangle$ to be a pure state.
Next the photon is supposed to be in the state
$|\psi\rangle = \frac{1}{\sqrt{2}}|x\rangle + \frac{1}{\sqrt{2}}|y\rangle$, Eq.(7.99).
With Eqs. (7.100) and (7.101) it is proved $|\psi\rangle$ is a pure state since the density operator $\widehat{W}$ appears to be equal to the projection operator $|\psi\rangle\langle\psi|$.
Note: $\widehat{W}$ is found by assuming $\widehat{W} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, and $|x\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|y\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Plug this into Eq.(7.100) and Eq.(7.101) is obtained.
Furthermore, a more general state has been analysed
$|\psi\rangle = a|x\rangle + b|y\rangle$ , Eq.(7.102),
and
$|a|^2 = |b|^2 = \frac{1}{2},$
with ambiguity about the phase of $a$ and $b$.
To find out about $\langle\hat{A}\rangle$ use is made of the average over the relative phase:
$\int_0^{2\pi} e^{iz}\, dz = 0$, where $z$ is the relative phase.

This leads, using average of the relative phase, to the conclusion that $|\psi\rangle = a|x\rangle + b|y\rangle$ is a nonpure state with

$\hat{W} = |a|^2|x\rangle\langle x| + |b|^2|y\rangle\langle y|$.

### 7.2.5 Unpolarized Light

Boccio analysed an experiment with monochromatic light(photons) of two sources and which source any particular photon come from.

Conclusion of this section: *Unpolarized light has equal probability of being in any polarization state.*

### 7.2.6 How Does the Polarization State Vector Change?

In this section *devices are considered where all the photons get through no matter what their polarization state is, but during transit, the device changes the incident polarization in some way.*

Calcite is considered a crystal with preferred direction: the optic axis.

A orthonormal basis $\{|o\rangle, |e\rangle\}$ is chosen. Photons polarized perpendicular to the optic axis are in the state $|o\rangle$ . Photons polarized parallel to the optic axis are in state $|e\rangle$. Photons interacting with the crystal are written as superpositions of the aforementioned basis states.

Measuring device for the observable $\hat{Q}$ is used. The eigenvectors of $\hat{Q}$ are the basis for all states.

I suppose Eq. (7.108) should read

$k = \frac{2\pi}{\lambda} - \frac{n\omega}{c}$ .

The phase in Eq.(7.107) depends on the index of refraction. Passing through the crystal means the relative phase of the set $\{|o\rangle, |e\rangle\}$ changes.

The initial state of the photon is given in Eq.(7.109).

The two basis states have different indices of refraction.

In Eq.(7.110) the state upon leaving the crystal is presented with a time development operator $\hat{U}_z$, Eq.(7.111).

Then, Boccio defined two new quantities to be remembered:

- a transition amplitude,
- the corresponding transition probability.

Next, Boccio started to further analyse the time development operator, page 497.

Notice in Eq.(7.113), expressions like

$e^{ik_e\epsilon}|e\rangle\langle e|e^{ik_o\epsilon}|o\rangle\langle o|$,

do not contribute.

Eq.(7.115) is obtained with Eq.(7.112).

Boccio obtained a differential equation, Eq.(7.112), similar to the differential equation from the time devilment operator. Remember the Schrödinger equation.

With Eq.(7.123), the representation of the identity operator is used again:

$\hat{I} = |x\rangle\langle x| + |y\rangle\langle y|$.

Then, Boccio showed the operator $\hat{K}$ to be Hermitian.

**Remark:**

With Eqs.(7.115) and (7.116), we can write

$|\psi_{z+\epsilon}\rangle = \hat{U}_\epsilon|\psi_z\rangle \Longrightarrow (\hat{I} + i\epsilon\hat{K})|\psi_z\rangle$.

Furthermore

$\langle\psi_{z+\epsilon}|\psi_{z+\epsilon}\rangle = \langle\psi_z|\hat{U}_\epsilon{}^*\hat{U}_\epsilon|\psi_z\rangle$.

To order $\epsilon$:

$\left(\hat{I} + i\epsilon\hat{K}\right)^*\left(\hat{I} + i\epsilon\hat{K}\right) = \hat{I} + i\epsilon\hat{I}\hat{K} - i\epsilon\hat{K}^*$.

Then,
$\langle\psi_z|(\hat{I} + i\epsilon\hat{I}\hat{K} - i\epsilon I\hat{K}^*)|\psi_z\rangle = \langle\psi_z|\psi_z\rangle + i\epsilon\langle\psi_z|\hat{I}\hat{K}|\psi_z\rangle - i\epsilon\langle\psi_z|I\hat{K}^*|\psi_z\rangle =$
$= \langle\psi_z|\psi_z\rangle + i\epsilon\langle\psi_z|\hat{K}|x\rangle\langle x|\psi_z\rangle + i\epsilon\langle\psi_z|\hat{K}|y\rangle\langle y|\psi_z\rangle - i\epsilon\langle\psi_z|\hat{K}^*|x\rangle\langle x|\psi_z\rangle +$
$-i\epsilon\langle\psi_z|\hat{K}^*|y\rangle\langle y|\psi_z\rangle.$
Hence, with $\langle\psi_{z+\epsilon}|\psi_{z+\epsilon}\rangle = \langle\psi_z|\psi_z\rangle$ , Eq.(7.114), it follows
$\langle\psi_z|\hat{K}|x\rangle - \langle\psi_z|\hat{K}^*|x\rangle = 0,$
or
$\langle\psi_z|\hat{K} - \hat{K}^*|x\rangle = 0 \Longrightarrow \hat{K} = \hat{K}^* \Longrightarrow \hat{K}$ is Hermitian.
Note: $\hat{K}^* \Longrightarrow \hat{K}^\dagger$.
$\hat{U}_z$ a unitary operator:
Eq.(7.111):
$\hat{U}_z = e^{ik_e z}|e\rangle\langle e| + e^{ik_o z}|o\rangle\langle o|.$
Eq.(7.117):
$\hat{I} = |e\rangle\langle e| + |o\rangle\langle o|.$
Then, orthogonality
$\hat{U}_z^\dagger\hat{U}_z = \left(e^{-ik_e z}|e\rangle\langle e| + e^{-ik_o z}|o\rangle\langle o|\right)\left(e^{ik_e z}|e\rangle\langle e| + e^{ik_o z}|o\rangle\langle o|\right) =$
$= |e\rangle\langle e| + |o\rangle\langle o| = \hat{I}.$

### 7.2.7 Calculating the Transition Probability, page 498

At the bottom of page 496 the transition probability has been defined. And presented in Eq.(7.126).
Boccio demonstrated the transition probability for the problem of a photon entering the calcite crystal as an LCP photon. LCP: Left-Circularly-Polarized.

### 7.2.8 Some More Bayesian Thoughts, page 499

This section is about retrodiction: the outcomes of a test are known and then it is about to guess the initial state. So, the opposite of forecasting.
Boccio presented an experimental setup in Figure 7.2, page 500, the inverse probability problem. This situation is ideal for using Bayesian methods, see Chapter 5.
In Eq.(7.134), Baye's theorem is presented.
Note:
Eq.(7.137) should read $P(B) = \sum_j P(B|A_j)P(A_j)$.
This is about the principle of indifference or insufficient reasoning.
The results of the example are illustrated in Figure 7.3.

## 7.3 The Strange world of Neutral K-Mesons, page 503

The formalism as developed for photon polarization can be used to study K-mesons.
Note:
near the bottom of page 503, the sentence on $K^0$mesons should read: *"For the $K^0$, the antiparticle is called $\bar{K}^0. The\ \bar{K}^0$-mesons have a strangeness equal to $-1$."*
On page 504 Boccio introduced a basis for the 2-dimensional vector space $\{|K^0\rangle, |\bar{K}^0\rangle\}$.
In the Eqs.(7.144)-(7.148) the strangeness operator and charge conjugation.
The similarity with polarization is demonstrated.
Then, Boccio presented the standard approach, 4 steps, for studying physical systems using quantum mechanics. This standard approach is similar to the recipe presented by Susskind page 124-125. The point here is to derive or guess an appropriate Hamiltonian. Susskind presented an additional possibility: steal the Hamiltonian.

In Eq.(7.154) the most general form of the Hamiltonian is constructed from all the relevant operators. This is a matrix in the $\{|K^0\rangle, |\bar{K}^0\rangle\}$ basis. The consequences of the assumption of the Hamiltonian is analysed in 4 steps. These latter 4 steps are related with the 4 steps of the standard approach.

**Step 1** Investigate the commutators.

For example, with Eqs.(7.145) and (7.154),

$$[\hat{H},\hat{S}] = \hat{H}\hat{S} - \hat{S}\hat{H} = \begin{pmatrix} M+B & A \\ A & M-B \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} M+B & A \\ A & M-B \end{pmatrix} =$$

$$= \begin{pmatrix} M+B & -A \\ A & -M+B \end{pmatrix} - \begin{pmatrix} M+B & A \\ -A & -M+B \end{pmatrix} = \begin{pmatrix} 0 & -2A \\ 2A & 0 \end{pmatrix}.$$

Hence

$$[\hat{H},\hat{S}] \neq 0.$$

**Step 2** Investigate special cases

- $A = 0$.

Then, using what we found under step 1,

$$[\hat{H},\hat{S}] = 0.$$

Boccio underlined the following: $\hat{H}$ and $\hat{S}$ share common eigenvectors for this case.

What about $[\hat{H},\hat{C}]$? With Eqs.(7.147) and (7.154)

$$[\hat{H},\hat{C}] = \begin{pmatrix} M+B & 0 \\ 0 & M-B \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} M+B & 0 \\ 0 & M-B \end{pmatrix} =$$

$$= \begin{pmatrix} 0 & M+B \\ M-B & 0 \end{pmatrix} - \begin{pmatrix} 0 & M-B \\ M+B & 0 \end{pmatrix} = \begin{pmatrix} 0 & 2B \\ -2B & 0 \end{pmatrix}.$$

Hence

$$[\hat{H},\hat{C}] \neq 0.$$

- $B = 0$.

$$[\hat{H},\hat{C}] = \begin{pmatrix} M & A \\ A & M \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} M & A \\ A & M \end{pmatrix} = \begin{pmatrix} A & M \\ M & A \end{pmatrix} - \begin{pmatrix} A & M \\ M & A \end{pmatrix} = 0.$$

Hence

$$[\hat{H},\hat{C}] = 0.$$

Reminder:

- the eigenvalues of $\hat{C}$ are $\pm 1$,
- the eigenvectors are Eqs.(7.151) - (7.153), page 505

$$+1: |K_S\rangle = \tfrac{1}{\sqrt{2}}(|K^0\rangle + |\bar{K}^0\rangle),$$

$$-1: |K_L\rangle = \tfrac{1}{\sqrt{2}}(|K^0\rangle - |\bar{K}^0\rangle).$$

Note: $|K_S\rangle \equiv |K^S\rangle$, and $|K_L\rangle \equiv |K^L\rangle$. Why? The subscript is used in Eq.(7.164).

As mentioned by Boccio, $\hat{H}$ and $\hat{C}$ share a common set of eigenvectors.

The eigenvalues of $\hat{H}$:

$$\begin{vmatrix} M-\lambda & A \\ A & M-\lambda \end{vmatrix} = 0 \Rightarrow (M-\lambda)^2 = A^2 \Rightarrow \lambda = M \pm A, \text{ Eq. (7.167).}$$

Eq.(7.164), with Eq.(7.153),

$$\hat{H}\,|K_S\rangle = M\hat{I}|K_S\rangle + A\hat{C}\,|K_S\rangle = M\,|K_S\rangle + A\,|K_S\rangle = (M+A)|K_S\rangle,$$

$$\hat{H}\,|K_L\rangle = M\hat{I}|K_L\rangle + A\hat{C}\,|K_L\rangle = M\,|K_L\rangle - A\,|K_L\rangle = (M-A)|K_S\rangle.$$

The eigenvalues are obtained.

The diagonalized Hamiltonian operator becomes:

$$\hat{H} = \begin{pmatrix} M+A & 0 \\ 0 & M-A \end{pmatrix}, \text{ Eq.(7.165).}$$

Boccio presented in Eq. (7.169) the time dependent state vector.

**Step 3**

Solve the general Hamiltonian problem.

The general Hamiltonian is given in Eq.(7.154), and presented here Eq.(7.170).

The eigenvector equation is written as:

$\hat{H}|\phi\rangle = E|\phi\rangle$.

With Eqs.(7.170)-(7.175), the energy eigenvalues $E_{\pm}$ are obtained.

Note: Eq. (7.174) should read:

$$\begin{vmatrix} M+B-E & A \\ A & M-B-E \end{vmatrix} = 0 \Longrightarrow \begin{vmatrix} (M-E)+B & A \\ A & (M-E)-B \end{vmatrix} = 0 \Longrightarrow$$

$\Longrightarrow (M-E)^2 - B^2 = A^2 \Longrightarrow$ Eq.(7.175).

The eigen vector in column vector representation:

$|\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$, Eq.(1.171).

Expressions for the elements of this column vector can be found by substituting the eigenvalues $E_{\pm}$ into the eigenvalue equation, Eq.(7.176).

The ratio of the elements of the eigenvector are given in Eq.(7.177).

Note: this equation should read:

$\phi_{1+} = \frac{-A}{M+B-E_{\pm}} = \frac{-A}{B+\sqrt{A^2+B^2}}\phi_{2+} = \frac{B+\sqrt{A^2+B^2}}{A}\phi_{2+}$ ,

and

$\phi_{1-} = \frac{-A}{M+B-E_{-}} = \frac{-A}{B-\sqrt{A^2+B^2}}\phi_{2-} = \frac{B-\sqrt{A^2+B^2}}{A}\phi_{2-}$.

Applying normalization

$\phi_{1\pm}^2 + \phi_{2\pm}^2 = 1$,

results in the elements of the eigenvector expressed in $A$ and $B$.

The results of normalization is presented in Eqs.(7.183)-(7.185)

Next, Boccio analysed the effect of the special cases on the elements of the eigenvector:

- $B = 0 \Longrightarrow$ Eq.(7.179).
- $A = 0 \Longrightarrow$ Eq.(7.181).

**Step 4**

A realistic physical system is considered.

In this case $B \ll A$.

Boccio mentioned *in this case the states* $\{|K_S\rangle, |K_L\rangle\}$ *to be almost energy eigenstates*, Eqs.(7.168)-(7.169).

In Eq.(7.186) Boccio presented the approximation of $B \approx 0$ .The small quantity $\theta$ is defined as

$\theta = \frac{B}{A} = 2\delta$ , Eq.(7.188).

Boccio presented the experimental results for $B = 0$ .In this case charge conjugation is conserved.

Next, Boccio investigated Quantum Interference Effects in the K-meson system.

In Eq.(7.200) use has been made of Eqs.(7.151)-(7.152):

$\langle \bar{K}^0 | K_S \rangle = \frac{1}{\sqrt{2}}$, and $\langle \bar{K}^0 | K_L \rangle = \frac{1}{\sqrt{2}}$.
At the end of this section 7.3, Boccio explained the physics.

## 7.4 Stern-Gerlach Experiments and Measurement, page 512

See *The Feynman Lectures on Physics*, Vol. II, Chapter 35 *Paramagnetism and Magnetic Resonance.*
Boccio investigated the angular momentum component of a spin-1/2 particle.
This is done in a series of experiments. Some of the experiment are described by Susskind in section 3 of chapter 1.
Experiment 1: This experiment is about state preparation.
Experiment 2: This experiment is about randomize a state.
Experiment 3: This experiment shows once more randomizing a state.

Note about this experiment. Boccio: “We also block the $| +\hat{x}\rangle$ ….”.
What I learned from Figure 7 is $| -\hat{x}\rangle$ to be blocked.

Deriving the quantum mechanical expression for $P(\downarrow_z \mid \uparrow_z)$
middle of page 518, use has been made of
$\hat{I} = |\uparrow_x\rangle\langle\uparrow_x| + |\downarrow_x\rangle\langle\downarrow_x|$.
**What constitutes an experiment?**⟹A measurement is something that removes coherence.
Experiment 4: This experiment is about coherence. See Figure 7.8, page 519.
Experiment 5: This experiment is about confirming the result of Experiment 4.
Experiment 6: This experiment is again about randomize a state.

Note: “*The incoming beam is from the first SG$\hat{z}$ device, where we blocked the $| -\hat{\mathbf{z}}\rangle$ path, and therefore, we have $N$ particles in the state $| +\hat{\mathbf{z}}\rangle$.” In experiment 1: “$N$ particles into a SG$\hat{z}$ device and select out the beam where the particles are in the state $| +\hat{\mathbf{z}}\rangle$ (we block the other beam) It contains $N/2$ particles.”* Well, I miss a factor 1/2 .

In Chapter 79 Boccio will discuss the results of section 7.4 more rigorously.

## 7.5 Problems, page 523

### 7.5.1 Change the Basis, page 523

In examining light polarization light polarization in the text, we have been working in the $\{|x\rangle, |y\rangle\}$ basis.
**a)** Just to show how easy it is to work in other bases, express $\{|x\rangle, |y\rangle\}$, in the $\{|R\rangle, |L\rangle\}$, and $\left\{\left|\frac{\pi}{4}\right\rangle, \left|\frac{3\pi}{4}\right\rangle\right\}$, bases. See pages 466-468 and page 477 of the Course.
In the text: Two standard sets of orthonormal polarization vectors are often chosen when one discusses polarization. One of the two sets is

$$\hat{e}_x = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \hat{e}_y = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \text{ Eq.(7.3)}, \Longrightarrow \{|x\rangle, |y\rangle\} \text{ basis.}$$

- $\{|x\rangle, |y\rangle\}$ basis:

$|x\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \longrightarrow$ linear polarized photon

$|y\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \longrightarrow$ linear polarized photon

- $\{|R\rangle, |L\rangle\}$ basis:
$|R\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} \longrightarrow$ right circular polarized
$|L\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} \longrightarrow$ left circular polarized
Then,
$\{|R\rangle, |L\rangle\}$ expressed in the $\{|x\rangle, |y\rangle\}$ basis:
$|R\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix} + i\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}(|x\rangle + i|y\rangle),$
and
$|L\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix} - i\begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}(|x\rangle - i|y\rangle).$
Inverting:
$|R\rangle + |L\rangle = \frac{2}{\sqrt{2}}|x\rangle \Leftrightarrow |x\rangle = \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle).$
On the other hand:
$|x\rangle = \alpha_1|R\rangle + \alpha_2|L\rangle \Longrightarrow \langle R|x\rangle = \alpha_1\langle R|R\rangle + \alpha_2\langle R|L\rangle = \alpha_1,$
and similarly
$\langle L|x\rangle = \alpha_1\langle L|R\rangle + \alpha_2\langle L|L\rangle = \alpha_2.$
So, with $|x\rangle = \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle)$
$|x\rangle = \langle R|x\rangle|R\rangle + \langle L|x\rangle|L\rangle = \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle).$
Now, the complex conjugate of
$|R\rangle = \frac{1}{\sqrt{2}}(|x\rangle + i|y\rangle) \Longrightarrow \langle R| = \frac{1}{\sqrt{2}}(\langle x| - i\langle y|) \Longrightarrow \langle R|x\rangle = \frac{1}{\sqrt{2}}(\langle x|x\rangle - i\langle y|x\rangle) = \frac{1}{\sqrt{2}},$
$|L\rangle = \frac{1}{\sqrt{2}}(|x\rangle - i|y\rangle) \Longrightarrow \langle L| = \frac{1}{\sqrt{2}}(\langle x| + i\langle y|) \Longrightarrow \langle L|x\rangle = \frac{1}{\sqrt{2}}(\langle x|x\rangle + i\langle y|x\rangle) = \frac{1}{\sqrt{2}}.$
The expression for $|y\rangle$
$|R\rangle - \ |L\rangle = \frac{2i}{\sqrt{2}}|y\rangle \Leftrightarrow |y\rangle = \frac{i}{\sqrt{2}}(-|R\rangle + |L\rangle).$
On the other hand
$|y\rangle = \beta_1|R\rangle + \beta_2|L\rangle \Longrightarrow \langle R|y\rangle = \beta_1\langle R|R\rangle + \beta_2\langle R|L\rangle = \beta_1,$
and similarly
$\langle L|y\rangle = \beta_1\langle L|R\rangle + \beta_2\langle L|L\rangle = \beta_2.$
So, with $|y\rangle = \frac{i}{\sqrt{2}}(-|R\rangle + |L\rangle)$
$|y\rangle = \langle R|y\rangle|R\rangle + \langle L|y\rangle|L\rangle = \frac{i}{\sqrt{2}}(-|R\rangle + |L\rangle).$
Now, the complex conjugate of
$|R\rangle = \frac{1}{\sqrt{2}}(|x\rangle + i|y\rangle) \Longrightarrow \langle R| = \frac{1}{\sqrt{2}}(\langle x| - i\langle y|) \Longrightarrow \langle R|y\rangle = \frac{1}{\sqrt{2}}(\langle x|y\rangle - i\langle y|y\rangle) = -\frac{i}{\sqrt{2}},$
$|L\rangle = \frac{1}{\sqrt{2}}(|x\rangle - i|y\rangle) \Longrightarrow \langle L| = \frac{1}{\sqrt{2}}(\langle x| + i\langle y|) \Longrightarrow \langle L|y\rangle = \frac{1}{\sqrt{2}}(\langle x|y\rangle + i\langle y|y\rangle) = \frac{i}{\sqrt{2}}.$
- $\left\{\left|\frac{\pi}{4}\right\rangle, \left|\frac{3\pi}{4}\right\rangle\right\}$:
$\left|\frac{\pi}{4}\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \longrightarrow$ linear polarized photon at $\frac{\pi}{4}$ to the x-axis
$\left|\frac{3\pi}{4}\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \longrightarrow$ linear polarized photon at $\frac{3\pi}{4}$ to the x-axis
$\left\{\left|\frac{\pi}{4}\right\rangle, \left|\frac{3\pi}{4}\right\rangle\right\}$ expressed in the $\{|x\rangle, |y\rangle\}$ basis:
$\left|\frac{\pi}{4}\right\rangle = \frac{1}{\sqrt{2}}(|x\rangle + |y\rangle),$
$\left|\frac{3\pi}{4}\right\rangle = \frac{1}{\sqrt{2}}(|x\rangle - |y\rangle).$

Then $|x\rangle$ and $|y\rangle$ expressed in the $\left\{|\frac{\pi}{4}\right\rangle, |\left.\frac{3\pi}{4}\right\rangle\}$ basis

$$|\tfrac{\pi}{4}\rangle + |\tfrac{3\pi}{4}\rangle = \tfrac{2}{\sqrt{2}}|x\rangle \Leftrightarrow |x\rangle = \tfrac{1}{\sqrt{2}}\left(|\tfrac{\pi}{4}\rangle + |\tfrac{3\pi}{4}\rangle\right),$$

$$|\tfrac{\pi}{4}\rangle - |\tfrac{3\pi}{4}\rangle = \tfrac{2}{\sqrt{2}}|x\rangle \Leftrightarrow |y\rangle = \tfrac{1}{\sqrt{2}}\left(|\tfrac{\pi}{4}\rangle - |\tfrac{3\pi}{4}\rangle\right).$$

Furthermore, completely similarly to the analysis of the $\{|R\rangle, |L\rangle\}$ basis, we have

$$|x\rangle = \left\langle\tfrac{\pi}{4}\middle|x\right\rangle|\tfrac{\pi}{4}\rangle + \left\langle\tfrac{3\pi}{4}\middle|x\right\rangle|\tfrac{3\pi}{4}\rangle = \tfrac{1}{\sqrt{2}}\left(|\tfrac{\pi}{4}\rangle + |\tfrac{3\pi}{4}\rangle\right),$$

and

$$|y\rangle = \left\langle\tfrac{\pi}{4}\middle|y\right\rangle|\tfrac{\pi}{4}\rangle + \left\langle\tfrac{3\pi}{4}\middle|y\right\rangle|\tfrac{3\pi}{4}\rangle = \tfrac{1}{\sqrt{2}}\left(|\tfrac{\pi}{4}\rangle - |\tfrac{3\pi}{4}\rangle\right).$$

**b)** If you are working in the $\{|R\rangle, |L\rangle\}$ basis, what would the operator representing a vertical polaroid look like?

We know

$$\hat{P}_{vert} = \hat{P}_y = |y\rangle\langle y|.$$

In the $\{|R\rangle, |L\rangle\}$ basis, the matrix representation of $\hat{P}_y$ reads

$$\hat{P}_y = \begin{pmatrix} \langle R|y\rangle\langle y|R\rangle & \langle R|y\rangle\langle y|L\rangle \\ \langle L|y\rangle\langle y|R\rangle & \langle L|y\rangle\langle y|L\rangle \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

On the other hand, Boccio,

$$\hat{P}_{vert} = \hat{P}_y = |y\rangle\langle y| = [\tfrac{i}{\sqrt{2}}(-|R\rangle + |L\rangle)]\left[\tfrac{-i}{\sqrt{2}}(-\langle R| + \langle L|)\right] =$$

$$= \tfrac{1}{2}(|R\rangle\langle R| - |R\rangle\langle L| - |L\rangle\langle R| + |L\rangle\langle L|) =$$

$$= \tfrac{1}{2}[\tfrac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} - \tfrac{1}{2}\begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} - \tfrac{1}{2}\begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} + \tfrac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}(0 \ \ 1) = |y\rangle\langle y|.$$

Now what?

### 7.5.2 Polaroids, page 523

Imagine a situation in which a photon in the $|x\rangle$ state strikes a vertically oriented polaroid. Clearly the probability of the photon getting through the vertically oriented polaroid is 0.

- Now consider the case of two polaroid's with the photon in the $|x\rangle$ state striking a polaroid oriented at $\frac{\pi}{4}$, and then striking a vertically oriented polaroid.

Show that the probability of the photon getting through both polaroid's is 1/4 .

As a base we use $\{|x\rangle, |y\rangle\}$.

For the state $|\theta\rangle$ of the photon polarized at an angle $\theta$ we have in the $\{|x\rangle, |y\rangle\}$ basis:

$$|\theta\rangle = \cos\theta\,|x\rangle + \sin\theta\,|y\rangle.$$

So,

$$|\pi/4\rangle = \tfrac{1}{\sqrt{2}}|x\rangle + \tfrac{1}{\sqrt{2}}|y\rangle.$$

Consequently

$$P\left(x \to \tfrac{\pi}{4} \to y\right) = |\left\langle y\middle|\tfrac{\pi}{4}\right\rangle\left\langle\tfrac{\pi}{4}\middle|x\right\rangle|^2 = (\tfrac{1}{\sqrt{2}}\cdot\tfrac{1}{\sqrt{2}})^2 = \tfrac{1}{4}.$$

- Consider now the case of three polaroid's with the photon in the $|x\rangle$ state strikes a polaroid oriented at $\frac{\pi}{6}$ first, then a polaroid at $\frac{\pi}{3}$, and finally a vertically oriented polaroid.

The probability of the photon getting through?

We have two new states:

$$|\pi/6\rangle = \tfrac{\sqrt{3}}{2}|x\rangle + \tfrac{1}{2}|y\rangle,$$

and

$$|\pi/3\rangle = \tfrac{1}{2}|x\rangle + \tfrac{\sqrt{3}}{2}|y\rangle.$$

Consequently

$P\left(x \to \frac{\pi}{6} \to \frac{\pi}{3} \to y\right) = |\left\langle y \middle| \frac{\pi}{3}\right\rangle \left\langle \frac{\pi}{3} \middle| \frac{\pi}{6}\right\rangle \left\langle \frac{\pi}{6} \middle| x\right\rangle|^2 = (\frac{\sqrt{3}}{2}\frac{\sqrt{3}}{2}\frac{\sqrt{3}}{2})^2 = \frac{27}{64}$,

with, i.e.,

$\left\langle \frac{\pi}{3} \middle| \frac{\pi}{6}\right\rangle = \left(\frac{1}{2}\langle x| + \frac{\sqrt{3}}{2}\langle y|\right)\left(\frac{\sqrt{3}}{2}|x\rangle + \frac{1}{2}|y\rangle\right) = \frac{\sqrt{3}}{4}\langle x|x\rangle + \frac{1}{4}\langle x|y\rangle + \frac{3}{4}\langle y|x\rangle + \frac{\sqrt{3}}{4}\langle y|y\rangle =$

$= \frac{\sqrt{3}}{4}\langle x|x\rangle + \frac{\sqrt{3}}{4}\langle y|y\rangle = \frac{\sqrt{3}}{2}$.

### 7.5.3 Calcite Crystal

A photon polarized at an angle $\theta$ to the optic axis is sent through a slab of calcite crystal. Assume the thickness of the slab to be $10^{-2}$ cm, the direction of the photon propagation is the $z$-axis and the and the optic axis lies in the $x$-$y$ plane.

Calculate, as a function of $\theta$, the transition probability for the photon left circular polarized. Let the frequency of the light be given by $\frac{c}{\omega} = 5000\text{Å}$, and let $n_e = 1.50$, and $n_o = 1.65$, for the calcite indices of refraction.

Course page 495: "*Photons polarized perpendicular to the optic axis are called ordinary and are in the state $|o\rangle$, and photons polarized parallel to the optic axis are called extraordinary and are in the state $|e\rangle$. The set $\{|o\rangle, |e\rangle\}$, forms an orthonormal basis and general photon states interacting with a calcite crystal are written as superpositions of these basis states.*"

Furthermore, see page 496 of the Course.

Now, with Eq.(7.109):

$|in\rangle = \langle e|in\rangle|in\rangle + \langle o|in\rangle|o\rangle$.

*The two components of this state have different indices of refraction $n_e$ and $n_o$.*

$|in\rangle = \cos\theta\,|o\rangle + \sin\theta\,|e\rangle$ .

Using the time evolution operator $\hat{T}$, Eq.(7.111)

$|out\rangle = \hat{T}|in\rangle = (e^{ik_o l}|o\rangle\langle o| + e^{ik_e l}|e\rangle\langle e|)|in\rangle$.

The photon being left circular polarized, Eq.(7.127)

$|final\rangle = |L\rangle = \frac{1}{\sqrt{2}}(|o\rangle - i|e\rangle)$.

Note : compare this with Eq.(7.129) for a RCP photon, $|R\rangle$ state, page 499.

The probability $P$ of emerging in the $|L\rangle$ state, the left circularized state,

$P = |\langle L|out\rangle|^2$.

$|out\rangle = \hat{T}|in\rangle = (e^{ik_o l}|o\rangle\langle o| + e^{ik_e l}|e\rangle\langle e|)|in\rangle =$

$= \left(e^{ik_o l}|o\rangle\langle o| + e^{ik_e l}|e\rangle\langle e|\right)(\cos\theta\,|o\rangle + \sin\theta\,|e\rangle) = \cos\theta\, e^{ik_o l}|o\rangle + \sin\theta\, e^{ik_e l}|e\rangle$.

Then,

$\langle L|out\rangle = \frac{1}{\sqrt{2}}(\langle o| + i\langle e|)\left(\cos\theta\, e^{ik_o l}|o\rangle + \sin\theta\, e^{ik_e l}|e\rangle\right) =$

$= \frac{1}{\sqrt{2}}(\cos\theta\, e^{ik_o l} + i\sin\theta\, e^{ik_e l})$.

Hence

$P = |\langle L|out\rangle|^2 = \frac{1}{2}\left(\cos\theta\, e^{-ik_o l} - i\sin\theta\, e^{-ik_e l}\right)\left(\cos\theta\, e^{ik_o l} + i\sin\theta\, e^{ik_e l}\right) =$

$= \frac{1}{2}[1 + \sin 2\theta \sin(k_0 - k_e)l$ .

With the numerical values, we can calculate $(k_0 - k_e)l$ >

Given $1\text{Å} = 10^{-8}$ cm:

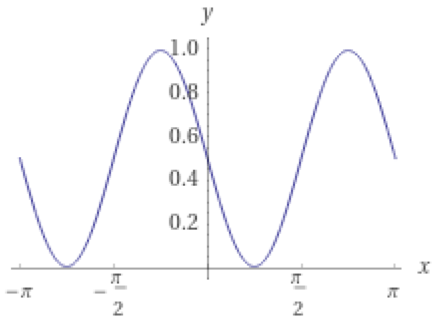
$k_0 l = \frac{\omega}{c} n_o l = \frac{1}{5000} 1.65 \cdot 10^{-2} = 330$,

and

$k_e l = \frac{\omega}{c} n_e l = \frac{1}{5000} 1.5 \cdot 10^{-2} = 300$.

Then

$\sin(k_0 - k_e)l = \sin 30 = -0.988.$
Consequently
$P = \frac{1}{2}(1 - 0.988 \sin 2\theta).$
Below the probability dependency of $\theta$ is illustrated:
$y = \frac{1}{2}(1 - 0.988 \sin 2x)$




($x$ from -3.1 to 3.1)

### 7.5.4 Turpentine

Turpentine is an optically active substance. If we send polarized light into turpentine then it emerges with its plane of polarization rotated. Specifically, turpentine induces a left-hand rotation of 5° per cm of turpentine that the light traverses. Write down the transition matrix that relates the incident polarization state to the emergent polarization state. Show that this matrix is unitary. Why is that important? Find its eigenvectors and eigenvalues, as a function of the length of the turpentine traversed.
We know
$|out\rangle = R(\theta)|in\rangle,$
where, see Eq.(7.41),
$R(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \Longrightarrow$ rotation operator.
Per cm $-5°$left-hand rotation$\Longrightarrow$per cm $-\frac{5 \cdot 2\pi}{360} = -\frac{\pi}{36}$ rotation.
So, per $l$ cm $-\frac{\pi}{36} l = \theta$ rotation.
$R(\theta)$ unitary? $R(\theta)R(\theta)^\dagger = 1?$
$\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} =$
$\begin{pmatrix} \cos^2\theta + \sin^2\theta & -\cos\theta\sin\theta + \sin\theta\cos\theta \\ -\sin\theta\cos\theta + \cos\theta\sin\theta & \sin^2\theta + \cos^2\theta \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$

Unitarity is about the conservation of distinction(Susskind): so the length of the vector and the probability of the length squared is conserved.
Eigenvalues of $R(\theta)$:
$\begin{vmatrix} \cos\theta - \lambda & \sin\theta \\ -\sin\theta & \cos\theta - \lambda \end{vmatrix} = 0 \Longrightarrow (\cos\theta - \lambda)^2 + \sin^2\theta = 0.$
Then,
$\cos\theta - \lambda = \pm i \sin\theta \Longrightarrow \lambda_\pm = \cos\theta \pm i \sin\theta = e^{\pm i\theta}.$
The eigenvectors in column representation
$\begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix}$, and with $\lambda_\pm = \cos\theta \pm i \sin\theta$, we obtain
$b_\pm = i a_\pm.$
With normalization
$\begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = a_\pm \begin{pmatrix} 1 \\ \pm i \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm i \end{pmatrix}.$

So,

$|\lambda_+\rangle = |e^{i\theta}\rangle = \frac{1}{\sqrt{2}}\binom{1}{i} = |R\rangle,$

and

$|\lambda_-\rangle = |e^{-i\theta}\rangle = \frac{1}{\sqrt{2}}\binom{1}{-i} = |L\rangle$ .

The emergent polarization state as a function of the length of the turpentine traversed:

$|out\rangle = R(\theta)|in\rangle = R(\theta)\hat{I}|in\rangle = e^{i\theta}|R\rangle\langle R|in\rangle + e^{-i\theta}|L\rangle\langle L|in\rangle =$

$= e^{-i\frac{\pi}{36}l}|R\rangle\langle R|in\rangle + e^{i\frac{\pi}{36}l}|L\rangle\langle L|in\rangle.$

### 7.5.5 What QM is all about – Two Views

Photons polarized at 30° to the $x$-axis are sent through a $y$-polaroid. An attempt is made to determine how frequently the photons that pass through the polaroid, pass through as right circularly polarized photons and how frequently they pass through as left circularly polarized photons. This attempt is made as follows:

First, a prism that passes only right circularly polarized light is placed between the source of the 30° polarized photons and the $y$-polaroid, and is determined how frequently the 30° polarized photons pass through the $y$-polaroid. Then, this experiment is repeated with a prism that passes only left circularly polarized photons instead of the one that passes only right.

**a)** Show by explicit calculation using standard amplitude mechanics that the sum of the probabilities for passing through the $y$-polaroid measured in these two experiments is different from the probability that one would measure if there were no prism in the path of the photon and only the $y$-polaroid.

We have

$|in\rangle = R(\theta)|x\rangle = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\theta \\ -\sin\theta \end{pmatrix} = \cos\theta\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \sin\theta\begin{pmatrix} 0 \\ 1 \end{pmatrix} =$

$= \cos\theta\,|x\rangle - \sin\theta\,|y\rangle.$

Note: I have here the minus sign. With probabilities this is not important.

$P_{Ry} = |\langle y \mid R\rangle\langle R \mid in\rangle|^2 = \text{probabilityof } |out\rangle = |y\rangle \text{ via } |R\rangle$

$P_{Ly} = |\langle y \mid L\rangle\langle L \mid in\rangle|^2 = \text{probabilityof } |out\rangle = |y\rangle \text{ via } |L\rangle$

$P_y = |\langle y \mid in\rangle|^2 = \text{probabilityof } |out\rangle = |y\rangle$

(independent of internal (unmeasurable properties))

Now

$$P_y = |\langle y \mid in\rangle|^2 = \left|\langle y|\,\hat{I}\,|in\rangle\right|^2 = |\langle y|\,(|R\rangle\langle R| + |R\rangle\langle R|)\,|in\rangle|^2$$
$$= |\langle y \mid R\rangle\langle R \mid in\rangle + \langle y \mid L\rangle\langle L \mid in\rangle|^2$$

where

$$\langle y \mid R\rangle\langle R \mid in\rangle = \text{ amplitude for } |out\rangle = |y\rangle \text{ via } |R\rangle$$
$$\langle y \mid L\rangle\langle L \mid in\rangle = \text{ amplitude for } |out\rangle = |y\rangle \text{ via } |L\rangle$$

With these expressions we can write

$P_y = P_{Ry} + P_{Ly} + 2\text{Real}[(\langle y|R\rangle\langle R|in\rangle)^*(\langle y|L\rangle\langle L|in\rangle)]$ .

We have, page 477,

$|R\rangle = \frac{1}{\sqrt{2}}\binom{1}{i}$ and $|L\rangle = \frac{1}{\sqrt{2}}\binom{1}{-i}$,

then

$\langle y|R\rangle = \frac{i}{\sqrt{2}}$,
$\langle y|L\rangle = -\frac{i}{\sqrt{2}}$,
$\langle R|in\rangle = \langle R|R(\theta)|x\rangle = e^{i\theta}\langle R|x\rangle = \frac{1}{\sqrt{2}}e^{i\theta}$,
$\langle L|in\rangle = \langle L|R(\theta)|x\rangle = e^{-i\theta}\langle R|x\rangle = \frac{1}{\sqrt{2}}e^{-i\theta}$.
Consequently the classical result is:
$P_{Ry} = \frac{1}{4} = P_{Ly} \Longrightarrow P_{Ry} + P_{Ly} = \frac{1}{2}$.
The quantum mechanical result is
$P_y = \frac{1}{2} + 2\text{Real}[(\langle y|R\rangle\langle R|in\rangle)^*(\langle y|L\rangle\langle L|in\rangle)] =$
$= \frac{1}{2} + 2\text{Real}[\left(\frac{i}{\sqrt{2}}\frac{1}{\sqrt{2}}e^{i\theta}\right)^*(-\frac{i}{\sqrt{2}}\frac{1}{\sqrt{2}}e^{-i\theta})] = \frac{1}{2} - \frac{1}{2}\cos 2\theta$.
A result dependent on $\theta$.
**b)** Repeat the calculations using density matrix methods instead of amplitude mechanics.
The outer product or projection operator
$\hat{\rho}_{in} = |in\rangle\langle in|$.
$|in\rangle = R(\theta)|x\rangle = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\theta \\ -\sin\theta \end{pmatrix} = \cos\theta\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \sin\theta\begin{pmatrix} 0 \\ 1 \end{pmatrix} =$
$= \cos\theta\,|x\rangle - \sin\theta\,|y\rangle$,
or
$|in\rangle = \cos\theta\,|x\rangle + \sin\theta\,|y\rangle$, Eq.(7.39)?
I choose
$|in\rangle = \cos\theta\,|x\rangle - \sin\theta\,|y\rangle$.
So, with $\theta = \frac{\pi}{6}$,
$|in\rangle = \frac{\sqrt{3}}{2}|x\rangle - \frac{1}{2}|y\rangle$.
From Problem 7.5.1 *Change the Basis,* we learned:
$|x\rangle = \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle)$,
$|y\rangle = \frac{i}{\sqrt{2}}(-|R\rangle + |L\rangle)$.
So,
$|in\rangle = \frac{\sqrt{3}}{2}|x\rangle - \frac{1}{2}|y\rangle = \frac{1}{2\sqrt{2}}[(\sqrt{3}+i)|R\rangle + ((\sqrt{3}-i)|L\rangle]$ .
$\hat{\rho}_{in} = |in\rangle\langle in| = (\frac{\sqrt{3}}{2}|x\rangle - \frac{1}{2}|y\rangle)(\frac{\sqrt{3}}{2}\langle x| - \frac{1}{2}\langle y|) =$
$= \frac{3}{4}|x\rangle\langle x| - \frac{\sqrt{3}}{4}|x\rangle\langle y| - \frac{\sqrt{3}}{4}|y\rangle\langle x| + \frac{1}{4}|y\rangle\langle y| =$
$= \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - \frac{\sqrt{3}}{4}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - \frac{\sqrt{3}}{4}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \frac{1}{4}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 3 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$.

Comparing this result with the result obtained by Boccio, it appeared Boccio used
$|in\rangle = \cos\theta\,|x\rangle + \sin\theta\,|y\rangle$.
However, this result contradicts
$|in\rangle = \frac{1}{2\sqrt{2}}[(\sqrt{3}+i)|R\rangle + ((\sqrt{3}-i)|L\rangle]$.
Then you will obtain
$|in\rangle = \frac{1}{2\sqrt{2}}[(\sqrt{3}-i)|R\rangle + ((\sqrt{3}+i)|L\rangle]$.

With the matrix representation of $\hat{\rho}_{in}$, we have

$Prob(x) = \frac{3}{4}$, and $Prob(y) = \frac{1}{4}$. A quantum result.

Alternatively, we can think of a measurement taking place in the $xy$ basis. This measurement cannot be done in the quantum world without destroying the phase relationships and hence eliminating any interference effects, that is, measurement separates orthogonal states making them classically distinct and all interference between orthogonal states (represented by the off-diagonal terms in $\hat{\rho}$) is destroyed.

Summarize: measurement diagonalizes $\hat{\rho}_{in}$ in the basis of the measurement.
Then, in the $xy$ basis

$\frac{1}{4}\begin{pmatrix} 3 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}$, after measurement $\frac{1}{4}\begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix}$.

To see what happens if we attempt to find out whether the photons are passing through the apparatus as $R$ or $L$ photons, we must first rewrite $\hat{\rho}_{in}$ in the $(R, L)$ basis, so that

$$\hat{\rho}_{in} = |in\rangle\langle in| = \frac{1}{8}\left[\left(\sqrt{3}+i\right)|R\rangle + \left(\sqrt{3}-i\right)|L\rangle\right]\left[\left(\sqrt{3}-i\right)\langle R| + \left(\sqrt{3}+i\right)\langle L|\right] =$$
$$= \frac{1}{2}|R\rangle\langle R| + \frac{1}{4}\left(1+i\sqrt{3}\right)|R\rangle\langle L| + \frac{1}{4}\left(1-i\sqrt{3}\right)|L\rangle\langle R| + \frac{1}{2}|L\rangle\langle L|.$$

$\hat{\rho}_{in}$ matrix representation, in the $(R, L)$ basis, $|R\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|L\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$,

$$\hat{\rho}_{in} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1+i\sqrt{3}}{4}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \frac{1-i\sqrt{3}}{4}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} =$$
$$= \frac{1}{4}\begin{pmatrix} 2 & 1+i\sqrt{3} \\ 1-i\sqrt{3} & 2 \end{pmatrix}.$$

Hence

$Prob(R) = \frac{1}{2}$, $Prob(L) = \frac{1}{2}$.

Now we measure in the $(R, L)$ basis (since we are trying to determine if the photon passes through the apparatus as a $R$ or $L$ photon). Again, this measurement cannot be done in the quantum world without destroying the phase relationships and hence eliminating any interference effects, that is, measurement separates orthogonal states making them classically distinct and all interference between orthogonal states (represented by the off-diagonal terms in $\hat{\rho}$) is destroyed.

Summarize: measurement diagonalizes $\hat{\rho}_{in}$ in the basis of the measurement.
Then, in the $(R, L)$ basis

$\hat{\rho}_{in} = \frac{1}{4}\begin{pmatrix} 2 & 1+i\sqrt{3} \\ 1-i\sqrt{3} & 2 \end{pmatrix}$, after measurement $\hat{\rho}_{out} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

The measurement changes

$\hat{\rho}_{out} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}|R\rangle\langle R| + \frac{1}{2}|L\rangle\langle L| \rightarrow$ a mixed state.

This represents a mixed state.
We change back to the $(x, y)$ basis.

$$|R\rangle = \frac{1}{\sqrt{2}}\left(|x\rangle + i|y\rangle\right),$$
$$|L\rangle = \frac{1}{\sqrt{2}}\left(|x\rangle - i|y\rangle\right).$$
$$\hat{\rho}_{out} = \frac{1}{4}\left(|x\rangle + i|y\rangle\right)\left(\langle x| - i\langle y|\right) + \frac{1}{4}\left(|x\rangle - i|y\rangle\right)\left(\langle x| + i\langle y|\right) =$$
$$= \frac{1}{4}|x\rangle\langle x| - \frac{i}{4}|x\rangle\langle y| + \frac{i}{4}|y\rangle\langle x| + \frac{1}{4}|y\rangle\langle y| + \frac{1}{4}|x\rangle\langle x| + \frac{i}{4}|x\rangle\langle y| - \frac{i}{4}|y\rangle\langle x| + \frac{1}{4}|y\rangle\langle y| =$$

$= \frac{1}{2}|x\rangle\langle x| + \frac{1}{2}|y\rangle\langle y| = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \rightarrow$ a mixed state.

$Prob(x) = \frac{1}{2}$ , $Prob(y) = 1/2 \rightarrow$ classical result.

The measurement turns pure states into mixed states with coefficients equal to measurement probabilities!

This problem is the same as the two-slit diffraction experiment if one tries to determine which slit the photon went through - that measurement will destroy the interference pattern!

### 7.5.6 Photons and Polarizers

A polarization state for a photon propagating in the $z$-direction is given by

$|\psi\rangle = \sqrt{\frac{2}{3}}|x\rangle + \frac{i}{\sqrt{3}}|y\rangle$ .

**a)** What is the probability that a photon in the above state will pass through a polaroid with its transmission axis in the $y$-direction?

$\langle y|\psi\rangle = \frac{i}{\sqrt{3}} \Longrightarrow P_y = |\langle y|\psi\rangle|^2 = \frac{1}{3}$ .

**b)** What is the probability that a photon in the state $|\psi\rangle$ will pass through a polaroid with its transmission axis $y'$ making an angle $\varphi$ with the $y$-axis?

$|y'\rangle = -\sin\varphi\,|x\rangle + \cos\varphi\,|y\rangle$.

$\langle y'|\psi\rangle = (-\sin\varphi\,\langle x| + \cos\varphi\,\langle y|)\left(\sqrt{\frac{2}{3}}|x\rangle + \frac{i}{\sqrt{3}}|y\rangle\right) = -\sqrt{\frac{2}{3}}\sin\varphi + \frac{i}{\sqrt{3}}\cos\varphi$.

$P_{y'} = |\langle y'|\psi\rangle|^2 = \frac{2}{3}\sin^2\varphi + \frac{1}{3}\cos^2\varphi = \frac{1}{3}(2 - \cos^2\varphi)$.

**c)** A beam carrying $N$ photons per second, each in state $|\psi\rangle$, is totally absorbed by a black disk with its surface in the $z$-direction. How large is the torque exerted on the disk?

**Reminder**: The photons states $|R\rangle$ and $|L\rangle$ each carry a unit $\hbar$ of angular momentum parallel and antiparallel, respectively, to the direction of propagation of the photon.

In the $\{x, y\}$ basis:

$|R\rangle = \frac{1}{\sqrt{2}}(|x\rangle + i|y\rangle \Longrightarrow \langle R|\psi\rangle = \frac{1}{\sqrt{2}}(\langle x| - i\langle y|)\left(\sqrt{\frac{2}{3}}|x\rangle + \frac{i}{\sqrt{3}}|y\rangle\right) = \frac{1}{\sqrt{3}}(1 + \frac{1}{\sqrt{2}})$.

$P_R = |\frac{1}{\sqrt{3}}(1 + \frac{1}{\sqrt{2}})|^2 = \frac{1}{2} + \frac{\sqrt{2}}{3} \Longrightarrow P_L = 1 - P_R = \frac{1}{2} - \frac{\sqrt{2}}{3}$ .

Th toque on the disk is the angular momentum transferred per second which is the amount transferred by $|R\rangle$ per second plus the amount transferred by $|L\rangle$ per second:

$N[\hbar(P(\hbar) - \hbar P(-\hbar)] \Longrightarrow N[\hbar(P(R) - \hbar P(-L)] = \frac{2\sqrt{2}}{3}N\hbar$ .

### 7.5.7 Time Evolution

The matrix representation of the Hamiltonian for a photon propagating along the optic axis (taken to be the $z$-axis) of a quartz crystal using the linear polarization states $|x\rangle$ and $|y\rangle$ as a basis is given by

$\hat{H} = \begin{pmatrix} 0 & -iE_0 \\ iE_0 & 0 \end{pmatrix}$.

**a)** The eigenvalues:

$\begin{vmatrix} -\lambda & -iE_0 \\ iE_0 & -\lambda \end{vmatrix} = 0 \Longrightarrow \lambda^2 - E_0^2 = 0 \Longrightarrow \lambda_1 = E_0, \lambda_2 = -E_0$.

For the coefficients of the eigenstates with the given basis we have with $\lambda_1 = E_0$:

$\langle y|\lambda_1\rangle = i\langle x|\lambda_1\rangle$ , with normalization:

$|\lambda_1\rangle = \frac{1}{\sqrt{2}}[|x\rangle + i|y\rangle] = |R\rangle$.

With $\lambda_1 = -E_0$:

$\langle y|\lambda_2\rangle = -i\langle x|\lambda_1\rangle$.

Then with normalization:

$|\lambda_2\rangle = \frac{1}{\sqrt{2}}[|x\rangle - i|y\rangle] = |L\rangle$ .

**b)** A photon enters the crystal linearly polarized in the $x$-direction, i.e., $|\psi_0\rangle = |x\rangle$. What is $|\psi(t)\rangle$ , the state of the photon at time $t$ expressed in the $\{|x\rangle, |y\rangle\}$ basis?

$|\psi_0\rangle = |in\rangle = |x\rangle = \langle\lambda_1|x\rangle|\lambda_1\rangle + \langle\lambda_2|x\rangle|\lambda_2\rangle$ .

With expressions above , we learned:

$\langle\lambda_1|x\rangle = \frac{1}{\sqrt{2}}[\langle x|x\rangle - i\langle y|x\rangle] = \frac{1}{\sqrt{2}}$,

$\langle\lambda_2|x\rangle = \frac{1}{\sqrt{2}}[\langle x|x\rangle + i\langle y|x\rangle] = \frac{1}{\sqrt{2}}$.

Hence

$|\psi_0\rangle = |in\rangle = |x\rangle = \langle\lambda_1|x\rangle|\lambda_1\rangle + \langle\lambda_2|x\rangle|\lambda_2\rangle = \frac{1}{\sqrt{2}}[|\lambda_1\rangle + |\lambda_2\rangle]$.

With the Hamiltonian, the eigenvalues and the time development

$|out\rangle = e^{-i\hat{H}t/\hbar}|in\rangle = \frac{1}{\sqrt{2}}\left(e^{-\frac{iE_0t}{\hbar}}|\lambda_1\rangle + e^{\frac{iE_0t}{\hbar}}|\lambda_2\rangle\right) = \frac{1}{2}(e^{-\frac{iE_0t}{\hbar}}[|x\rangle + i|y\rangle]$

$= \frac{1}{2}\left(e^{-\frac{iE_0t}{\hbar}}[|x\rangle + i|y\rangle] + e^{\frac{iE_0t}{\hbar}}[|x\rangle - i|y\rangle]\right) = \cos(\frac{E_0t}{\hbar})|x\rangle + \sin\frac{E_0t}{\hbar}|y\rangle = |\psi(t)\rangle$.

**c)** What is happening to the polarization of the photon as it travels through the crystal?

In general we know that a linearized state with polarization along $x'$ is

$|x'\rangle = \cos\theta|x\rangle + \sin\theta|y\rangle$.

Compare this with the result for $|\psi(t)\rangle$, we see with the progress of time the direction of polarization rotates when the photon propagates through the crystal.

### 7.5.8 K-Meson Oscillations

An additional effect to worry about when thinking about the time development of K-meson states is that $|K_L\rangle$ and $|K_S\rangle$ states decay with time. Thus we expect the states should have the time dependence

$|K_L(t)\rangle = e^{-i\omega_L t - t/2\tau_L}|K_L\rangle$ ,

and

$|K_S(t)\rangle = e^{-i\omega_S t - t/2\tau_S}|K_S\rangle$.

With

$\omega_L = \frac{E_L}{\hbar} = (p^2c^2 + m_L^2c^4)^{\frac{1}{2}}$,

$\omega_S = \frac{E_L}{\hbar} = (p^2c^2 + m_S^2c^4)^{\frac{1}{2}}$ ,

$\tau_S \approx 0.9 \cdot 10^{-10}$ sec, and $\tau_L \approx 560 \cdot 10^{-10}$ sec.

Suppose that a pure $K_L$ beam is sent through a thin absorber whose only effect is to change the relative phase of the $K^0$ particle and the $\bar{K}^0$ antiparticle amplitudes by $10°$.

Calculate the number of $K_S$ decays, relative to the incident number of particles, that will be observed in the first 5 cm after the absorber. The particles have momentum $mc$.

**Note**: the subscript $S$ indicate *Strange* of the strangeness operator of which $|K^0\rangle$ and $|\bar{K}^0\rangle$ are eigenvectors, page 504 of the Undergraduate Course.

Before the absorber we have

$|\psi_{before}\rangle = |K_L\rangle = \frac{1}{\sqrt{2}}[|K^0\rangle - |\bar{K}^0\rangle]$, Eq.(7.152).

The effect of the absorber is expressed by the development operator represented by the sun of the projection operators and the relative phase shift $\frac{\pi}{18}$ :

$\hat{A} = |K^0\rangle\langle K^0|e^{i\theta} + |\bar{K}^0\rangle\langle\bar{K}^0|e^{i(\theta+\frac{\pi}{18})}$.
Therefore, the absorber state is
$$|\psi_{after}\rangle = \hat{A}|\psi_{before}\rangle = \left(|K^0\rangle\langle K^0|e^{i\theta} + |\bar{K}^0\rangle\langle\bar{K}^0\right|e^{i\left(\theta+\frac{\pi}{18}\right)}\right)\frac{1}{\sqrt{2}}[|K^0\rangle - |\bar{K}^0\rangle] =$$
$$\frac{e^{i\theta}}{\sqrt{2}}\left(|K^0\rangle - e^{\frac{i\pi}{18}}|\bar{K}^0\rangle\right).$$
Above, the time dependence of the $|K_L\rangle$ and $|K_S\rangle$ states are given. So, we rewrite $|\psi_{after}\rangle$ in the $\{|K_L\rangle, |K_S\rangle\}$ basis.
With Eqs.(7.151) and (7.152)
$$|K_S\rangle = \frac{1}{\sqrt{2}}[|K^0\rangle + |\bar{K}^0\rangle],$$
$$|K_L\rangle = \frac{1}{\sqrt{2}}[|K^0\rangle - |\bar{K}^0\rangle],$$
we find
$$|K^0\rangle = \frac{1}{\sqrt{2}}[|K_S\rangle + |K_L\rangle],$$
$$|\bar{K}^0\rangle = \frac{1}{\sqrt{2}}[|K_S\rangle - |K_L\rangle].$$
Then,
$$|\psi_{after}\rangle = \frac{e^{i\theta}}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}[|K_S\rangle + |K_L\rangle] - \frac{1}{\sqrt{2}}e^{\frac{i\pi}{18}}[|K_S\rangle - |K_L\rangle]\right) =$$
$$= \frac{e^{i\theta}}{2}\left(\left[1 - e^{\frac{i\pi}{18}}\right]|K_S\rangle + \left[1 + e^{\frac{i\pi}{18}}\right]|K_L\rangle\right).$$
At $t = 0$, we have $|\psi(0)\rangle = |\psi_{after}\rangle$, just after leaving the absorber.
We have
$$|K_L(t)\rangle = e^{-i\omega_L t - t/2\tau_L}|K_L\rangle\ ,$$
and
$$|K_S(t)\rangle = e^{-i\omega_S t - t/2\tau_S}|K_S\rangle.$$
Then,
$$|\psi(t)\rangle = \frac{e^{i\theta}}{2}\left(\left[1 - e^{\frac{i\pi}{18}}\right]e^{-i\omega_S t - t/2\tau_S}|K_S\rangle + \left[1 + e^{\frac{i\pi}{18}}\right]e^{-i\omega_S t - t/2\tau_S}|K_L\rangle\right).$$
Next, the probability amplitude
$$\langle K_S|\psi(t)\rangle = \frac{e^{i\theta}}{2}(1 - e^{\frac{i\pi}{18}})e^{-i\omega_S t - t/2\tau_S}.$$
The probability
$$P_S = |\langle K_S|\psi(t)\rangle|^2 = \frac{e^{i\theta}}{2}\left(1 - e^{\frac{i\pi}{18}}\right)e^{-i\omega_S t - \frac{t}{2\tau_S}} \cdot \frac{e^{-i\theta}}{2}\left(1 - e^{\frac{-i\pi}{18}}\right)e^{+i\omega_S t - \frac{t}{2\tau_S}} =$$
$$= \frac{1}{2}(1 - \cos\frac{\pi}{18})\, e^{-\frac{t}{\tau_S}}.$$
The numerical example, Boccio:
$$d = 5\,cm \to t_d = \frac{d}{v} \approx \frac{d}{c} = 1.6 \times 10^{-10}\ \text{sec}$$
$$\tau_S = 0.9 \times 10^{-10}\ \text{sec} \to \frac{t_d}{\tau_S} = \frac{16}{9}$$
Now the number of transitions per sec at time $t$ is given by $N(0)P_S(t)$. This says that the
$$\text{total number of transitions}(0 \to t_d) = \bar{N} = \int_0^{t_d} N(0)P_S(t)dt$$
$$\bar{N} = \frac{1}{2}\left(1 - \cos\frac{\pi}{18}\right)N(0)\int_0^{t_d} e^{-t/\tau_S}dt = \frac{1}{2}\left(1 - \cos\frac{\pi}{18}\right)\tau_S N(0)(1 - e^{-16/9}) = 0.0063\tau_S N(0)$$
where we assumed $N(0)$ = constant since the total number of decays is very small compared to $N(0)$. Therefore,
$$\text{fraction} = \frac{\bar{N}}{N(0)} = 0.0063\tau_S = 5.69 \times 10^{-13}$$

## 7.5.9 What Comes Out?

A beam of spin ½ particles is sent through a series of three Stern-Gerlach measuring devices as shown in the Figure(Boccio) below(see also page 513 of the Undergraduate Course):

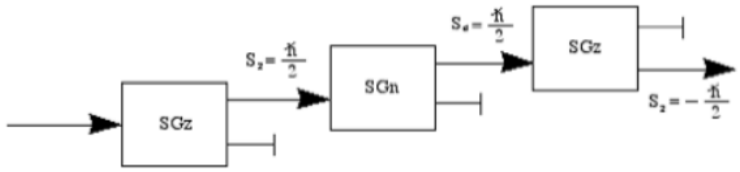



Figure 7.1: Stern-Gerlach Setup

The first SGz device transmits particles with $\hat{S}_z = \frac{\hbar}{2}$ and filters out particles with $\hat{S}_z = -\frac{\hbar}{2}$.
The second device, an SGn device transmits particle with $\hat{S}_z = \frac{\hbar}{2}$ and filters out particles with $\hat{S}_z = -\frac{\hbar}{2}$, where the axis $\hat{n}$ make an angle $\theta$ in the $x$-$z$ plane with respect to the $z$-axis.
Thus the particles passing through the SGn device are in the state
$|+\hat{n}\rangle = \cos\frac{\theta}{2}|+\hat{z}\rangle + e^{i\varphi}\sin\frac{\theta}{2}|-\hat{z}\rangle$.
The phase shift angle $\varphi$ is set equal to 0. A last SGz device transmits particles with $\hat{S}_z = -\frac{\hbar}{2}$ and filters out particles with $\hat{S}_z = \frac{\hbar}{2}$.
**a)** What fraction of the particle transmitted through the first SGz device will survive the third measurement? It is about the probability of having particles coming out with $\hat{S}_z = -\frac{\hbar}{2}$.
The diagonal basis $|\pm\hat{z}\rangle$. With the projection operator we have
$\widehat{M}(+\hat{z}) = |+\hat{z}\rangle\langle+\hat{z}|$.
With this projection operator, $|+\hat{z}\rangle$ is projected out.

**Remark:** The incoming beam of spin particles is described by the normalized state:
$|\pm\hat{z}\rangle = \frac{1}{\sqrt{2}}|+\hat{z}\rangle + \frac{1}{\sqrt{2}}|-\hat{z}\rangle$.
Then,
$\widehat{M}(+\hat{z})\,|\pm\hat{z}\rangle = |+\hat{z}\rangle\langle+\hat{z}|\left(\frac{1}{\sqrt{2}}|+\hat{z}\rangle + \frac{1}{\sqrt{2}}|-\hat{z}\rangle\right) = \frac{1}{\sqrt{2}}|+\hat{z}\rangle$.
Is there a contradiction? $\frac{1}{\sqrt{2}}|+\hat{z}\rangle$ is measured with a probability $\frac{1}{2}$. However, we know the device transmits particles with $\hat{S}_z = \frac{\hbar}{2}$ and particles with $\hat{S}_z = -\frac{\hbar}{2}$, are filtered out.
Consequently, the probability to measure $|+\hat{z}\rangle$ is 1. Meaning, $\widehat{M}(+\hat{z})\,|\pm\hat{z}\rangle = |+\hat{z}\rangle$.
This answer is found when neglecting normalization.
In the experiment 1 on page 515 of the Undergraduate Course, this probability is translated into the fraction of particles passing through the device. So, the fraction is $\frac{1}{2}$ with probability 1 coming out of the first device.

With the second measurement and the basis $|\pm\hat{n}\rangle$, we have the projection operator
$\widehat{M}(+\hat{n}) = |+\hat{n}\rangle\langle+\hat{n}|$, with the given angle $\theta$
$|+\hat{n}\rangle = \cos\frac{\theta}{2}|+\hat{z}\rangle + \sin\frac{\theta}{2}|-\hat{z}\rangle$.
Then,

$$\widehat{M}(+\hat{n}) = |+\hat{n}\rangle\langle+\hat{n}| = \left(\cos\frac{\theta}{2}|+\hat{z}\rangle + \sin\frac{\theta}{2}|-\hat{z}\rangle\right)\left(\cos\frac{\theta}{2}\langle+\hat{z}\big| + \sin\frac{\theta}{2}\langle-\hat{z}\big|\right) =$$

$$= \cos^2\frac{\theta}{2}|+\hat{z}\rangle\langle+\hat{z}\big| + \cos\frac{\theta}{2}\sin\frac{\theta}{2}\left(|+\hat{z}\rangle\langle-\hat{z}| + |-\hat{z}\rangle\langle+\hat{z}|\right) + \sin^2\frac{\theta}{2}|-\hat{z}\rangle\langle-\hat{z}\big|.$$

The third measurement and the basis $|\pm\hat{z}\rangle$ gives us for the operator
$\widehat{M}(-\hat{z}) = |-\hat{z}\rangle\langle-\hat{z}|$.
For the combined measurement we have the product operator
$\widehat{M}_T = \widehat{M}(-\hat{z})\widehat{M}(+\hat{n})\widehat{M}(+\hat{z})$.
Hence the fraction $f$ of the particles transmitted through the first SGz device that will survive the third measurement is
$f = \left|\left\langle -\hat{z}\middle|\widehat{M}(-\hat{z})\widehat{M}(+\hat{n})\middle|+\hat{z}\right\rangle\right|^2$.
In the preceding expression, the operation of $\widehat{M}(+\hat{z})$ is already incorporated into $|+\hat{z}\rangle$.

With the expression for
$\widehat{M}(+\hat{n}) = \cos^2\frac{\theta}{2}|+\hat{z}\rangle\langle+\hat{z}| + \cos\frac{\theta}{2}\sin\frac{\theta}{2}(|+\hat{z}\rangle\langle-\hat{z}| + |-\hat{z}\rangle\langle+\hat{z}|) + \sin^2\frac{\theta}{2}|-\hat{z}\rangle\langle-\hat{z}|$,
we obtain for
$\widehat{M}(+\hat{n})|+\hat{z}\rangle = \cos^2\frac{\theta}{2}|+\hat{z}\rangle + \cos\frac{\theta}{2}\sin\frac{\theta}{2}|-\hat{z}\rangle$.

So,
$\left\langle -\hat{z}\middle|\widehat{M}(-\hat{z})\widehat{M}(+\hat{n})\middle|+\hat{z}\right\rangle = \left\langle -\hat{z}\middle|\widehat{M}(-\hat{z})\cos^2\frac{\theta}{2}\middle|+\hat{z}\right\rangle + \left\langle -\hat{z}\middle|\widehat{M}(-\hat{z})\cos\frac{\theta}{2}\sin\frac{\theta}{2}\middle|-\hat{z}\right\rangle$.
With
$\langle-\hat{z}|\widehat{M}(-\hat{z}) = \langle-\hat{z}|-\hat{z}\rangle\langle-\hat{z}| = \langle-\hat{z}|$,
$\left\langle -\hat{z}\middle|\widehat{M}(-\hat{z})\widehat{M}(+\hat{n})\middle|+\hat{z}\right\rangle = \left\langle -\hat{z}\middle|\cos^2\frac{\theta}{2}\middle|+\hat{z}\right\rangle + \left\langle -\hat{z}\middle|\cos\frac{\theta}{2}\sin\frac{\theta}{2}\middle|-\hat{z}\right\rangle = \cos\frac{\theta}{2}\sin\frac{\theta}{2}$.

Hence,
the probability of measuring $|-\hat{z}\rangle$ after the third device is equal to the fraction
$f = \left|\left\langle -\hat{z}\middle|\widehat{M}(-\hat{z})\widehat{M}(+\hat{n})\middle|+\hat{z}\right\rangle\right|^2 = \cos^2\frac{\theta}{2}\sin^2\frac{\theta}{2} = \frac{1}{4}\sin^2\theta$.
**b)** How must the angle $\theta$ of the SGn device be oriented so as to maximise the number of particles that are transmitted by the final SGz device? What fraction of the particles survive the third measurement for this value of $\theta$?
$f = \frac{1}{4}\sin^2\theta$.
Hence, to maximise the fraction $\Longrightarrow \theta = \frac{\pi}{2}$.
Then, $f = \frac{1}{4}$.
**c)** What fraction of the particles survive the last measurement if the second SGz is removed?
With SGn device particles in the state $|+\hat{n}\rangle$ are transmitted.
The probability of measuring these particles is:
$f = \left|\left\langle +\hat{n}\middle|\widehat{M}(+\hat{n})\middle|+\hat{z}\right\rangle\right|^2$.
$\left\langle +\hat{n}\middle|\widehat{M}(+\hat{n})\middle|+\hat{z}\right\rangle = \left\langle +\hat{n}\middle|\cos^2\frac{\theta}{2}\middle|+\hat{z}\right\rangle + \left\langle +\hat{n}\middle|\cos\frac{\theta}{2}\sin\frac{\theta}{2}\middle|-\hat{z}\right\rangle$.
With
$|+\hat{n}\rangle = \cos\frac{\theta}{2}|+\hat{z}\rangle + \sin\frac{\theta}{2}|-\hat{z}\rangle$:
$\left\langle +\hat{n}\middle|\widehat{M}(+\hat{n})\middle|+\hat{z}\right\rangle = \cos^3\frac{\theta}{2} + \cos\frac{\theta}{2}\sin^2\frac{\theta}{2} = \cos\frac{\theta}{2}$.
The surviving fraction $\bar{f}$ is now:
$\bar{f} = \cos^2\frac{\theta}{2} = (1+\cos\theta)/2$.

### 7.5.10 Orientations

The kets $|h\rangle$ and $|v\rangle$ are horizontal and vertical polarization, respectively. Consider the states

$|\psi_1\rangle = -\frac{1}{2}(|h\rangle + \sqrt{3}|v\rangle)$,

$|\psi_2\rangle = -\frac{1}{2}(|h\rangle - \sqrt{3}|v\rangle)$,

and

$|\psi_3\rangle = |h\rangle$.

What are the relative orientations of the plane polarization for these three states?

For a generalized polarization state at angle $\theta$ we learned the state vector to be

$|\psi\rangle = \cos\theta\,|h\rangle + \sin\theta\,|v\rangle$.

- $|\psi_1\rangle = -\frac{1}{2}(|h\rangle + \sqrt{3}|v\rangle) \Longrightarrow \cos\theta = -\frac{1}{2}$, and $\sin\theta = -\frac{1}{2}\sqrt{3} \Longrightarrow \theta = 210°$.
- $|\psi_2\rangle = -\frac{1}{2}(|h\rangle - \sqrt{3}|v\rangle) \Longrightarrow \cos\theta = -\frac{1}{2}$, and $\sin\theta = \frac{1}{2}\sqrt{3} \Longrightarrow \theta = 150°$.
- $|\psi_3\rangle = |h\rangle \Longrightarrow \cos\theta = 1$ , and $\sin\theta = 0 \Longrightarrow \theta = 0°$.

### 7.5.11 Find the Phase Angle

If CP [6] is not conserved in the decay of neutral K mesons, then the states of definite energy are no longer the $|K_L\rangle$ , $|K_S\rangle$ states, but are slightly different states $|K_L'\rangle$ and $|K_S'\rangle$.

One can write, for example

$|K_L'\rangle = (1+\varepsilon)|K^0\rangle - (1-\varepsilon)|\bar{K}^0\rangle$ ,

where $\varepsilon$ is a very small complex number ( $|\varepsilon| \approx 2 \cdot 10^{-3}$) that is a measure of the lack of CP conservation in the decays. The amplitude for a particle to be in $|K_L'\rangle$(or $|K_S'\rangle$) varies as

$e^{-i\omega_L t - t/2\tau_L}$ (or $e^{-i\omega_S t - t/2\tau_S}$),

where

$\hbar\omega_L = (p^2c^2 + m_L^2c^4)^{1/2}$,

$\hbar\omega_S = (p^2c^2 + m_S^2c^4)^{1/2}$,

and

$\tau_L \gg \tau_S$ .

**a)** Normalized expressions for $|K_L'\rangle$ and $|K_S'\rangle$.

Use the normalization factor $A_L$ , then

$|K_L'\rangle = A_L[(1+\varepsilon)|K^0\rangle - (1-\varepsilon)|\bar{K}^0\rangle]$.

With $\langle K_L'|K_L'\rangle = 1$, we obtain:

$\langle K_L'|K_L'\rangle = |A_L|^2[(1+\varepsilon^*)\langle K^0| - (1-\varepsilon^*)\langle\bar{K}^0|][(1+\varepsilon)|K^0\rangle - (1-\varepsilon)|\bar{K}^0\rangle] =$

$= |A_L|^2[(1+\varepsilon^*)(1+\varepsilon) + (1-\varepsilon^*)(1-\varepsilon)] = 2|A_L|^2(1+|\varepsilon|^2) = 1.$

So,

$|A_L| = \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}$,

and we choose

$A_L = \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}$ .

In addition we have:

$\langle K_S'|K_S'\rangle = 1$, and $\langle K_S'|K_L'\rangle = 0$ .

For $|K_S'\rangle$ we write:

$|K_S'\rangle = [a|K^0\rangle + b|\bar{K}^0\rangle]$.

Then with normalization

$\langle K_S'|K_S'\rangle = [a^*\langle K^0| + b^*\langle\bar{K}^0|][a|K^0\rangle + b|\bar{K}^0\rangle] = |a|^2 + |b|^2 = 1$ .

---

[6] CP: Circular Polarization(Polarized).

With orthogonality

$\langle K_S'|K_L'\rangle = [a^*\langle K^0| + b^*\langle \bar{K}^0|]A_L[(1+\varepsilon)|K^0\rangle - (1-\varepsilon)|\bar{K}^0\rangle] =$

$= A_L[a^*(1+\varepsilon) - b^*(1-\varepsilon)] = 0 \rightarrow a^*(1+\varepsilon) - b^*(1-\varepsilon) = 0.$

For $a$ and $b$ we choose

$a = \frac{1-\varepsilon^*}{\sqrt{2(1+|\varepsilon|^2)}}$, and $b = \frac{1+\varepsilon^*}{\sqrt{2(1+|\varepsilon|^2)}}$.

For the perturbed states we have

$$|K_L'\rangle = \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}[(1+\varepsilon)|K^0\rangle - (1-\varepsilon)|\bar{K}^0\rangle].$$

With $a$ and $b$

$$|K_S'\rangle = \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}[(1-\varepsilon^*)|K^0\rangle + (1+\varepsilon^*)|\bar{K}^0\rangle].$$

Now we use

$$|K^0\rangle = \frac{1}{\sqrt{2}}(\,|K_S\rangle + |K_L\rangle),$$

and

$$|\bar{K}^0\rangle = \frac{1}{\sqrt{2}}(\,|K_S\rangle - |K_L\rangle),$$

to rewrite $|K_L'\rangle$ and $|K_S'\rangle$ in the $\{|K_L\rangle, |K_S\rangle\}$ basis

$$|K_L'\rangle = \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}\left[(1+\varepsilon)\frac{1}{\sqrt{2}}(\,|K_S\rangle + |K_L\rangle) - (1-\varepsilon)\frac{1}{\sqrt{2}}(\,|K_S\rangle - |K_L\rangle)\right] =$$

$$= \frac{1}{\sqrt{(1+|\varepsilon|^2)}}(|K_L\rangle + \varepsilon|K_S\rangle).$$

$$|K_S'\rangle = \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}[(1-\varepsilon^*)\frac{1}{\sqrt{2}}(\,|K_S\rangle + |K_L\rangle) + (1+\varepsilon^*)\frac{1}{\sqrt{2}}(\,|K_S\rangle - |K_L\rangle)] =$$

$$= \frac{1}{\sqrt{(1+|\varepsilon|^2)}}(|K_S\rangle - \varepsilon^*|K_S\rangle).$$

Including time dependency:

$$|K_L'(t)\rangle = \frac{1}{\sqrt{(1+|\varepsilon|^2)}}(\,e^{-i\omega_L t - t/2\tau_L}|K_L\rangle + \varepsilon e^{-i\omega_S t - t/2\tau_S}|K_S\rangle),$$

and

$$|K_S'(t)\rangle = \frac{1}{\sqrt{(1+|\varepsilon|^2)}}(e^{-i\omega_S t - t/2\tau_S}|K_S\rangle - \varepsilon^* e^{-i\omega_L t - t/2\tau_L}|K_L\rangle).$$

**b)** Calculate the ratio for a long-lived $K$-meson to decay to two pions (a CP$= +1) \equiv |K_S\rangle$ state to the amplitude for a short-lived $K$-meson to de cay to two pions (a CP$= -1) \equiv |K_L\rangle$ state.

It is about the perturbed states.

So, we work with $|K_L'\rangle$ and $|K_S'\rangle$.

The ratio $R$ of the square of the amplitudes:

$$R = \frac{|\langle\langle K_S|K_L'(t)\rangle|^2}{|\langle K_L|K_L'(t)\rangle|^2}.$$

**Note Boccio:**

Notice that if $|K_L'\rangle \rightarrow |K_L\rangle$, then the probability for it to behave like a $|K_S\rangle$ would be zero. This means that if we see any effect (any $CP = +1$ decays), that is, if $\varepsilon \neq 0$, this result implies non-conservation of $CP$.

$$\langle\langle K_S|K_L'(t)\rangle = \frac{1}{\sqrt{(1+|\varepsilon|^2)}}\langle K_S|\left(e^{-i\omega_L t - \frac{t}{2\tau_L}}|K_L\rangle + \varepsilon e^{-i\omega_S t - \frac{t}{2\tau_S}}|K_S\rangle\right) =$$

$$= \frac{1}{\sqrt{(1+|\varepsilon|^2)}}\,\varepsilon e^{-i\omega_S t - \frac{t}{2\tau_S}},$$

and

$\langle K_L|K_L'(t)\rangle = \frac{1}{\sqrt{(1+|\varepsilon|^2)}}\langle K_L|\left(e^{-i\omega_L t-\frac{t}{2\tau_L}}|K_L\rangle + \varepsilon e^{-i\omega_S t-\frac{t}{2\tau_S}}|K_S\rangle\right) =$

$= \frac{1}{\sqrt{(1+|\varepsilon|^2)}} e^{-i\omega_L t-\frac{t}{2\tau_L}}$ .

Then,

$$R = \frac{|\langle K_S|K_L'(t)\rangle|^2}{|\langle K_L|K_L'(t)\rangle|^2} = \frac{\frac{1}{(1+|\varepsilon|^2)}|\varepsilon|^2 e^{-\frac{t}{\tau_S}}}{\frac{1}{(1+|\varepsilon|^2)}e^{-\frac{t}{\tau_L}}} = |\varepsilon|^2 e^{-t(\frac{1}{\tau_S}-\frac{1}{\tau_L})},$$

with $\tau_L \gg \tau_S$

$R \approx |\varepsilon|^2 e^{-\frac{t}{\tau_S}}$ .

Measuring $R \Longrightarrow \varepsilon$ .

**c)** Suppose that a beam of purely long-lived $K$ mesons is sent through an absorber whose only effect is to change the relative phase of the $|K^0\rangle$ and $|\bar{K}^0\rangle$ by $\delta$. Derive an expression for the number of two pion events observed as a function of time travel from the absorber. How well would such a measurement (given $\delta$) enable one to determine the phase of $\varepsilon$?

The probability for the long-lived $K$ mesons(see **b)**) to decay to two pions (a CP$=+1$) $\equiv |K_S\rangle$:

$P_{K_l' \to K_S}(t) = |\langle K_S|K_L'(t)\rangle|^2$.

We know, before the absorber

$|\psi_{before}\rangle = |K_L'\rangle = \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}[(1+\varepsilon)|K^0\rangle - (1-\varepsilon)|\bar{K}^0\rangle]$.

After the absorber

$|\psi_{after}\rangle = |\psi_0\rangle = \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}[(1+\varepsilon)|K^0\rangle - e^{-i\delta}(1-\varepsilon)|\bar{K}^0\rangle]$.

Changing the basis

$|K^0\rangle = \frac{1}{\sqrt{2}}(|K_S\rangle + |K_L\rangle)$,

and

$|\bar{K}^0\rangle = \frac{1}{\sqrt{2}}(|K_S\rangle - |K_L\rangle)$:

$|\psi_0\rangle = \frac{1}{\sqrt{2(1+|\varepsilon|^2)}}[(1+\varepsilon)\frac{1}{\sqrt{2}}(|K_S\rangle + |K_L\rangle) - e^{-i\delta}(1-\varepsilon)\frac{1}{\sqrt{2}}(|K_S\rangle - |K_L\rangle)]$.

Include time dependency, oscillations and decay

$|K_L'(t)\rangle = \frac{1}{2\sqrt{(1+|\varepsilon|^2)}}[\{(1+\varepsilon) - e^{-i\delta}(1-\varepsilon)\}e^{-i\omega_S t-\frac{t}{2\tau_S}}|K_S\rangle +$

$+\{(1+\varepsilon) + e^{-i\delta}(1-\varepsilon)\}e^{-i\omega_L t-\frac{t}{2\tau_L}}|K_L\rangle]$ .

$\langle K_S|K_L'(t)\rangle = \frac{1}{2\sqrt{(1+|\varepsilon|^2)}}\{(1+\varepsilon) - e^{-i\delta}(1-\varepsilon)\}e^{-i\omega_S t-\frac{t}{2\tau_S}}$,

and

$P_{K_l' \to K_S}(t) = |\langle K_S|K_L'(t)\rangle|^2 = \frac{1}{4(1+|\varepsilon|^2)}|(1+\varepsilon) - e^{-i\delta}(1-\varepsilon)|^2 e^{-\frac{t}{\tau_S}}$ .

Next, evaluate

$|(1+\varepsilon) - e^{-i\delta}(1-\varepsilon)|^2 = 2(1+|\varepsilon|^2) - 2(1-|\varepsilon|^2)\cos\delta + 2i(\varepsilon^* - \varepsilon)\sin\delta =$

$= 2(1-\cos\delta) + 2|\varepsilon|^2(1+\cos\delta) + 2\text{Im}(\varepsilon)\sin\delta$.

So,

$P_{K_l' \to K_S}(t) = |\langle K_S|K_L'(t)\rangle|^2 = \frac{1}{2(1+|\varepsilon|^2)}[(1-\cos\delta) + |\varepsilon|^2(1+\cos\delta) + \text{Im}(\varepsilon)\sin\delta]\, e^{-\frac{t}{\tau_S}}$.

After a measuring $R$ giving us $\varepsilon$.

Then measuring $P_{K_l' \to K_S}(t) \Longrightarrow \text{Im}(\varepsilon)$.

We finally obtain phase $(\varphi) = \tan^{-1}\frac{\mathrm{Re}(\varepsilon)}{\mathrm{Im}(\varepsilon)}$.

where $\mathrm{Re}(\varepsilon) = \sqrt{|\varepsilon|^2 - [\mathrm{Im}(\varepsilon)]^2}$.

Note: the preceding expression is based on the complex number $a + ib$, where $a$ and $b$ are real numbers:

$a^2 = |a + ib|^2 - b^2$.

### 7.5.12 Quarter-Wave Plate

A beam of linearly polarized light is incident on a quarter-wave plate(changes the relative phase by 90°) with its direction of polarization oriented at 30° to the optic axis. Subsequently, the beam is absorbed by a black disk. Determine the rate angular momentum is transferred to the disk, assuming the beam carries $N$ photons per second.

In the $\{|x\rangle, |y\rangle\}$ basis, the operator

$\hat{Q} = |x\rangle\langle x| + e^{i\pi/2}|y\rangle\langle y|$,

changes the relative phase by $\frac{\pi}{2}$.

The incident wave, input state

$|in\rangle = \cos 30°\,|x\rangle + \sin 30°\,|y\rangle = \frac{\sqrt{3}}{2}|x\rangle + \frac{1}{2}|y\rangle$.

After the ¼-wave plate

$|out\rangle = \hat{Q}|in\rangle = \left(|x\rangle\langle x| + e^{\frac{i\pi}{2}}|y\rangle\langle y|\right)\left(\frac{\sqrt{3}}{2}|x\rangle + \frac{1}{2}|y\rangle\right) = \frac{\sqrt{3}}{2}|x\rangle + \frac{i}{2}|y\rangle$.

Now, see Problem 7.5.6 **c)**,

$$|R\rangle = \frac{1}{\sqrt{2}}(|x\rangle + i\,|y\rangle) \to \langle R \mid \psi\rangle = \frac{1}{\sqrt{3}}\left(1 + \frac{\sqrt{2}}{2}\right)$$

$$P_R = |\langle R \mid \psi\rangle|^2 = \frac{1}{2} + \frac{\sqrt{2}}{3} \to P_L = 1 - P_R = \frac{1}{2} - \frac{\sqrt{2}}{3}$$

The torque on the disk is the angular momentum transferred per second, which is

amount transferred by $|R\rangle$ per sec + amount transferred by $|L\rangle$ per sec

or

$$N(\hbar P(\hbar) - \hbar P(-\hbar))$$
$$N(\hbar P(R) - \hbar P(L))$$
$$N\hbar\left(\frac{1}{2} + \frac{\sqrt{2}}{3}\right) - N\hbar\left(\frac{1}{2} - \frac{\sqrt{2}}{3}\right) = \frac{2\sqrt{2}}{3}N\hbar$$

Thus, the torque is positive, which implies that the disk will rotate CCW as viewed from the positive $z$-axis.

the photon state $|R\rangle$ carry a unit $\hbar$ of angular momentum parallel to the direction of propagation of the photon.

$|R\rangle = \frac{1}{\sqrt{2}}(|x\rangle + i|y\rangle$.

Then,

$\langle R|out\rangle = \frac{1}{\sqrt{2}}(\langle x| - i\langle y|)\left(\frac{\sqrt{3}}{2}|x\rangle + \frac{i}{2}|y\rangle\right) = \frac{\sqrt{3}+1}{2\sqrt{2}}$.

$P_R = |\langle R|out\rangle|^2 = \frac{2+\sqrt{3}}{4}$,

and

$P_L = 1 - P_3 = 1 - \frac{2+\sqrt{3}}{4} = \frac{2-\sqrt{3}}{4}$.

Or

$\langle L|out\rangle = \frac{1}{\sqrt{2}}(\langle x| + i\langle y|)\left(\frac{\sqrt{3}}{2}|x\rangle + \frac{i}{2}|y\rangle\right) = \frac{\sqrt{3}-1}{2\sqrt{2}}$,

and

$P_L = |\langle L|out\rangle|^2 = \frac{2-\sqrt{3}}{4}$.

The rate at which the angular momentum is absorbed by the black disk

$N\hbar(P_R - P_L) = \frac{\sqrt{3}}{2} \cdot N\hbar$ .

The torque is positive and will rotate counter clock wise as viewed from the positive $z$-axis.

### 7.5.13 What is happening

A system of $N$ ideal linear polarizers is arranged in sequence. The transmission axis of the first polarizer makes an angle $\frac{\varphi}{N}$ with the $y$-axis. The transmission axis of every other polarizer makes an angle $\frac{\varphi}{N}$ with respect to the axis of the preceding polarizer. Thus, the transmission axis of the final polarizer makes an angle $\varphi$ with the $y$-axis. A beam of $y$-polarized photons is incident on the first polarizer

**a)** What is the probability that an incident photon is transmitted by the array of polarizers?

Photons exiting the last polaroid are in the state

$|y'(\varphi)\rangle$.

So, after the first polarizer a photon is in the state $|y'(\varphi/N)\rangle = \cos\frac{\varphi}{N}|y\rangle$ .

Consequently, the probability passing through the first polaroid

$\left|\left\langle y'\left(\frac{\varphi}{N}\right)\middle|y\right\rangle\right|^2 = \cos^2\frac{\varphi}{N}$ .

Then, the probability of being transmitted through the entire array is

$\left(\cos^2\frac{\varphi}{N}\right)^N$.

**b)** The probability of transmission for $\frac{\varphi}{N} \ll 1$.

We expand $\cos\frac{\varphi}{N}$

$\cos\frac{\varphi}{N} \approx 1 - \frac{1}{2}\left(\frac{\varphi}{N}\right)^2 \Longrightarrow \cos^2\frac{\varphi}{N} = 1 - (\frac{\varphi}{N})^2$

Using this result we expand $\left(\cos^2\frac{\varphi}{N}\right)^N$:

$\lim_{N\to\infty}\left(\cos^2\frac{\varphi}{N}\right)^N = \lim_{N\to\infty}(1-(\frac{\varphi}{N})^2)^N = \lim_{N\to\infty}[1 - N\left(\frac{\varphi}{N}\right)^2] = \lim_{N\to\infty}(1-\frac{\varphi^2}{N})$.

**c)** Now, consider the special case with the angle 90°.

For $\varphi = 90°$ ,

$|out\rangle = |y'\rangle = |x\rangle$.

So, one could think the probability could become 0:

$\langle x|y\rangle = 0$.

However, look at the result under b). The probability becomes $\lim_{N\to\infty}(1-\frac{\varphi^2}{N}) = 1$.

### 7.5.14 Interference

Photons freely propagating through a vacuum have one value for their energy:

$E = h\nu$. This is therefore 1-D quantum mechanical system, and since the energy of a freely propagating photon does not change, it must be an eigenstate of the energy operator. So, if the state of the photon at $t = 0$ is denoted as $|\psi(0)\rangle$, then the eigenstate can be written as

$\hat{H}|\psi(0)\rangle = E|\psi(0)\rangle$.

To see what happens to the state of the photon with time, we apply the evolution time operator

$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle = e^{-ih\nu t/\hbar}|\psi(0)\rangle = e^{-i2\pi\nu t}|\psi(0)\rangle =$

$= e^{-i2\pi x/\lambda}|\psi(0)\rangle$,

where use has been made of $\nu = c/\lambda$ and the distance travelled is $x = ct$. Furthermore, the probability of finding the photon at various points is homogeneous distributed, i.e., no dependence on the position.

Consider the following situation: Two sources of identical photons face each other and emit photons at the same time. The distance between the sources is $L$. The setup is illustrated in the Figure below.

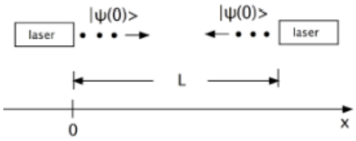



Figure 7.2: Interference Setup

Notice that we are assuming the photons emerge from each source in state $|\psi(0)\rangle$. In between the two light sources we can detect photons but we do not know from which source they originated. Therefore, we have to treat the photons at a point along the $x$-axis as a superposition of the time-evolved state from the left source and the time-evolved state from the right source.

**a)** What is the superposition state $|\psi(t)\rangle$ at a point $x$ between the two sources? The wave length of the photons is $\lambda$.

The super position of the two sources at $x$ is:

$|\psi(t)\rangle = (e^{-\frac{i2\pi x}{\lambda}} + e^{-\frac{i2\pi(L-x)}{\lambda}})|\psi(0)\rangle$.

**b)** Find the relative probability $P(x)$ of detecting a photon at point $x$ by evaluating $|\langle\psi(t)|\psi(t)\rangle|^2$ at point $x$.

$$P(x) = |\langle\psi(t)|\psi(t)\rangle|^2 = |e^{-\frac{i2\pi x}{\lambda}} + e^{-\frac{i2\pi(L-x)}{\lambda}}|^2|\langle\psi(0)|\psi(0)\rangle|^2 =$$

$$= \left(e^{\frac{i2\pi x}{\lambda}} + e^{\frac{i2\pi(L-x)}{\lambda}}\right)\left(e^{-\frac{i2\pi x}{\lambda}} + e^{-\frac{i2\pi(L-x)}{\lambda}}\right) = 2 + e^{\frac{i2\pi(2x-L)}{\lambda}} + e^{-\frac{i2\pi(2x-L)}{\lambda}} =$$

$$= 2 + 2\cos[\frac{2\pi}{\lambda}(2x-L)] = 4\cos^2[\frac{2\pi}{\lambda}(x-\frac{L}{2}] ,$$

where use has been made of

$2\cos^2\varphi = \cos 2\varphi + 1$.

**c)** $4\cos^2[\frac{2\pi}{\lambda}(x-\frac{L}{2}]$ describes an interference pattern between the two sources. Dark and bright spots.

### 7.5.15 More interference

The interference result above draws our attention to the two slit experiment. The situation is illustrated below:

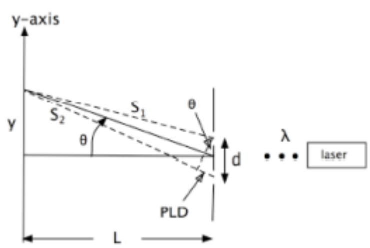



Figure 7.3: Double-Slit Interference Setup

The distance between the slits, $d$ is quite small (less than a $mm$) and the distance up the $y$-axis(screen) where the photons arrive is much, much less than $L$( the distance between the slits and the screen). In the Figure above, $S_1$ and $S_2$ are the lengths of the photon paths from the two slits to a point a distance $y$ up the $y$-axis from the midpoint of the slits. The most important quantity is the difference in length(PLD) between $S_1$ and $S_2$. The path length difference(PLD) is shown in the Figure above.

PLD:

$S_1^2 = (y - \frac{d}{2})^2 + L^2$,

and

$S_2^2 = (y + \frac{d}{2})^2 + L^2$.

With the approximations applied:

$S_2^2 - S_1^2 \approx 2yd \Longrightarrow (S_2 - S_1)(S_2 + S_1) \approx 2yd \Longrightarrow$PLD$\approx \frac{2yd}{S_2+S_1}$.

With the approximation $y \ll L \Longrightarrow S_2 + S_1 \approx 2L$,

PLD$\approx \frac{2yd}{S_2+S_1} \approx \frac{yd}{L}$.

With the classical interference of light waves, Fitzpatrick page 21 Undergraduate Course, *the light intensity $I(y)$ on the screen a distance y from the center-line is*

$I(y) \propto \cos^2(\frac{\pi yd}{\lambda L})$.

What do we find for the relative probability $P(y)$ of detecting a photon at various points along the screen).

Now, we use the result of Problem 7.5.14 with the two wave functions:

$|screen\ at\ y\rangle = |\psi(y)\rangle = (e^{-\frac{i2\pi S_1}{\lambda}} + e^{-\frac{i2\pi S_2}{\lambda}})|\psi(0)\rangle$.

Then

$P(y) = |\langle\psi(y)|\psi(y)\rangle|^2 = |(e^{-\frac{i2\pi S_1}{\lambda}} + e^{-\frac{i2\pi S_2}{\lambda}})|^2 = 2 + 2\cos[\frac{2\pi}{\lambda}(S_2 - S_1)] =$

$= 4\cos^2[\frac{\pi}{\lambda}(S_2 - S_1)]$.

We obtained above

$(S_2 - S_1)(S_2 + S_1) \approx 2yd$,

and with $S_2 + S_1 \approx 2L$,

$(S_2 - S_1) = \frac{yd}{L}$.

So,

$P(y) = |\langle\psi(y)|\psi(y)\rangle|^2 = 4\cos^2[\frac{\pi yd}{\lambda L}]$.

### 7.5.16 The Mach-Zehnder Interferometer and Quantum Interference

**Background information**: Consider a single photon incident on a 50-50 beam splitter (that is, a partially transmitting, partially reflecting mirror, with equal coefficients). Whereas classical electromagnetic energy divides equally, the photon is indivisible. That is, if a photon-counting detector is placed at each of the output ports (see figure below), only one of them clicks. Which one clicks is completely random (that is, we have no better guess for one over the other).

Figure 7.4: Beam Splitter

The input-output transformation of the waves incident on 50-50 beam splitters and perfectly reflecting mirrors are shown in the figure below.

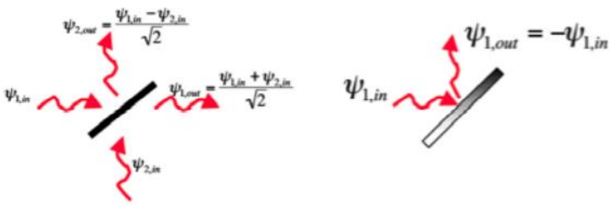



Figure 7.5: Input-Output transformation

**a)** Show that with the above results, there is a 50-50 chance of either of the detectors, shown in Figure 7.4, to click.

$|\psi_{in}\rangle = \frac{1}{\sqrt{2}}|\psi_{1,out}\rangle + \frac{1}{\sqrt{2}}|\psi_{2,out}\rangle$.

Then,

$|\psi_{1,out}\rangle = \frac{1}{\sqrt{2}}|\psi_{in}\rangle$, and $|\psi_{2,out}\rangle = \frac{1}{\sqrt{2}}|\psi_{in}\rangle$ .

The probabilities

$P_{1,out} = |\langle\psi_{1,out}|\psi_{1,out}\rangle|^2 = \frac{1}{2}|\langle\psi_{in}|\psi_{in}\rangle|^2 = \frac{1}{2}$,

or in terms of wave function

$P_{1,out} = \int |\psi_{1,out}|^2 dx = \frac{1}{2}$,

and

$P_{2,out} = |\langle\psi_{2,out}|\psi_{2,out}\rangle|^2 = \frac{1}{2}|\langle\psi_{in}|\psi_{in}\rangle|^2 = \frac{1}{2}$,

or in terms of wave function

$P_{2,out} = \int |\psi_{2,out}|^2 dx = \frac{1}{2}$.

Note Boccio:

NOTE: The photon is found at one detector *or* the other, never both. The photon is indivisible. This contrasts with classical waves where half of the intensity goes along one way and half the other; an antenna would also receive energy. We interpret this as the mean value of a large number of photons.

**b)** Now we set up a Mach-Zehnder interferometer, Figure below,

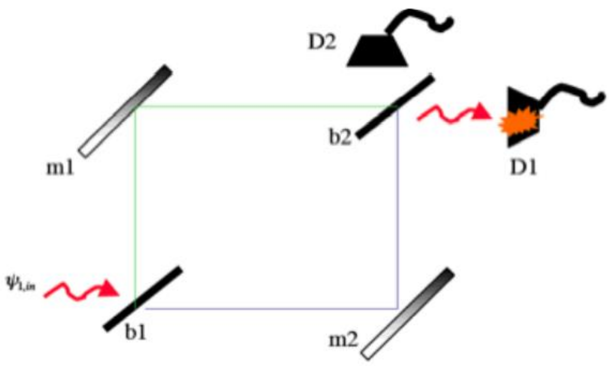


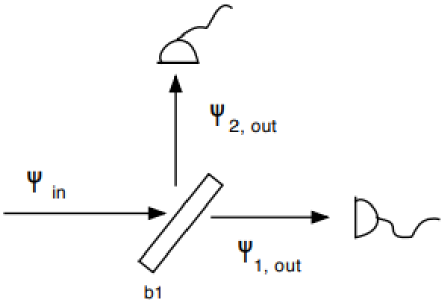

Figure 7.6: Input-Output transformation

The wave is split at beam-splitter b1, where it travels either path b1-m1-b2(call it the green path) or the path b1-m2-b2 (call it the blue path). Mirrors are then used to recombine the beams on a second beam splitter, b2. Detectors D1 and D2 are placed at the two output ports of b2.

**a)** Assuming the paths are perfectly balanced(i.e., equal length), show that the probability for detector D1 to click is 100% - *no randomness.*

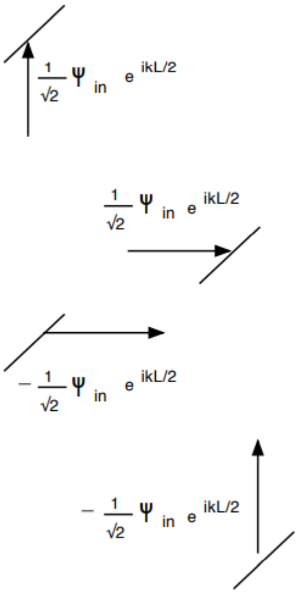
The wave function is split at b1, sent along two different paths, and recombined at b2. To find the wave functions impinging on D1 and D2 the transformation rules are sequentially applied.

- Beam splitter b1

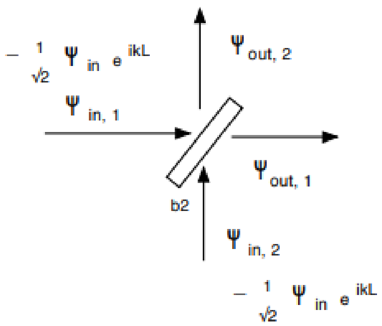



Then propagation over a distance $L/2$ giving a phase of $e^{ikL/2}$.

- Bounce of mirrors m1 and m2




- Then propagation over another distance $L/2$ giving as total phase $e^{ikL}$, and
- Beam splitter b2




**Remark:** I copied the above Figure from the Undergraduate Course $\psi_{in} \Longrightarrow -\frac{1}{\sqrt{2}}\psi_{in}e^{ikL}$.

Now $\psi_{1,out}$ is the sum of two wave functions:

$\psi_{out,1} = \frac{\psi_{in,1}+\psi_{in,2}}{\sqrt{2}} = e^{ikL}\psi_{in}$,
and
$\psi_{out,2} = \frac{\psi_{in,1}-\psi_{in,2}}{\sqrt{2}} = 0$.
Consequently,
$P_{out,1} = \int |\psi_{in}|^2 dx = 1$,
and
$P_{out,2} = \int |\psi_{in}|^2 dx = 0$ .
**c)** Classical reasoning would predict a probability for D1 to click given by
$P_{D1} = P(transmission\ at\ b2|greenpath)P(green\ path) +$
$+P(reflection\ at\ b2|blue\ path)P(blue\ path)$.
We know there to be a 50-50 probability for the photon to take the blue or green path which implies
$P(blue) = P(green) = \frac{1}{2}$ .
Along the green path at b2 we have a 50% chance of transmission(similarly for reflection of the blue path):
$P(transmission\ at\ b2|green\ path) = P(reflection\ at\ b2|blue\ path) = \frac{1}{2}$ .
Hence
$P_{D1} = \frac{1}{2}\cdot\frac{1}{2} + \frac{1}{2}\cdot\frac{1}{2} = \frac{1}{2}$.
Conclusion: the chance of D1 firing is 50-50 $\Longrightarrow$ Random.
Now the quantum case:
The two paths leading to D1 are indistinguishable, so there is interference and the wave function is
$\psi_{total} = (\frac{1}{\sqrt{2}}\psi_{in}e^{ikL} + \frac{1}{\sqrt{2}}\psi_{in}e^{ikL})/\sqrt{2}$ .
Then,
$P_{D1} = \int |\psi_{total}|^2 dx = \frac{1}{4}(4\int|\psi_{in}|^2 dx = 1$.
With the path to D2 we have: $P_{D2} = 0$ .
**d)** How to change the set up so that the detector D2 clicked with 100% probability? How to make D2 click at random? The basic geometry remains the same.
Now we want constructive interference for the paths leading to D2 and destructive interference for the paths leading to D1.
The only possibility we have to do the job is changing the relative phase by changing the length of the path by moving m1 or m2. Resulting in the following two expressions:
$\psi_{out,1} = (\frac{1}{\sqrt{2}}\psi_{in}e^{ik(L+\Delta L)} + \frac{1}{\sqrt{2}}\psi_{in}e^{ikL})/\sqrt{2}$ ,
and
$\psi_{out,2} = (\frac{1}{\sqrt{2}}\psi_{in}e^{ik(L+\Delta L)} - \frac{1}{\sqrt{2}}\psi_{in}e^{ikL})/\sqrt{2}$ .
For the probabilities we have,
$P_{D1} = \int |\psi_{out,1}|^2 dx = \frac{1}{4}\int |\psi_{in}e^{ik(L+\Delta L)} + \psi_{in}e^{ikL}|^2\, dx =$
$= \frac{1}{4}\left(2 + e^{ik\Delta L} + e^{-ik\Delta L}\right)\int|\psi_{in}|^2 dx = \frac{1}{2}[1+\cos(k\Delta L)] = \cos^2(\frac{k\Delta L}{2})$ .
Similarly
$P_{D2} = \int |\psi_{out,2}|^2 dx = \sin^2(\frac{k\Delta L}{2})$ .
To obtain
$P_{D1} = 0$ ,

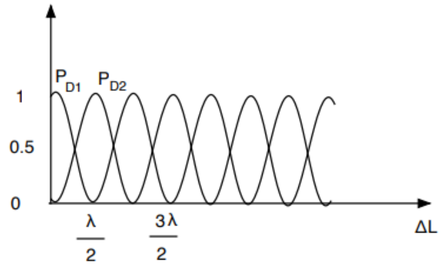
and

$P_{D2} = 1,$

we have to set, with $\sin^2(\frac{k\Delta L}{2}) = 1,$

$k\Delta L = m\pi, m$ odd, $\Longrightarrow \Delta L = m\lambda/2.$

In the figure below the probability of detecting a signal in D1 and D2 as a function of $\Delta L$ is presented, Boccio,




### 7.5.17 More Mach-Zehnder

An experimenter sets up two optical devices for single photons. The first, (i) in the figure below, is a standard balanced Mach-Zehnder interferometer with equal path lengths, perfectly reflecting mirrors (M) and 50-50- beam splitters (BS).

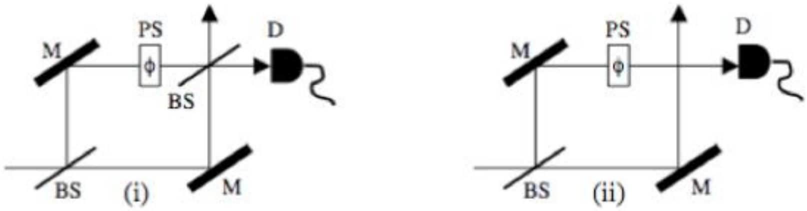



*Figure 7.7 Boccio: Mach-Zehnder Setups*

A transparent piece of glass which imparts a phase shift (PS) $\phi$ is placed in one arm. Photons are detected (D) at one port. The second interferometer, (ii) in the figure above, is the same except that the final beam splitter is omitted.

Sketch the probability of detecting the photon as a function of $\phi$ for each device.

Interferometer (i) is similar to Problem 7.5.16 **d)**. There, the phase shift $\phi$ is obtained by a difference in path length $\Delta L$.

Two cases in 7.15.16 **d),** let us denote $\frac{k\Delta L}{2} = \phi,$

- In phase $\phi = 0, \pi, 2\pi, \ldots$..
- Out of phase $\phi = \frac{\pi}{2}, \frac{3\pi}{2}$ , ...

In (ii), without the final beam splitter, there is only one path that leads to D ( the top path). Consequently there is no interference. Hence, $P_D = \frac{1}{2}$.

# 8 Schrödinger Wave Equation 1-Dimensional Quantum Systems, Page 533

## 8.1 The coordinate Representation

The steps to form a representation are presented:
- a complete orthonormal set of basis vectors,
- the identity operator,
- an arbitrary vector presented as a linear combination of basis vectors.

An important representation is by the eigenstates in position representation.
This is illustrated in Eqs. (8.3)-(8.6), pages 533 and 534.
The wave function is defined, Eq. (8.6).
The bra vector and normalization condition are given in Eqs.(8.7) and (8.8).
Position eigenvectors are not normalizable. For this reason Dirac introduced the delta-function to be used for normalization. Top page 535.
In addition to the position operator $\hat{Q}$ , we have the linear momentum operator $\hat{P}$, see Eq.(8.14) leading to the momentum representation.

**Note**: The second line of Eq.(8.19) should read
$\frac{1}{(2\pi\hbar)^3}\int |\langle\vec{p}|\psi\rangle|^2\, d\vec{p} = \frac{1}{(2\pi\hbar)^3}\int |\Psi(\vec{p})|^2\, d\vec{p}$ .

For normalization in the momentum representation, $\delta$-function normalization is applied, Eq. (8.22). In Eq. (8.23), the last line, $\langle\vec{p}\psi\rangle$ should read $\langle\vec{p}|\psi\rangle$.
At the top of page 537, Boccio referred to Eq.(4.413) where the connection between the position and momentum representation is introduced.:
$\langle\vec{x}|\vec{p}\rangle = e^{i\vec{p}\cdot\vec{x}/\hbar}$ , Eq.(8.25).
The relation with Fourier transform is rehearsed.
In Eq. (8.30) use is made of
$\hat{p} = -i\hbar\nabla$ .

**Note**: Eq.(8.30) $\Longrightarrow$ second line $\langle\vec{x}|\hat{P}|\psi\rangle = \frac{1}{(2\pi\hbar)^3}\int(-i\hbar\nabla)\langle\vec{x}|\vec{p}\rangle\langle\vec{p}|\psi\rangle d\vec{p} \Longrightarrow$
$\Longrightarrow \frac{-i\hbar\nabla}{(2\pi\hbar)^3}\int\langle\vec{x}|\vec{p}\rangle\langle\vec{p}|\psi\rangle d\vec{p} = -i\hbar\nabla\langle\vec{x}|\psi\rangle$.

Next the momentum operator as the generator for displacements is discussed, Eq. (8.33). then, with the results Schrödinger's wave equation is derived.
In Eq. (8.38) the time independent Schrödinger equation is presented using the Hamiltonian.

**Note:** Eq. (8.41) $|\vec{x}\rangle\hat{U}(t)|\psi_E\rangle$ should read $\langle\vec{x}|\hat{U}(t)|\psi_E\rangle$ .

The time dependent Schrödinger equation is presented in Eq. (8.42).

## 8.2 The Free Particle and Wave Packets

Boccio started this section with the potential energy in the one-particle Schrödinger equation to be zero: the free particle.
The eigenfunctions for this case are given in Eq. (8.45), the plane wave.

**Note**: Eq. (8.47)→ $|\vec{x},t\rangle = e^{-iEt/\hbar}|\vec{x},0\rangle$.

Then, $\langle \vec{x}, t|\psi_E\rangle = e^{-iEt/\hbar}\langle \vec{x}, 0|\psi_E\rangle$,
or should it be $\langle \vec{x}, t|\psi_E\rangle = e^{iEt/\hbar}\langle \vec{x}, 0|\psi_E\rangle$? Does it matter?
At the bottom of page 541, Boccio started the analysis of the wave packet with a width of $\Delta\vec{p}$, illustrated in Figure 8.1 :

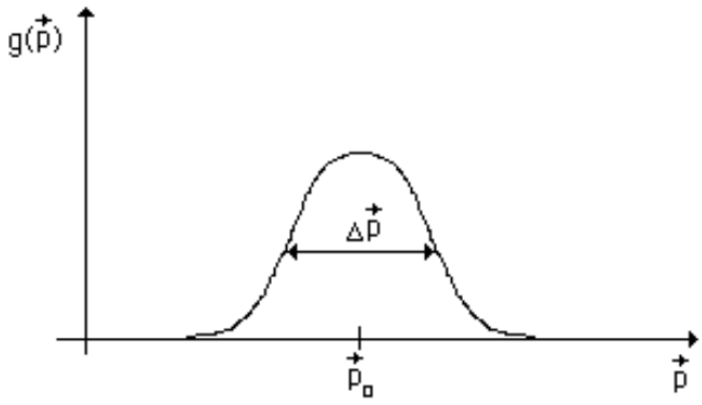



Figure 8.1: Weight Function

where $g(\vec{p})$ is the weight function.

Deriving Eq.(8.54) use has been made of $\nabla_{\vec{p}}(E) \cong \frac{\frac{d}{d\vec{p}_0}\vec{p}_0^2}{2m} = \frac{\vec{p}_0}{m} = \vec{v}$, the group velocity of the wave packet.
In Eq.(8.55): $\frac{\partial}{\partial p_x}(Et) = vt = x$.
This analysis resulted in the Heisenberg uncertainty principle, top page 544.

## 8.3 Derivation of the Uncertainty Relation in General

A new operator is introduced: the difference between an operator and its expectation value.
The mean standard deviation is derived, Eq.(8.59), where
$\frac{1}{N}\sum_{i=1}^{N}(q_i\, q_{average}) = q_{average} \cdot \frac{1}{N}\sum_{i=1}^{N} q_i = (q_{average})^2$.
In Eqs.(8.61) en (8.62), Boccio used the two new operators as defined in Eq.(8.58).
In Eq. (8.64) use has been made of
$[\hat{D}_A, \hat{B}] = [\hat{A} - \langle\hat{A}\rangle, \hat{B}] = \hat{A}\hat{B} - \langle\hat{A}\rangle\hat{B} - \hat{B}\hat{A} + \hat{B}\langle\hat{A}\rangle = [\hat{A}, \hat{B}]$,
since $-\langle\hat{A}\rangle\hat{B} + \hat{B}\langle\hat{A}\rangle = 0$ .
In Eq.(8.70), the anti-commutator has been used:
$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ .
Finally, (8.71) is obtained using Eqs(8.69)-(8.70).
Boccio concluded this section with:
*"…..commuting observables do not have an uncertainty principle!"*
Commuting observables can be measured simultaneously.

### 8.3.1 The Meaning of the Indeterminacy Relations

The significance of indeterminacy relations with respect to experiments is discussed.
Boccio showed the results of measurement of the position observable $Q$ and the momentum observable $P$. The results of these measurements are shown in Figure 8.2 page 547. The standard deviations $\Delta Q$ and $\Delta P$ are given.

Boccio paid attention to the difference between the standard deviations and the errors of measurement.

### 8.3.2 Time-Energy Uncertainty Relations

In Eq.(8.77) the relation for any operator in the Heisenberg picture is given. See also chapter 6 of the Undergraduate Course.
Then, Boccio explained the so-called Time-Energy Uncertainty Relation as presented in Eq.(8.85) not to have any meaning.

## 8.4 The Wave Function and Its Meaning

Boccio started this section with the time dependent Schrödinger equation and made the remark this equation not to be representing a real wave. This misinterpretation results from working with a simple one particle system.
Then, Boccio started working with a more complicated case of a system of $N$ particles, page 550. At the top of page 551, Boccio explained why in a $N$ particle system we are not dealing with $N$ individual interacting waves. Furthermore the statistical interpretation of $N$- particle wave function is demonstrated with the experimental setup as shown in Figure 8.3.

## 8.5 One-Dimensional Systems, page 553

The time-independent Schrödinger equation in 1-D is given in Eq.(8.97).
In this section Boccio analysed the general continuity properties of derivative of the wave function $\psi_E(x)$.
Boccio summarized a range of physical systems which can be studied using 1-D potential functions. In the following sections some examples are presented.

### 8.5.1 One-Dimensional Barrier

The potential energy function is in this case a step, presented in Eq.(8.110).
Figure (8.4), page 556 Boccio

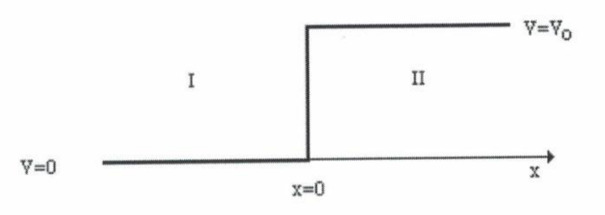



Figure 8.4: Finite Step barrier

The general solution for region I for $V = 0$, is presented in Eq. (8.117).
The solution in region I can be thought of as to be an incident wave in the positive $x$-direction and a reflected wave in the negative $x$-direction.
In region II we have the case with $V \neq 0$.
To find the unknown amplitudes of the travelling waves, the continuity conditions at $x = 0$, come into play.
In Eq. (8.126), the relations between the amplitudes are presented.
Keep in mind: the subscript $I$ and $II$ in Eqs. (8.132) and (8.133) refers to $x < 0$, and $x > 0$ respectively.
Next, Boccio introduced the reflection and transmission probabilities at the barrier, Eq. (8.134).

Eqs. (8.126) and (8.134) $\Longrightarrow$ Eqs.(8.135) and (8.136).
Then , Boccio analysed the wave packet case for $E > V_0$ .
After the wave packet analysis Boccio investigated the case $E < V_0$.

### 8.5.2 Tunneling

In this section the potential is a kind of Hat function: a potential barrier.
The case $E > V_0$ is similar to the case analysed in section 8.5.1.
With $E < V_0$, quantum tunneling is introduced.

### 8.5.3 Bound States

**Infinite Square Well**
Sometimes also called Infinite Potential Well.
This case is illustrated in the Figure 8.6 below (Boccio).

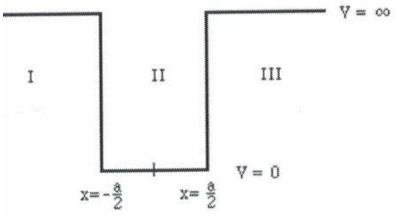



Figure 8.6: Infinite Square Well

**Note**: Eq.(8.190) should read
$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} = E\psi_{II}$,
where $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$ .

Eq.(8.198), normalization gives
$\tilde{A}_n = \sqrt{\frac{2}{a}}$.
So, Eq.(8.(202) reads
$\psi_{II}(x) = \sqrt{\frac{2}{a}}\sin k_n\,(x + \frac{a}{2})$ .
On page 569 the parity operator is introduced and defined in Eq.(8.214)
$\langle \vec{x}|\hat{\mathcal{P}}|\psi\rangle = \langle -\vec{x}|\psi\rangle$.
**The Finite Square Well**
Sometimes called the Square Potential Well.
Set $V = \infty \Longrightarrow V = 0$, and $V = 0 \Longrightarrow V = -V_0$, in Figure 8.6 .

**Note**:
- in Eq.(8.230) $fracp\hbar \equiv \frac{p}{\hbar}$,
- in Eq.(8.231) $fracp\hbar k \equiv \frac{p}{\hbar k}$ .

The solutions for the finite square well, $E < 0$ , are transcendental equations Eqs.(8.227)-(8.232).
Next, Boccio discussed the possible solutions of the transcendental equations.
- Graphical solutions are presented in Figure 8.8.

- Numerical solutions.

Eq. (8.239): $frac\alpha^2 \cos^2\frac{\alpha}{2} \equiv \frac{\alpha^2}{\cos^2\frac{\alpha}{2}}$.

**Transmission Resonances**

This sub section is about $E > 0$, the particle is unbounded. When the particle encounters the well it is either reflected or transmitted.

Boccio presented the wave equations for the three regions and calculated the transmission coefficient by applying the continuity conditions for the wave functions.

In Figure 8.9 a plot of the transmission coefficient over the square well is presented.

Boccio presented the results of a particle for the case given in Eq.(8.245)⟹no reflected wave.

**What do wave packets say?**

In this subsection Boccio discussed the results of a wave packet of-resonance and near-resonance.

**Time Delay at a Square Well**

The transmission of a wave packet through a square is considered., Figure 8.10.

The time delay of a wave packet has been discussed in section 8.5.1.

### 8.5.4 Delta Function Potentials page 581

The delta function potential energy is presented in Eq.(8.266).

Now the derivative of the wave function is not continuous at the delta function. The resulting discontinuity is found by integrating the Schrödinger equation over a small region at the position of the delta function potential.

**Transmission Problem.**

A delta function barrier is assumed.

The transmission probability, Eq.(8.275), and the reflection probability, Eq.(8.276), are derived.

**Bound-State Problem**

Now,

$V(x) = -A\delta(x-a)$.

The bound state energy is presented in Eq.(8.285).

**Double Delta Function Potential**

The potential is constructed from two delta functions, one at $x = -\frac{l}{2}$, and the other at $x = \frac{l}{2}$. Boccio investigate first the barrier potential.

**Transmission problem**

Now, there three regions to be considered.

Boccio calculated the transmission probability defined as the ratios of square of the amplitudes of the incoming wave from the left and the transmitted wave at the right of the duo barrier.

Here Boccio used the expression "*Much algebra gives….*"

**The Bound-State Problem**

The strength of the duo delta function $u < 0$ .

The solutions in the three regions are presented.

**Graphical Solutions**

In this subsection Boccio presented the graphical solutions of the transcendental functions of the double delta function bound states.

## 8.6 Harmonic Oscillators

The potential energy function is presented in Eq.(8.313).
Boccio analysed the system in position representation and *solve the Schrödinger equation using differential equations techniques.*

### 8.6.1 Differential Equation Method

With the polynomial expansion used, Boccio arrived at the Hermite polynomial represented by the differential equation Eq.(8.377).
The Schrödinger wave functions are given by Eq.(8.346).
Eq.(8.348):

$$\int_{-\infty}^{\infty} e^{-s^2+2sq-t^2+2tq-q^2} dq = e^{2st} \int_{-\infty}^{\infty} e^{-s^2+2sq-t^2+2tq-q^2-2st} dq =$$

$$= e^{2st} \int_{-\infty}^{\infty} e^{-(q-s-t)^2} \, dq = e^{2st}\sqrt{\pi} \, .$$

### 8.6.2 Algebraic Method

The algebraic method is based on two new operators given in Eq.(8.354).
Eqs.(8.354)- (8.356) are explained in more detail in Chapter 10.6 of Susskind.
At the bottom of page 595, the raising and lowering operators are introduced.

**Coherent States**

Boccio used the ladder formalism in an exercise.
The eigenstates of the lowering operator are looked for.
The result is presented in Eq.(8.390).
To derive Eq.(8.395) use has been made of Eq.(8.355).
On page 600, Boccio presented the results of the investigation into the expectation value of the position operator. *The expectation value behaves like a classical oscillator.*
Next, a term is added to the Hamiltonian, representing a charged oscillator in an electric field, Eq.(8.400).

**Using the Translation Operator.**

## 8.7 Green's Functions

This section is about the Green's function technique for solving differential equations.
The wave function solution with the Green's function technique is presented in Eq.(8.428).
Then two examples are discussed:

**Example #1- Single Delta Function**

"*A very important lesson to learn*", Boccio.
Here contour integration is used.

**Example #2 – Double Delta Function**

Here two integrals need to be evaluated.

## 8.8 Charged Particles in Electromagnetic Fields.

Boccio started with the classical representation. Then, with this information the Lagrangian and Hamiltonian are constructed.
On page 611 gauge transformation has been introduced.

**The Aharonov-Bohm Effect**

In Eq.(8.472) the Ampere$\tilde{O}$s law is presented.
Boccio illustrates: *"…. most powerfully it is the electromagnetic potential, rather than the electromagnetic fields,……., that are the fundamental physical quantities in quantum mechanics."* The vector potential is the fundamental physical filed.

## 8.9 Time Evolution of Probabilities

It is about the fundamental question: *If the system is in the state $|\alpha\rangle$ at time $t = 0$, what is the probability that it will be in the state $|\beta\rangle$ at time $t$?*

The answer to this question is given by Eq.(8.473). As usual, the time evolution operator comes into play.

Then, Boccio presented the most important rule in quantum mechanics:

*Evaluating an amplitude involving a particular operator switch to a basis for the space corresponding to the eigenvectors of that operator.*

Boccio presented the procedure in four steps and applied the procedure to the infinite square well.

**Note**: this procedure compares with the recipe which can be found in Susskind section 4.13.

**Note:** In Eq. (8.481) the results of the infinite well, $[-\frac{a}{4},\frac{a}{4}]$ are presented. The results in Eq.(8.482)-(8.484) are a mixture of a well $[-\frac{a}{4},\frac{a}{4}]$, and $[-\frac{a}{2},\frac{a}{2}]$. A bit confusing.

## 8.10 Numerical Techniques

A numerical scheme for solving the 1-D Schrödinger equation is presented.

The procedure is illustrated with the harmonic oscillator potential.

The steps of the solution method are presented on pages 620 1nd 621.

MATLAB language has been used, pages 621-622.

## 8.11 Translation Invariant Potential-Bands page 623

A potential which is periodic in space is considered. Think of an electron in a 1D crystal lattice.

**Example**

Boccio illustrated the analysis with a 1D periodic  array of delta functions.

## 8.12 Closed Commutator Algebras and Glauber's Theorem

The commutator algebra of the harmonic oscillator potential is presented in Eq.(8.524).

This equation represents a closed set of operators: a *closed commuter algebra.*

On page 628 Boccio proved *Glauber's Theorem*.

**Note**: In the proof the assumption Eq.(8.525) instead of (8.526) is used.

Deriving Eq. (8.528) use has been made of:

$\sum(-1)^n \frac{x^n}{(n-1)!}\hat{A}^{n-1} = x\sum(-1)^n \frac{x^{n-1}}{(n-1)!}\hat{A}^{n-1} = -x\sum(-1)^{n-1}\frac{x^{n-1}}{(n-1)!}\hat{A}^{n-1}$. This becomes with a "new" $n$ : $-x\sum(-1)^n\frac{x^n}{n!}\hat{A}^n = -xe^{-\hat{A}x}$ .

**Note:** Eqs. (8.528) and (8.529) $\rightarrow$ $[\hat{B}, e^{-\hat{A}x}] = \hat{B}\, e^{-\hat{A}x} - e^{-\hat{A}x}\hat{B} = -e^{-\hat{A}x}[\hat{B},\hat{A}]x$.

Multiply Eq.(8.529) to the left with $e^{\hat{A}x}$ and Eq.(8.530) is obtained.

Boccio demonstrated the Baker-Hausdorff identity for $x = 1$, Eq.(8.534), top of page 628.

## 8.13 Quantum Interference with Slits page 630

In this experiment the $y$-component of momentum of a particle passing through a system of slits is measured.

### 8.13.1 Introduction

Boccio presented some of the history of the double-slit experiment.

### 8.13.2 Probability functions and quantum interference
In Figure 8.20 a schematical representation of scattering from slits is shown.
Th basis vectors used by Boccio are the momentum eigenvectors $|p_y\rangle$.
Boccio evaluated in the following section the integral of the amplitude equation.
This is done for a four source-slit system, including the double slit.
### 8.13.3 Scattering from a narrow slit
The eigenfunction of position after emerging from the slit is the Dirac delta function, Eq.(8.541).
### 8.13.4 Scattering from a double slit(narrow)
The state vector for this experiment is given by Eq.(8.544).
The angular distribution of scattered particles is shown in Figure 8.21.
### 8.13.5 Scattering from a slit of finite width
A slit of finite width is, Boccio, "…..*an imperfect apparatus for measuring position."*

### 8.13.6 Scattering from a double finite-width slit
The angular distribution of scattered particles is shown in Figure 8.24
### 8.13.7 Conclusions
Boccio concluded *the results obtained are in agreement with wave optics*.
## 8.14 Algebraic Methods- Supersymmetric Quantum Mechanics
### 8.14.1 Generalized Ladder Operators
The question to be answered in this section is: Can the commutator algebra used for the harmonic oscillator be used for other Hamiltonians?
Eq.(8.564) follows from:
$\hat{H}_0\psi_0(x) = E_0\psi_0(x)$.
I explain the step in Eq.(8.572) between the second and the third line.
I assume $\psi_0'$ to be $\frac{d}{dx}\psi_0$ :
$\hat{a}f(x) = \pm\frac{d}{dx}\left(\frac{\psi_0'}{\psi_0}\right)f(x) \mp \left(\frac{\psi_0'}{\psi_0}\right)\frac{d}{dx}f(x)$,
where $\pm\frac{d}{dx}\left(\frac{\psi_0'}{\psi_0}\right)$ is part of the operator $\hat{a}$.
So, operate
$\pm\frac{d}{dx}\left(\frac{\psi_0'}{\psi_0}\right)$
on $f(x)$, and we have
$\pm\frac{\psi_0'}{\psi_0}\frac{d}{dx}f(x) \pm f(x)\frac{d}{dx}\left(\frac{\psi_0'}{\psi_0}\right)$.
The second line of Eq. (8.572) becomes
$\pm\frac{\psi_0'}{\psi_0}\frac{d}{dx}f(x) \mp \left(\frac{\psi_0'}{\psi_0}\right)\frac{d}{dx}f(x) \pm f(x)\frac{d}{dx}\left(\frac{\psi_0'}{\psi_0}\right)$.
Next, I assume the square brackets to represent the commutator notation.
Hence
$\left[\pm\frac{d}{dx}\left(\frac{\psi_0'}{\psi_0}\right)\right] = \left\{\pm\frac{d}{dx}\left(\frac{\psi_0'}{\psi_0}\right) \mp \left(\frac{\psi_0'}{\psi_0}\right)\frac{d}{dx}\right\}f(x) \to \pm\frac{d}{dx}\left(\frac{\psi_0'}{\psi_0}\right)f(x) \mp \left(\frac{\psi_0'}{\psi_0}\right)\frac{d}{dx}f(x) =$
$= \pm\frac{\psi_0'}{\psi_0}\frac{d}{dx}f(x) \pm f(x)\frac{d}{dx}\left(\frac{\psi_0'}{\psi_0}\right) \mp \left(\frac{\psi_0'}{\psi_0}\right)\frac{d}{dx}f(x)$,
and the second line of Eq.(8.572) is obtained from the third line.

On page 639 the supersymmetric partner and the supersymmetric potentials are introduced.
Then, Boccio introduced a new operator $\hat{\beta} = \frac{d}{dx}$, Eq.(8.578).

### 8.14.2 Examples

Boccio presented some examples of generalized ladder operators of section 8.14.1.
1) **Harmonic Oscillator**
The ground state is recovered, Eq.(8.610).
Iteration using the raising and lowering operators is illustrated in the Book by Susskind.
2) **Refection-Free Potentials**
In Eq.(8.613), Boccio introduced
$\Phi(x) = \tanh x$ .
I suppose $\Phi$ to be defined in Eq.(8.592):
$\Phi = -\frac{\psi_0^{0\prime}}{\psi_0^0}$,
and Eq.(8.599)
$\Phi(x) = \frac{d\psi_0^0}{\psi_0^0}$.
To obtain Eq(8.614), Eqs.(8.594) and (8.595) are used.

### 8.14.3 Generalizations

Boccio raised the question: *"…how does one find the $\Phi(x)$ functions relevant to a particular Hamiltonian $\hat{H}$ that one wants to solve?"*

### 8.14.4 Examples.

In this section examples of the generalization method are dealt with. It is about not guessing the function $\Phi(x)$.
1) **Harmonic Oscillator Revisited.**
Boccio showed the procedure to work for the Harmonic oscillator. Then, the procedure is applied to some more examples.
2) **One-Dimensional Infinite Square Well.**
Boccio showed the procedure to work for this case.
3) **Hydrogen Atom.**
The correct wave functions are obtained. Well, some knowledge about the correct wave functions should be available.

### 8.14.5 Supersymmetric Quantum Mechanics

Here the results of the study of the relationship between pairs of super partner potentials are presented.
Quantum mechanical systems are studied of which the Hamiltonian is constructed from anticommuting charges. Boccio showed the charge to be a conserved observable, using Eqs.(8.728) and (8.729).

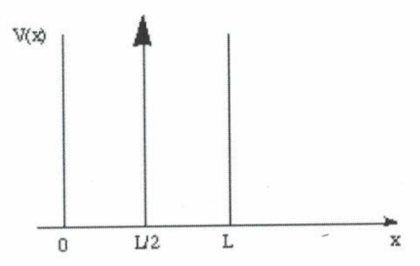
### 8.14.6 Additional Thoughts

The unitary operator is expressed in the charge operator, Eq. (8.737).
In this section Boccio illustrated spontaneous broken symmetry.

## 8.15 Problems page 660

### 8.15.1 Delta function in a well

A particle of mass $m$ moving in one dimension is confined to a space $0 < x < L$ by an infinite well potential. In addition, the particle experiences a delta function potential of strength $\lambda$ given by $\lambda\delta(x-\frac{L}{2})$ located at the center of the well as shown in Figure 8.26, page 660.




Find a transcendental equation for the energy eigenvalues in terms of the mass $m$ , the potential strength $\lambda$ and the size of the well.
From the picture above, we conclude to consider two regions:
**Region I**: $0 \le x \le L/2$ .
A general solution as found in the Undergraduate Course looks like:
$\psi_I(x) = A_I \sin kx$,
where the boundary condition at $x = 0$ is included, $\psi_I(0) = 0$.
**Region II**: $\frac{L}{2} \le x \le L$ .
A general solution for this region is
$\psi_{II}(x) = A_{II} \sin[\,k(L-x)]$.
Additional information is generated in the middle of the well at the potion of the delta function potential.
As we learned from the Course, there is continuity of the wave function
$\psi_I\left(x=\frac{L}{2}\right) = \psi_{II}\left(x=\frac{L}{2}\right) \therefore A_I = A_{II}$.
Furthermore we know the first derivative at the delta function potential to show a jump. The strength of which has been derived in the Course:
$\frac{d\psi_{II}}{dx}|_{L/2} - \frac{d\psi_I}{dx}|_{\frac{L}{2}} = \frac{2m\lambda}{\hbar^2}\psi_I|_{\frac{L}{2}}$ .
So,
$\frac{d\psi_{II}}{dx}|_{L/2} = -A_I k \cos\left(-\frac{kL}{2}\right) = -A_I k \cos(\frac{kL}{2})$,
$\frac{d\psi_I}{dx}|_{\frac{L}{2}} = A_I k \cos\left(-\frac{kL}{2}\right) = A_I k \cos(\frac{kL}{2})$.
Then
$\frac{d\psi_{II}}{dx}|_{L/2} - \frac{d\psi_I}{dx}|_{\frac{L}{2}} = \frac{2m\lambda}{\hbar^2}\psi_I|_{\frac{L}{2}} \Longrightarrow -A_I k \cos\left(\frac{kL}{2}\right) - A_I k \cos\left(\frac{kL}{2}\right) = \frac{2m\lambda}{\hbar^2} A_I \sin\frac{kL}{2} \Longrightarrow$
$\Longrightarrow \tan\frac{kL}{2} = -\frac{\hbar^2 k}{m\lambda}$ .
So with $k^2 = \frac{2mE}{\hbar^2}$ , we have the system of equations to solve for the energy eigenvalues in terms of the mass $m$ , the potential strength $\lambda$ and the size of the well.
**Note:**
We could have set
$\psi_{II}(x) = A_{II} \sin[\,k(x-L)]$.
Then, continuity of the wave function at the delta function potential gives:
$\psi_I\left(x=\frac{L}{2}\right) = \psi_{II}\left(x=\frac{L}{2}\right) \Longrightarrow A_I \sin\frac{kL}{2} = A_{II} \sin\,[\,k(\,-L/2)] = -A_{II}\sin\frac{kL}{2} \therefore A_I = -A_{II}$ .
Hence,
$\frac{d\psi_{II}}{dx}|_{L/2} = -A_I k \cos\left(-\frac{kL}{2}\right) = -A_I k \cos(\frac{kL}{2})$,

$\frac{d\psi_I}{dx}|_{\frac{L}{2}} = A_I k \cos\left(-\frac{kL}{2}\right) = A_I k \cos(\frac{kL}{2})$.
Consequently, leading to the same transcendental equation and conclusion.

### 8.15.2 Properties of the wave function

A particle of mass $m$ is confined to a one-dimensional region $0 < x < a$ ( an infinite square well potential). At $t = 0$ a normalized wave function is:

$\psi(x, t = 0) = \sqrt{\frac{8}{5a}}(1 + \cos\frac{\pi x}{a}) \sin\frac{\pi x}{a}$.

**a)** What is the wave function at a later time $t = t_0$.

For the infinite square well we obtained in the Course 8.5.3, page 566[7].

$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}$,

with

$E_n = \frac{1}{2m}(\frac{n\pi\hbar}{a})^2, n = 1,2,3, \ldots$

The time evolution is imported by the factor $e^{-iE_n t/\hbar}$.

Now, we can formulate an arbitrary wave function by expanding the arbitrary wave function with the eigenfunctions as basis multiplied by the time development factor:

$\psi(x, t) = \sum_n A_n\, e^{-iE_n t/\hbar}\psi_n(x)$.

To relate

$\psi(x, t = 0) = \sqrt{\frac{8}{5a}}(1 + \cos\frac{\pi x}{a}) \sin\frac{\pi x}{a}$ and $\psi(x, t) = \sum_n A_n\, e^{-iE_n t/\hbar}\psi_n(x)$,

we use $\sin 2\alpha = 2 \sin\alpha \cos\alpha$.

So,

$\psi(x, t = 0) = \sqrt{\frac{8}{5a}}\left(1 + \cos\frac{\pi x}{a}\right) \sin\frac{\pi x}{a} = \sqrt{\frac{8}{5a}} \sin\frac{\pi x}{a} + \sqrt{\frac{2}{5a}} \sin\frac{2\pi x}{a}$.

It becomes clear with $n = 1,2$ in $\psi(x, t) = \sum_n A_n\, e^{-iE_n t/\hbar}\psi_n(x)$:

$\psi(x, t) = A_1 e^{-iE_1 t/\hbar}\psi_1(x) + A_2 e^{-iE_2 t/\hbar}\psi_2(x)$.

Hence, using $\psi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}$

$\psi(x, t_0) = \sqrt{\frac{4}{5}} e^{-iE_1 t_0/\hbar}\psi_1(x) + \sqrt{\frac{1}{5}} e^{-iE_2 t_0/\hbar}\psi_2(x)$ .

**b)** The average energy of the system at $t = 0$ and $t = t_0$ .

The average energy, expectation value, is time independent. Consequently , the average energy does not change.

$\langle E\rangle = \langle\psi|\hat{H}|\psi\rangle = \sum_n A_n^*\, e^{iE_n t/\hbar}\psi_n^*(x) \sum_n A_n\, e^{-iE_n t/\hbar}\hat{H}\psi_n(x) = \sum_n |A_n|^2\, E_n \psi_n^* \psi_n(x) =$

$= \sum_n |A_n|^2\, E_n = |A_1|^2 E_1 + |A_2|^2 E_2 = \frac{4}{5}E_1 + \frac{1}{5}E_1 = \frac{4}{5}\frac{1}{2m}(\frac{\pi\hbar}{a})^2 + \frac{1}{5}\frac{1}{2m}(\frac{2\pi\hbar}{a})^2 = \frac{4}{5}\frac{1}{m}(\frac{\pi\hbar}{a})^2$.

**c)** What is the probability that the particle is found in the left half of the infinite well at $t = t_0$?

The probability is:

$P\left(0 \le x \le \frac{a}{2}; t_0\right) = \int_0^{a/2} |\psi(x, t_0)|^2\, dx$.

$|\psi(x, t_0)|^2 = |\sqrt{\frac{4}{5}} e^{-iE_1 t_0/\hbar}\psi_1(x) + \sqrt{\frac{1}{5}} e^{-iE_2 t_0/\hbar}\psi_2(x)|^2 =$

---

[7] the $x$-axis is at $a = 0$.

$= |\sqrt{\frac{8}{5a}} e^{-\frac{iE_1 t_0}{\hbar}} \sin\frac{\pi x}{a} + \sqrt{\frac{2}{5a}} e^{-iE_2 t_0/\hbar} \sin\frac{2\pi x}{a}|^2.$

$P\left(0 \leq x \leq \frac{a}{2}; t_0\right) = \int_0^{a/2} |\sqrt{\frac{8}{5a}} e^{-\frac{iE_1 t_0}{\hbar}} \sin\frac{\pi x}{a} + \sqrt{\frac{2}{5a}} e^{-iE_2 t_0/\hbar} \sin\frac{2\pi x}{a}|^2 dx$ .

After some calculus and algebra, we find the probability to be constituted of a constant equal to $\frac{1}{2}$ plus an oscillating term. As te be expected.

### 8.15.3 Repulsive potential

A repulsive short-range potential with a strongly attractive core can be approximated by a square barrier with a delta function at its center, namely,

$V(x) = V_0 \Theta(|x| - a) - \frac{\hbar^2 g^2}{2m}\delta(x)$ .

**a)** Show that there is a negative energy eigen state, i.e., the ground state.

We have two regions:

$|x| > a,$

$|x| < a.$

For convenience we define the following quantities:

- $k^2 = \frac{2m|E|}{\hbar^2}$,

- $q^2 = \frac{2m(|E|+V_0)}{\hbar^2}$,

And

- $\beta^2 = \frac{2mV_0}{\hbar^2}$ .

For the two regions we have the two Schrödinger equations:

- $|x| > a$: $\frac{d^2}{dx^2}\psi = k^2\psi$ ,

- $|x| < a$: $\frac{d^2}{dx^2}\psi = q^2\psi$ .

The delta function at $x = 0$, gives the discontinuity relation

$\frac{d}{dx}\psi|_{x=+0} - \frac{d}{dx}\psi|_{x=-0} = -g^2\psi|_{x=0}.$

For the region $|x| > a$ the solution for the wave function is:

- $\psi(x) = Ae^{-k|x|}$, the wave function must vanish as $|x| \to \infty$,

for the region $|x| < a$ the solution for the wave function is:

- $\psi(x) = Be^{q|x|} + Ce^{-q|x|}$.

With (dis)continuity relations we have at $x = a$

- $Be^{qa} + Ce^{-qa} = Ae^{-ka}$,

- $Bqe^{qa} - Cqe^{-qa} = -Ake^{-ka}$.

At $x = 0$

$\frac{d}{dx}\psi|_{x=+0} - \frac{d}{dx}\psi|_{x=-0} = -g^2\psi|_{x=0} \Longrightarrow 2q(B - C) = -g^2(B + C) \Longrightarrow$

$\Longrightarrow \frac{(B-C)}{(B+C)} = -\frac{g^2}{2q}$ .

$\frac{Be^{qa}+Ce^{-qa}}{Bqe^{qa}-Cqe^{-qa}} = -\frac{1}{k} \Longrightarrow k(Be^{2qa} + C) = -Bqe^{2qa} + Cq \Longrightarrow Be^{2qa}(k + q) = C(-k + q)$

$\frac{(B-C)}{(B+C)} = -\frac{g^2}{2q} \Longrightarrow B - C = -\frac{g^2}{2q}(B + C) \Longrightarrow B\left(1 + \frac{g^2}{2q}\right) = C\left(1 - \frac{g^2}{2q}\right) \Longrightarrow \frac{B}{C} = \frac{1-\frac{g^2}{2q}}{1+\frac{g^2}{2q}}$ .

$Be^{2qa}(k + q) = C(-k + q) \Longrightarrow \frac{B}{C} = e^{-2qa}\frac{-k+q}{k+q}$ .

Equate the two expressions of $\frac{B}{C}$

$\frac{1-\frac{g^2}{2q}}{1+\frac{g^2}{2q}} = e^{-2qa}\frac{-k+q}{k+q} \Longrightarrow e^{2qa}\frac{1-\frac{g^2}{2q}}{1+\frac{g^2}{2q}} = \frac{-k+q}{k+q}$ .

With a vanishing $V_0$we have the delta function potential

$V(x) = -\frac{\hbar^2 g^2}{2m}\delta(x)$.

The wave function is for $x \neq 0$

$\psi(x) = De^{-\alpha|x|}$, a cusp type of wave function,

where $\alpha^2 = -\frac{2mE}{\hbar^2}$ , $E < 0$,

with $E < 0$ .

At $x = 0$:

$\frac{d}{dx}\psi|_{x=+0} - \frac{d}{dx}\psi|_{x=-0} = -g^2\psi|_{x=0}$.

Then,

$-\alpha D - \alpha D = -g^2 D \Longrightarrow \alpha = \frac{g^2}{2}$ .

With $\alpha^2 = -\frac{2mE}{\hbar^2} = -\frac{2mE_0}{\hbar^2}$ ,

$E_0 = -\frac{\hbar^2}{2m}\alpha^2 = -\frac{\hbar^2}{2m}\frac{g^4}{4}$ .

Or, with $q = k \rightarrow$ the vanishing potential:

$1 - \frac{g^2}{2q} = 0 \Longrightarrow q^2 = \frac{g^4}{4}$ , or $E_0 = -\frac{\hbar^2}{2m}\frac{g^4}{4}$ .

**b)** If $E_0$ is the ground-state energy of the delta-function potential in the absence of the positive potential barrier, then the ground-state energy of the present system satisfies the relation $E \geq E_0 + V_0$ .

What is the particular value of $V_0$ for which we have the limiting case of a ground-state with zero energy?

The right hand side of the eigenvalue equation is positive.

Hence

$1 - \frac{g^2}{2q} \geq 0$.

Include the potential $V_0$ in the preceding expression:

$1 - \frac{g^2}{2q} \geq 0 \Longrightarrow q \geq \frac{g^2}{2} \Longrightarrow q^2 \geq \frac{g^4}{4}$:

the right hand side of the Schrödinger equation $\frac{2m}{\hbar^2}(-E + V_0) \geq \frac{g^4}{4} \Longrightarrow -E + V_0 \geq \frac{\hbar^2}{2m}\frac{g^4}{4} \therefore$

$E \leq V_0 - \frac{\hbar^2}{2m}\frac{g^4}{4}$.

The eigenvalue equation

$e^{2qa}\frac{1-\frac{g^2}{2q}}{1+\frac{g^2}{2q}} = \frac{-k+q}{k+q}$

can be investigated graphically . It follows one solution to exist.

To find out, it is convenient to use the following substitution and plug these into the eigenvalue equation:

$\xi = qa,\ \lambda = \frac{g^2 a}{2}, b = \beta a\ , \beta^2 = \frac{2mV_0}{\hbar^2}$ and $q^2 = \frac{2m(|E|+V_0)}{\hbar^2}$ .

The eigenvalue equation becomes:

$e^{2\xi}\frac{\xi-\lambda}{\xi+\lambda} = \frac{\xi-\sqrt{\xi^2-b^2}}{\xi-\sqrt{\xi^2+b^2}}$ .

Necessarily, $\lambda \geq b$.

For $\lambda = b$ , we have

$$\beta a = \frac{g^2 a}{2} \Longrightarrow \beta^2 = \frac{g^4}{4} = \frac{2mV_0}{\hbar^2}.$$

8.15.4 Step and Delta Functions

Consider a one-dimensional potential with a Heaviside step-function component and an attractive delta function component just at the edge of the step, namely

$$V(x) = V_0 \Theta(x) - \frac{\hbar^2 g}{2m}\delta(x)$$

**a)** For $E > V$, compute the reflection coefficient for particle incident from the left. How does this result differ from that of the step barriers alone at high energy?

The wave function for $x < 0$

$$\psi(x) = e^{ikx} + Be^{-ikx},$$

for $x > 0$

$$\psi(x) = Ce^{iqx}.$$

with

$$k = \sqrt{\frac{2mE}{\hbar^2}}\ ,\ \ q = \sqrt{\frac{2m(E-V)}{\hbar^2}}.$$

Continuity at $x = 0$:

$$e^{ikx} + Be^{-ikx} = Ce^{iqx} \Longrightarrow 1 + B = C.$$

Now the effect of the delta function at $x = 0$, a discontinuity of the derivatives

$$-\frac{\hbar^2}{2m}\int_{-0}^{+0} dx \frac{d^2\psi}{dx^2} = -\frac{\hbar^2}{2m}\left(\frac{d}{dx}\psi|_{x=+0} - \frac{d}{dx}\psi|_{x=-0}\right) = \int_{-0}^{+0} dx[E - V(x)]\psi(x) = \frac{\hbar^2 g}{2m}\psi(0) \Longrightarrow$$

$$\Longrightarrow \frac{d}{dx}\psi|_{x=+0} - \frac{d}{dx}\psi|_{x=-0} = -g\psi(0) \Longrightarrow ik(1-B) = (iq+g)C \Longrightarrow$$

$$\Longrightarrow 1 - B = -\frac{i}{k}(iq+g)C.$$

With the two equations for $B$ and $C$

$$B = \frac{1-\frac{q}{k}+\frac{ig}{k}}{1+\frac{q}{k}-\frac{ig}{k}},$$

and

$$C = \frac{2}{1+\frac{q}{k}-\frac{ig}{k}}.$$

The reflection coefficient $\mathfrak{R}$ is defined as

$$\mathfrak{R} = \left|\frac{j_r}{j_l}\right|,$$

where $j_r$ is the particle current(probability current) reflected to the left and $j_l$ is the incoming particle current from the left.

$$j = \frac{i\hbar}{2m}\left(\psi\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial\psi}{\partial x}\right)$$

Hence, with the wave function $\psi(x) = e^{ikx} + Be^{-ikx}$

$$\mathfrak{R} = \left|\frac{j_r}{j_l}\right| = \frac{\frac{\hbar k}{m}|B|^2}{\frac{\hbar k}{m}} = |B|^2 = \left|\frac{1-\frac{q}{k}+\frac{ig}{k}}{1+\frac{q}{k}-\frac{ig}{k}}\right|^2 = \frac{\left(1-\frac{q}{k}\right)^2+\left(\frac{g}{k}\right)^2}{\left(1+\frac{q}{k}\right)^2+\left(\frac{g}{k}\right)^2}.$$

To find out about the difference between the refection coefficient above and the reflection coefficient for the step barrier (without delta function) at high energy, $E \gg V$ :

$$\left(1-\frac{q}{k}\right)^2 = \left(1-\sqrt{\frac{E-V}{E}}\right)^2 \cong \left(1-1+\frac{1}{2}\frac{V}{E}\right)^2 = \frac{1}{4}\left(\frac{V}{E}\right)^2,$$

and

$$\left(1+\frac{q}{k}\right)^2 = \left(1+\sqrt{\frac{E-V}{E}}\right)^2 \cong \left(1+1-\frac{1}{2}\frac{V}{E}\right)^2 \cong 4.$$

Then

$\Re = \frac{1}{16}\left(\frac{V}{E}\right)^2$.

**b)** For $E < 0$ determine the energy eigenvalues and eigenfunctions of any bound-state solutions.

The following numbers are used:

$k = \sqrt{\frac{2m|E|}{\hbar^2}}$, and $q = \sqrt{\frac{2m(V+|E|)}{\hbar^2}}$.

The wave function for $x < 0$

$\psi(x) = Ae^{kx}$,

for $x > 0$

$\psi(x) = Ae^{-qx}$ .

The effect of the delta function at $x = 0$, a discontinuity of the derivatives

$$-\frac{\hbar^2}{2m}\int_{-0}^{+0} dx \frac{d^2\psi}{dx^2} = -\frac{\hbar^2}{2m}\left(\frac{d}{dx}\psi|_{x=+0} - \frac{d}{dx}\psi|_{x=-0}\right) = \int_{-0}^{+0} dx[E - V(x)]\psi(x) = \frac{\hbar^2 g}{2m}\psi(0) \Longrightarrow$$

$$\Longrightarrow \frac{d}{dx}\psi|_{x=+0} - \frac{d}{dx}\psi|_{x=-0} = -g\psi(0) \Longrightarrow q + k = g.$$

So

$$\sqrt{\frac{2m(V+|E|)}{\hbar^2}} + \sqrt{\frac{2m|E|}{\hbar^2}} = g \Longrightarrow \sqrt{V + |E|} + \sqrt{|E|} = g\sqrt{\frac{\hbar^2}{2m}}.$$

With the preceding expression $E$ is found, using with $k$ and $q$.

With normalization

$$1 = \int_{-\infty}^{\infty} dx\, |\psi(x)|^2 = A^2\left(\int_{-\infty}^{0} dx e^{2kx} + \int_{0}^{\infty} dx e^{-2qx}\right) = A^2\frac{1}{2}\left(\frac{1}{k} + \frac{1}{q}\right) \Longrightarrow$$

$$\Longrightarrow A = \sqrt{\frac{2kq}{k+q}} = \sqrt{\frac{2kq}{g}}.$$

the prefactor $A$ is determined.

### 8.15.5 Atomic Model

An approximate model for an atom near a wall is to consider a particle moving under the influence of the one-dimensional potential given by

$x > -d$

$V(x) = -V_0\delta(x)$,

with $V_0 > 0$,

and $x < -d$

$V(x) = \infty$.

**a)** Find the transcendental equation for the bound state energies.

The Schrödinger equation for $x > -d$:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\big(E + V_0\delta(x)\big)\psi = 0 .$$

Use $k = \sqrt{-\frac{2mE}{\hbar^2}}$,

where $E < 0$ .

In the region $-d < x < 0$, the solution is

$\psi_1 = ae^{kx} + be^{-kx}$.

In the region $x > 0$, the solution is

$\psi_2 = e^{kx}$.

Continuity of the wave function at $x = 0$ , gives with $\psi_1(0) = \psi_2(0)$

$a + b = 1$.

The discontinuity at the potential well

$$-\frac{\hbar^2}{2m}\int_{-0}^{+0} dx\,\frac{d^2\psi}{dx^2} = -\frac{\hbar^2}{2m}\left(\frac{d}{dx}\psi|_{x=+0} - \frac{d}{dx}\psi|_{x=-0}\right) = \int_{-0}^{+0} dx[E - V(x)]\psi(x) \Longrightarrow$$
$$\Longrightarrow -\frac{\hbar^2}{2m}\left(\frac{d}{dx}\psi|_{x=+0} - \frac{d}{dx}\psi|_{x=-0}\right) = \int_{-0}^{+0} dx[E + V_0\delta(x)]\psi(x) \Longrightarrow$$
$$\Longrightarrow \frac{d}{dx}\psi|_{x=+0} - \frac{d}{dx}\psi|_{x=-0} = -\frac{2m}{\hbar^2}V_0\psi_2(0) \Longrightarrow \frac{d\psi_2}{dx}(0) - \frac{d\psi_1}{dx}(0) = -\frac{2m}{\hbar^2}V_0 \Longrightarrow$$
$$\Longrightarrow -k - k(a-b) = -\frac{2m}{\hbar^2}V_0.$$
In addition we have at $x = -d$ an infinite potential. Consequently,
$\psi_1(-d) = ae^{-kd} + be^{kd} = 0.$
We have three expressions for $a, b$ and $k$.
Start with the simple one:
$a = -be^{2kd}$ and $a = 1 - b$, gives:
$b = \frac{1}{1-e^{2kd}} \Longrightarrow a = -\frac{e^{2kd}}{1-e^{2kd}}.$
Next
$k(1 + a - b) = -\frac{2m}{\hbar^2}V_0 \Longrightarrow k = \frac{m}{\hbar^2}V_0(1 - e^{-2kd}).$
With $E = -\frac{\hbar^2 k^2}{2m}$,
$E = -\frac{m}{2\hbar^2}V_0^2(1 - e^{-2kd})^2.$

**b)** Find an approximation for the modification of the bound-state energy caused by the wall when the wall is far away. A careful definition of faraway is needed.
The wall is faraway$\Longrightarrow$ $kd \gg 1$.
Hence,
$E = -\frac{m}{2\hbar^2}V_0^2(1 - e^{-2kd})^2 \cong -\frac{m}{2\hbar^2}V_0^2.$
This is the bound state energy from a delta function potential well, without a wall(see Mahan, pages 46-47).
A better approximation is
$(1 - e^{-2kd})^2 \cong 1 - 2e^{-2kd}.$
Then
$E = -\frac{m}{2\hbar^2}V_0^2(1 - e^{-2kd})^2 \cong -\frac{m}{2\hbar^2}V_0^2(1 - 2e^{-2kd}).$
Consequently, the correction of bound-state energy of to the solitary delta function potential well by the wall faraway is:
$\frac{m}{\hbar^2}V_0^2 e^{-2kd}.$
Without a wall,
$k = \frac{m}{\hbar^2}V_0.$
With a wall
$k \cong \frac{m}{\hbar^2}V_0.$
So the reciprocal of $k$ is a measure of the distance
$\frac{1}{k} \cong \frac{\hbar^2}{mV_0},$
gives an idea of faraway.

**c)** What is the exact condition on $V_0$ and $d$ for the existence of at least one bound state?
We can examine:
- $k = \frac{m}{\hbar^2}V_0(1 - e^{-2kd}),$
or
- $E = -\frac{m}{2\hbar^2}V_0^2(1 - e^{-2kd})^2.$
We choose

$k = \frac{m}{\hbar^2} V_0 (1 - e^{-2kd})$.
The solution for $k$ can be obtained by, precollege mathematics, graphical iteration. So, use $x = k$, and $x = \frac{m}{\hbar^2} V_0 (1 - e^{-2kd})$.
However, for to use iteration you need to know a few numbers.
What we are basically looking for is the existence of a solution: is there a point of intersection of $x = k$ and $x = \frac{m}{\hbar^2} V_0 (1 - e^{-2kd})$? If so, a section of $x = \frac{m}{\hbar^2} V_0 (1 - e^{-2kd})$ should be above $x = k$. In other words the slope of $x = \frac{m}{\hbar^2} V_0 (1 - e^{-2kd})$ should be above the slope of $x = k$, at $k = 0$.
Hence:
$\frac{d}{dk} \frac{m}{\hbar^2} V_0 (1 - e^{-2kd}) > \frac{d}{dk} k$,
or
$\frac{m}{\hbar^2} V_0 2d > 1$.
Consequently, the exact condition on $V_0$ and $d$ for the existence of at least one bound state is:
$V_0 d > \frac{\hbar^2}{2m}$.

### 8.15.6 A confined particle

A particle of mass $m$ is confined to a space $0 < x < a$, in one dimension by infinite high walls at $x = 0$ and $x = a$. At $t = 0$ the particle is initially in the left half of the well with a wave function given by
- $0 < x < \frac{a}{2}$ : $\psi(x, 0) = \sqrt{\frac{2}{a}}$,

and
- $\frac{a}{2} < x < 0$ : $\psi(x, 0) = 0$.

**a)** Find the time-dependent wave function $\psi(x, t)$. The eigenfunctions and eigenvalues for the Hamiltonian $\hat{H}$ for the above presented system are:
$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$, and $E_n = \frac{\hbar^2}{2m} (\frac{n\pi}{a})^2$, $n = 1,2,3$ ( section 8.5.3 page 566).
With the basis $\psi_n$, we have the general expansion
$\psi(x, t) = \sum_{n=1}^{\infty} a_n \, \psi_n e^{-iE_n t/\hbar}$.
Next we use the initial condition:
$\psi(x, 0) = \sum_{n=1}^{\infty} a_n \, \psi_n$.
Orthogonality:
$\int_0^a \psi(x, 0) \psi_k dx = \sum_{n=1}^{\infty} a_n \int_0^a \psi_n \psi_k dx = \sum_{n=1}^{\infty} a_n \delta_{nk} = a_k \Longrightarrow$
$\Longrightarrow a_k = \int_0^a \psi(x, 0) \psi_k dx = \int_0^{\frac{a}{2}} \sqrt{\frac{2}{a}} \sqrt{\frac{2}{a}} \sin \frac{k\pi x}{a} dx = \frac{2}{a} \int_0^{\frac{a}{2}} \sin \frac{k\pi x}{a} dx = \frac{2}{k\pi} (1 - \cos \frac{k\pi}{2})$.
So, $\psi(x, t) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{a} \, e^{-iE_n t/\hbar}$
$\psi(x, t) = \frac{2}{\pi} \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} \frac{1}{n} (1 - \cos \frac{n\pi}{2}) \sin \frac{n\pi x}{a} \, e^{-iE_n t/\hbar}$.
**b)** What is the probability that the particle is in the $n^{th}$ eigenstate of the well at time $t$?
The probability is:
$P_n = |a_n|^2 = [\frac{2}{n\pi} (1 - \cos \frac{n\pi}{2})]^2$.
**c)** Derive an expression for the average value of particle energy.

The expectation value:
$\langle E\rangle = \langle\psi|\hat{H}|\psi\rangle = \langle\psi|\sum_n E_n\psi_n\rangle = \sum_n E_n\,|\psi_n|^2 = \sum_n E_n\,|a_n|^2 =$
$= \frac{\hbar^2}{2m}\sum_n(\frac{n\pi}{a})^2[\frac{2}{n\pi}(1-\cos\frac{n\pi}{2})]^2 \ = \frac{2\hbar^2}{ma^2}\sum_n(1-\cos\frac{n\pi}{2})^2$ .
This quadratic expansion does not converge.

### 8.15.7 $1/x$ potential

An electron moves in one dimension and is confined to the right halve space, $x > 0$, where it has potential energy
$V(x) = -\frac{e^2}{4x}$,
where $e$ is the charge of the electron.
The 1-D Schrödinger equation
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \frac{e^2}{4x}\psi = -|E|\psi$ ,
for bound states.
**a)** What is the solution of the Schrödinger equation at large $x$?
Since it is about bound states $\frac{e^2}{4x}\psi \to 0$,
and the differential equation becomes
$\frac{d^2\psi}{dx^2} - \frac{2m|E|}{\hbar^2}\psi = 0$,
with solution:
$\psi = e^{-x\cdot\sqrt{\frac{2m|E|}{\hbar^2}}} = e^{-\alpha x}$
for $x \to \infty$ and $\alpha = \sqrt{\frac{2m|E|}{\hbar^2}}$ .
**b)** What is the boundary condition at $x = 0$?
The potential of the charge becomes infinite, consequently $\psi(0) = 0$.
**c)** Use the result of a) and b) to guess the ground state solution of
$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \frac{e^2}{4x}\psi = -|E|\psi$,
with the ground-state wave function being zero at the boundaries.
A trial function is used:
$\psi = f(x)e^{-\alpha x}$ .
The boundary conditions:
$f(0) = 0$,
and
$\lim_{x\to\infty} f(x)e^{-\alpha x} = 0$ .
$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left(\frac{df}{dx}e^{-\alpha x} - \alpha f e^{-\alpha x}\right) = \frac{d^2 f}{dx^2}e^{-\alpha x} - \alpha\frac{df}{dx}e^{-\alpha x} - \alpha\frac{df}{dx}e^{-\alpha x} + \alpha^2 f e^{-\alpha x} =$
$= \left(\frac{d^2 f}{dx^2} - 2\,\alpha\frac{df}{dx} + \alpha^2 f\right)e^{-\alpha x}$.
Plug $\psi = f(x)e^{-\alpha x}$, into $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \frac{e^2}{4x}\psi = -|E|\psi$,
$\frac{\hbar^2}{2m}\left(\frac{d^2 f}{dx^2} - 2\,\alpha\frac{df}{dx} + \alpha^2 f\right)e^{-\alpha x} + \frac{e^2}{4x}f(x)e^{-\alpha x} = |E|\,f(x)e^{-\alpha x} \Longrightarrow$
$\Longrightarrow \left(\frac{d^2 f}{dx^2} - 2\,\alpha\frac{df}{dx} + \alpha^2 f\right)e^{-\alpha x} + \frac{2me^2}{4x\hbar^2}fe^{-\alpha x} = \frac{2m}{\hbar^2}|E|\,fe^{-\alpha x}$.
With $\frac{2m}{\hbar^2}|E| = \alpha^2$, the preceding equation becomes
$\left(\frac{d^2 f}{dx^2} - 2\,\alpha\frac{df}{dx} + \frac{2me^2}{4x\hbar^2}f\right)e^{-\alpha x} = 0$.
Now, an educated guess of $f(x) = x$ .

The boundary conditions are complied with.
So, the solution for the wave function reads:
$\psi = Axe^{-\alpha x}$,
where $A$ is the normalization constant.
Normalization:
$A^2 \int_0^\infty |\psi|^2 dx = A^2 \int_0^\infty x^2 e^{-2\alpha x} dx = 1.$
Using integration by parts:
$A^2 \frac{1}{4\alpha^3} = 1 \to A = 2\alpha^{3/2.}$
**d)** The ground-state energy
With $\alpha = \sqrt{\frac{2m|E|}{\hbar^2}} \Longrightarrow E_0 = -\frac{\hbar^2\alpha^2}{2m}$ .
Furthermore
$\left(\frac{d^2 f}{dx^2} - 2\,\alpha \frac{df}{dx} + \frac{2me^2}{4x\hbar^2} f\right) = 0,$
gives with $f = x$
$\alpha = \frac{me^2}{4\hbar^2}.$
Then
$E_0 = -\frac{\hbar^2\alpha^2}{2m} = -\frac{\hbar^2\left(\frac{me^2}{4\hbar^2}\right)^2}{2m} = -\frac{me^4}{32\hbar^2}$ .
**e)** Find the expectation value of the position operator $\langle \hat{x} \rangle$
Using the position projection operators, we obtain
$\langle \psi|\hat{x}|\psi\rangle = \int_0^\infty \int_0^\infty \langle \psi|x'\rangle\langle x'|\hat{x}|x\rangle \langle x|\psi\rangle dx dx' = \int_0^\infty \int_0^\infty \langle \psi|x'\rangle x\delta(x-x') \langle x|\psi\rangle dx dx' =$
$= \int_0^\infty \langle \psi|x\rangle\, x\langle x|\psi\rangle dx = \int_0^\infty x|\psi|^2 dx = 4\alpha^3 \int_0^\infty x^3 e^{-2\alpha x} dx.$
With integration by parts
$\int_0^\infty x|\psi|^2 dx = 4\alpha^3 \int_0^\infty x^3 e^{-2\alpha x} dx = 4\alpha^3 \cdot \frac{3}{8\alpha^4} = \frac{3}{2\alpha}.$

### 8.15.8 Using the commutator

Using coordinate-momentum commutation relation prove that
$\sum_n (E_n - E_0)|\langle E_n|\hat{x}|E_0\rangle|^2 =$ constant,
where $E_0$ is the energy corresponding to the eigenstate $|E_0\rangle$. Determine the value of the constant. The above expression suggets the use of the projection operators $|E_n\rangle\langle E_n|$.
$\sum_n (E_n - E_0)|\langle E_n|\hat{x}|E_0\rangle|^2 = \sum_n (E_n - E_0)\langle E_0|\hat{x}|E_n\rangle\langle E_n|\hat{x}|E_0\rangle \Longrightarrow$
$\Longrightarrow \sum_n E_n \langle E_0|\hat{x}|E_n\rangle\langle E_n|\hat{x}|E_0\rangle - \sum_n E_0 \langle E_0|\hat{x}|E_n\rangle\langle E_n|\hat{x}|E_0\rangle \Longrightarrow$
$\Longrightarrow \sum_n \langle E_0|\hat{x}E_n|E_n\rangle\langle E_n|\hat{x}|E_0\rangle - E_0 \langle E_0|\hat{x}\hat{x}|E_0\rangle =$
$= \sum_n \langle E_0|\hat{x}\hat{H}|E_n\rangle\langle E_n|\hat{x}|E_0\rangle - E_0 \langle E_0|\hat{x}\hat{x}|E_0\rangle = \langle E_0|\hat{x}\hat{H}\hat{x}|E_0\rangle - \langle E_0|\hat{x}\hat{x}\hat{H}|E_0\rangle =$
$= \langle E_0|\hat{x}\hat{H}\hat{x} - \hat{x}\hat{x}\hat{H}|E_0\rangle = \langle E_0|\hat{x}(\hat{H}\hat{x} - \hat{x}\hat{H})|E_0\rangle = \langle E_0|\hat{x}[\hat{H},\hat{x}]|E_0\rangle.$
The same procedure can be used,slightly differently, giving
$\sum_n \langle E_0|\hat{x}|E_n\rangle\langle E_n|E_n\hat{x}|E_0\rangle - \langle E_0|E_0\hat{x}\hat{x}|E_0\rangle = \langle E_0|\hat{x}\hat{H}\hat{x}|E_0\rangle - \langle E_0|\hat{H}\hat{x}\hat{x}|E_0\rangle =$
$= \langle E_0|\hat{x}\hat{H}\hat{x} - \hat{H}\hat{x}\hat{x}|E_0\rangle = \langle E_0|(\hat{x}\hat{H} - \hat{H}\hat{x})\hat{x}|E_0\rangle = -\langle E_0|[\hat{H},\hat{x}]\hat{x}|E_0\rangle \Longrightarrow$
$\Longrightarrow \sum_n (E_n - E_0)|\langle E_n|\hat{x}|E_0\rangle|^2 = -\langle E_0|[\hat{H},\hat{x}]\hat{x}|E_0\rangle.$
Adding both expressions of $\sum_n (E_n - E_0)|\langle E_n|\hat{x}|E_0\rangle|^2$:
$2\sum_n (E_n - E_0)|\langle E_n|\hat{x}|E_0\rangle|^2 = \langle E_0|\hat{x}[\hat{H},\hat{x}]|E_0\rangle - \langle E_0|[\hat{H},\hat{x}]\hat{x}|E_0\rangle =$
$= \langle E_0|\hat{x},[\hat{H},\hat{x}]|E_0\rangle.$

Below, commutators of the momentum and position operators are derived, resulting into

$$[[\hat{H},\hat{x}],\hat{x}] = -\frac{i\hbar}{m}[\hat{p},\hat{x}] = -\frac{i\hbar}{m}\cdot(-i\hbar) = -\frac{\hbar^2}{m}.$$

Consequently

$$2\sum_n(E_n - E_0)|\langle E_n|\hat{x}|E_0\rangle|^2 = \langle E_0|\hat{x},[\hat{H},\hat{x}]|E_0\rangle = \frac{\hbar^2}{m}\langle E_0|E_0\rangle \Longrightarrow$$

$$\Longrightarrow \sum_n(E_n - E_0)|\langle E_n|\hat{x}|E_0\rangle|^2 = \frac{\hbar^2}{2m}$$, a constant.

**Commutators of the momentum and position operators:**

Since the energy and eigenstate are general, we work with the general Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}).$$

The commutator

$$[\hat{H},\hat{x}] = \frac{\hat{p}^2}{2m}\hat{x} + V(\hat{x})\hat{x} - \hat{x}\frac{\hat{p}^2}{2m} - \hat{x}V(\hat{x}) = \frac{1}{2m}[\frac{\hat{p}^2}{2m},\hat{x}],$$

since $V(\hat{x})$ can be written as a polynomial of $\hat{x}$.

We know

$$\frac{1}{2m}[\hat{p},\hat{x}] = -\frac{i\hbar}{2m}.$$

Then

$$\hat{p}\hat{x}\hat{p} - \hat{p}^2\hat{x} = i\hbar\hat{p} \Longrightarrow \hat{p}\hat{x}\hat{p} - \hat{p}^2\hat{x} + \hat{x}\hat{p}^2 = i\hbar\hat{p} + \hat{x}\hat{p}^2 \Longrightarrow \hat{p}\hat{x}\hat{p} - \hat{x}\hat{p}^2 - \hat{p}^2\hat{x} + \hat{x}\hat{p}^2 = i\hbar\hat{p}.$$

Combining the terms in the preceding expression:

$$(\hat{p}\hat{x} - \hat{x}\hat{p})\hat{p} - [\hat{p}^2,\hat{x}] = i\hbar\hat{p} \Longrightarrow [\hat{p},\hat{x}]\hat{p} - [\hat{p}^2,\hat{x}] = i\hbar\hat{p} \Longrightarrow [\hat{p}^2,\hat{x}] = -2\,i\hbar\hat{p}.$$

Plug $[\hat{p}^2,\hat{x}] = -2\,i\hbar\hat{p}$ into

$$[\hat{H},\hat{x}] = [\frac{\hat{p}^2}{2m},\hat{x}],$$

giving

$$[\hat{H},\hat{x}] = -\frac{i\hbar\hat{p}}{m}.$$

Next,

$$[[\hat{H},\hat{x}],\hat{x}] = -\frac{i\hbar}{m}[\hat{p},\hat{x}] = -\frac{i\hbar}{m}\cdot(-i\hbar) = -\frac{\hbar^2}{m}.$$

### 8.5.9 Matrix Elements for Harmonic Oscillator

Section 8.6.2 Harmonic Oscillators and Algebraic methods.

Compute the following matrix elements:

$\langle n'|\hat{x}^3|n\rangle$ , and $\langle n'|\hat{x}\hat{p}|n\rangle$ .

I assume orthonormality:

$\langle n'|n\rangle = \delta_{nm}$.

We use raising and lowering operators as developed for the harmonic oscillator.

From the Course

$\hat{x} = x_0(\hat{a} + \hat{a}^+)$, Eqs.(8.355)

where $x_0 = \sqrt{\frac{\hbar}{2m\omega}}$.

The lowering operator

$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ .

The raising operator

$\hat{a}^+|n\rangle = \sqrt{n+1}|n+1\rangle$ .

So,

$\langle n'|\hat{x}|n\rangle = x_0\langle n'|(\hat{a} + \hat{a}^+)|n\rangle = x_0(\langle n'|\hat{a}|n\rangle + \langle n'|\hat{a}^+|n\rangle) =$

$= x_0(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1})$.
Using the preceding result and the projection operator
$\langle n'|\hat{x}^2|n\rangle = \sum_m \langle n'|\hat{x}|m\rangle\langle m|\hat{x}|n\rangle =$
$= x_0(\sqrt{m}\delta_{n',m-1} + \sqrt{m+1}\delta_{n',m+1})x_0(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}) =$
$= x_0^2[\sqrt{n(n-1)}\delta_{n',n-2} + \sqrt{n+1}\sqrt{n+2}\delta_{n',n+2} + (2n+1)\delta_{n',n}]$[8].

We can derive the preceding expression also in the following way:
$\langle n'|\hat{x}^2|n\rangle = \langle n'|\hat{x}\hat{x}|n\rangle = x_0\langle n'|\hat{x}(\hat{a}+\hat{a}^+)|n\rangle = x_0(\langle n'|\hat{x}\hat{a}|n\rangle + \langle n'|\hat{x}\hat{a}^+|n\rangle) =$
$= x_0(\langle n'|\hat{x}\hat{a}|n\rangle + \langle n'|\hat{x}\hat{a}^+|n\rangle) = x_0(\langle n'|\hat{x}\sqrt{n}|n-1\rangle + \langle n'|\hat{x}\sqrt{n+1}|n+1\rangle) =$
$= x_0^2[\langle n'|\sqrt{n}(\hat{a}+\hat{a}^+)|n-1\rangle + \langle n'|\sqrt{n+1}(\hat{a}+\hat{a}^+)|n+1\rangle] =$
$= x_0^2[\langle n'|\sqrt{n(n-1)}|n-2\rangle + \langle n'|\sqrt{n}\sqrt{n}|n\rangle + \langle n'|\sqrt{n+1}\sqrt{n+1}|n\rangle +$
$+\langle n'|\sqrt{n+1}\sqrt{n+2}|n+2\rangle]$ .
Then, using orthonormalization
$\langle n'|\hat{x}^2|n\rangle = x_0^2[\sqrt{n(n-1)}\delta_{n',n-2} + n\delta_{n',n} + (n+1)\delta_{n',n} + \sqrt{(n+1)(n+2)}\delta_{n',n+2}] =$
$= x_0^2[\sqrt{n(n-1)}\delta_{n',n-2} + (2n+1)\delta_{n',n} + \sqrt{(n+1)(n+2)}\delta_{n',n+2}]$.

With the preceding results, we can compute the matrix element $\langle m|\hat{x}^3|n\rangle$.
$\langle n'|\hat{x}^3|n\rangle = \langle n'|\hat{x}\hat{x}^2|n\rangle =$
$= x_0^2[\langle n'|\hat{x}\sqrt{n(n-1)}|n-2\rangle + \langle n'|\hat{x}\sqrt{n}\sqrt{n}|n\rangle + \langle n'|\hat{x}\sqrt{n+1}\sqrt{n+1}|n\rangle +$
$+\langle n'|\hat{x}\sqrt{n+1}\sqrt{n+2}|n+2\rangle]$ .
We investigate the terms of the preceding expression:
- $\langle n'|\hat{x}\sqrt{n(n-1)}|n-2\rangle = x_0\langle n'|\sqrt{n(n-1)}(\hat{a}+\hat{a}^+)|n-2\rangle =$
$= x_0[\langle n'|\sqrt{n(n-1)(n-2)}|n-3\rangle + \langle n'|\sqrt{n(n-1)^2}|n-1\rangle]$.

- $\langle n'|\hat{x}\sqrt{n}\sqrt{n}|n\rangle + \langle n'|\hat{x}\sqrt{n+1}\sqrt{n+1}|n\rangle = (2n+1)\langle n'|\hat{x}|n\rangle =$
$= x_0(2n+1)\langle n'|\hat{a}+\hat{a}^+|n\rangle = x_0(2n+1)[\langle n'|\sqrt{n}|n-1)\rangle + \langle n'|\sqrt{n+1}|n+1)\rangle$.

- $\langle n'|\hat{x}\sqrt{n+1}\sqrt{n+2}|n+2\rangle = x_0\sqrt{(n+1)(n+2)}\langle n'|\hat{a}+\hat{a}^+|n+2\rangle =$
$= x_0\sqrt{(n+1)(n+2)}[\langle n'|\sqrt{n+2}|n+1\rangle + \langle n'|\sqrt{n+3)}|n+3\rangle]$
Collecting all the terms and using orthonormalization:
$\langle n'|\hat{x}^3|n\rangle = x_0^3[\sqrt{n(n-1)(n-2)}\delta_{n',n-3} + (n-1)\sqrt{n}\delta_{n',n-1} +$
$+(2n+1)\sqrt{n}\delta_{n',n-1} + (2n+1)\sqrt{n+1}\delta_{n',n+1} + (n+2)\sqrt{n+1}\delta_{n',n+1} +$
$+\sqrt{(n+1)(n+2)(n+3)}\delta_{n',n+3}] =$
$= x_0^3[\sqrt{n(n-1)(n-2)}\delta_{n',n-3} + 3n\delta_{n',n-1} + (3n+3)\delta_{n',n+1} +$
$+\sqrt{(n+1)(n+2)(n+3)}\delta_{n',n+3}]$.

[8] An example of Kronecker delta multiplication: $\sqrt{m}\delta_{n',m-1}\sqrt{n}\delta_{m,n-1}$.
$\delta_{n',m-1}\delta_{m,n-1} = 1$, for $n' = m-1$, and $m = n-1$. So, $m-1 = n-2$.
Hence, $\delta_{n',n-2}\delta_{m,m} = \delta_{n',n-2}$. Consequently, $\sqrt{m}\delta_{n',m-1}\sqrt{n}\delta_{m,n-1} = \sqrt{n(n-1)}\delta_{n',n-2}$.

The next matrix element:
$\langle n'|\hat{x}\hat{p}|n\rangle$.Two methods:
- with projection operators
- multiplication of operators.
I choose for the last method.
The momentum operator:
With $\hat{p} = -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^+)$
$\langle n'|\hat{x}\hat{p}|n\rangle = -i\sqrt{\frac{m\omega\hbar}{2}}\langle n'|\hat{x}(\hat{a} - \hat{a}^+)|n\rangle = -i\sqrt{\frac{m\omega\hbar}{2}}[\langle n'|\hat{x}\sqrt{n}|n-1\rangle +$
$-\langle n'|\hat{x}\sqrt{n+1}|n+1\rangle]$.

- $\langle n'|\hat{x}\sqrt{n}|n-1\rangle = x_0\sqrt{n}\langle n'|(\hat{a} + \hat{a}^+)|n-1\rangle = x_0\sqrt{n}[\langle n'|\sqrt{n-1}|n-2\rangle +$
$+\langle n'|\sqrt{n}|n\rangle]$. .
- $\langle n'|\hat{x}\sqrt{n+1}|n+1\rangle = x_0\sqrt{n+1}\langle n'|(\hat{a} + \hat{a}^+)|n+1\rangle =$
$= x_0\sqrt{n+1}[\langle n'|\sqrt{n+1}|n\rangle + \langle n'|\sqrt{n+2}|n+2\rangle]$.
Collecting all the terms and using orthonormalization:
$\langle n'|\hat{x}\hat{p}|n\rangle = -i\frac{\hbar}{2}\left[\sqrt{(n-1)n}\delta_{n',n-2} + n\delta_{n',n} - (n+1)\delta_{n',n} - \sqrt{(n+1)(n+2)}\delta_{n',n+2}\right]$.
So,
$\langle n'|\hat{x}\hat{p}|n\rangle = -i\frac{\hbar}{2}[\sqrt{(n-1)n}\delta_{n',n-2} - \delta_{n',n} - \sqrt{(n+1)(n+2)}\delta_{n',n+2}]$.

### 8.15.10 A Matrix Element

Show for the one dimensional simple harmonic oscillator
$\langle 0|e^{ik\hat{x}}|0\rangle$ =exp[$-\frac{k^2\langle 0|\hat{x}^2|0\rangle}{2}$],
where $\hat{x}$ is the position operator.
We know, using the series expansion
$\langle 0|e^{ik\hat{x}}|0\rangle = \sum_{n=0}^{\infty}\frac{(ik)^n}{n!}\langle 0|\hat{x}^n|0\rangle$.
Use raising and lowering operator
$\hat{x} = x_0(\hat{a} + \hat{a}^+)$, Eqs.(8.355)
where $x_0 = \sqrt{\frac{\hbar}{2m\omega}}$.
The lowering operator
$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ .
The raising operator
$\hat{a}^+|n\rangle = \sqrt{n+1}|n+1\rangle$ .
The matrix elements in the series expansion:
$\langle 0|\hat{x}^0|0\rangle = \langle 0|0\rangle = 1$,
$\langle 0|\hat{x}^1|0\rangle = x_0\langle 0|(\hat{a} + \hat{a}^+)|0\rangle = x_0\langle 0|\hat{a}|0\rangle + x_0\langle 0|\hat{a}^+|0\rangle = 0 + x_0\langle 0|1|1\rangle = 0$,
$\langle 0|\hat{x}^2|0\rangle$, can be obtained with the projection operator $\sum|m\rangle\langle m|$ , or
$(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)$ giving $x_0^2\langle 0|1|0\rangle = x_0^2$.
$\langle 0|\hat{x}^3|0\rangle = x_0^3\langle 0|\hat{a} + \hat{a}^+|0\rangle = 0 \Longrightarrow \langle 0|\hat{x}^n|0\rangle = 0$, for $n$ is odd,
$\langle 0|\hat{x}^4|0\rangle = \langle 0|\hat{x}^2\hat{x}^2|0\rangle = x_0^2\langle 0|\hat{x}^2(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)|0\rangle$,
using the results of $\langle 0|\hat{x}^2|0\rangle$

$\langle 0|\hat{x}^4|0\rangle = x_0^2\left[\langle 0|\hat{x}^2|0\rangle + \sqrt{2}\langle 0|\hat{x}^2|2\rangle\right] = x_0^4\left[1 + \sqrt{2}\langle 0|(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)|2\rangle\right] =$
$= x_0^4[1 + 2\langle 0|(\hat{a} + \hat{a}^+)|1\rangle + \sqrt{6}\langle 0|(\hat{a} + \hat{a}^+)|3\rangle = x_0^4(1 + 2) = 3x_0^4$ .
$\langle 0|\hat{x}^6|0\rangle = \langle 0|\hat{x}^4\hat{x}^2|0\rangle = x_0^2\langle 0|\hat{x}^4(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)|0\rangle =$
$= x_0^2\langle 0|\hat{x}^4(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)|0\rangle = x_0^2\langle 0\big|\hat{x}^4[|0\rangle + \sqrt{2}\big|2\rangle] =$
$= x_0^4\langle 0\big|\hat{x}^2[3|0\rangle + 6\sqrt{2}\big|2\rangle + 2\sqrt{6}|4\rangle] = x_0^6\langle 0\big|[3|0\rangle + 6\sqrt{2}\big|2\rangle + 2\sqrt{6}|4\rangle] =$
$= x_0^6\langle 0\big|(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)[3|0\rangle + 6\sqrt{2}\big|2\rangle + 2\sqrt{6}|4\rangle] =$
$= x_0^6\left[\langle 0|12 + 3|0\rangle + 45\sqrt{2}|2\rangle + 30\sqrt{6}|4\rangle + 12\sqrt{5}|6\rangle\right] = 15x_0^6$

Is there already a pattern to discern?

We have to show

$\langle 0\big|e^{ik\hat{x}}\big|0\rangle$ =exp[$-\frac{k^2\langle 0|\hat{x}^2|0\rangle}{2}$].

The series expansion of

$\langle 0\big|e^{ik\hat{x}}\big|0\rangle = \left\langle 0\middle|\sum_{n=0}^{\infty}\frac{(ik)^n}{n!}\hat{x}^n\middle|0\right\rangle = \sum_{n=0}^{\infty}\frac{(ik)^n}{n!}\langle 0|\hat{x}^n|0\rangle.$

Four terms are obtained

$1 - \frac{k^2}{2!}\langle 0|\hat{x}^2|0\rangle + \frac{k^4}{4!}\langle 0|\hat{x}^4|0\rangle - \frac{k^6}{6!}\langle 0|\hat{x}^6|0\rangle =$
$1 - \frac{k^2}{2!}x_0^2 + \frac{k^4}{4!}3\cdot x_0^4 - \frac{k^6}{6!}15\cdot x_0^6 =$
$= 1 - \frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle + \frac{1}{2!}\left(\frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle\right)^2 - \frac{1}{3!}\left(\frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle\right)^3.$

Nota Bene:

$\frac{1}{6!}\cdot 15 = \frac{1}{1\cdot 2\cdot 4\cdot 6} = \frac{1}{1\cdot 2\cdot 3\cdot 2^3} = \frac{1}{3!\cdot 2^3}$ ,

and

$x_0^6 = (x_0^2)^3.$

$\langle 0|\hat{x}^8|0\rangle = \langle 0|\hat{x}^2\hat{x}^6|0\rangle = x_0^8\langle 0|(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)\big[15|0\rangle + 45\sqrt{2}|2\rangle + 30\sqrt{6}|4\rangle +$
$12\sqrt{5}|6\rangle\big] = x_0^8\langle 0|[105|0\rangle + 420\sqrt{2}|2\rangle + 420\sqrt{6}|4\rangle + 236\sqrt{5}|6\rangle + 12\sqrt{70}|8\rangle] = 105x_0^8.$

The next term in the series expansion:

$\frac{k^8}{8!}105x_0^8 = \frac{k^8}{4!}\cdot\frac{1}{2^4}x_0^8 = \frac{1}{4!}\left(\frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle\right)^4.$

For the expansion so far, we have

$1 - \frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle + \frac{1}{2!}\left(\frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle\right)^2 - \frac{1}{3!}\left(\frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle\right)^3 + \frac{1}{4!}\left(\frac{k^2}{2}\langle 0|\hat{x}^2|0\rangle\right)^4.$

So, we showed the first 5 term to represent the series expansion.

Hence,

I assume

$\langle 0\big|e^{ik\hat{x}}\big|0\rangle$ =exp[$-\frac{k^2\langle 0|\hat{x}^2|0\rangle}{2}$] to be correct.

**Remark:**

$\langle 0|\hat{x}^4|0\rangle = \langle 0|\hat{x}^2\hat{x}^2|0\rangle = \sum_{j=0}^{\infty}\langle 0|\hat{x}^2|j\rangle\langle j|\hat{x}^2|0\rangle = \langle 0|\hat{x}^2|0\rangle\langle 0|\hat{x}^2|0\rangle + \langle 0|\hat{x}^2|1\rangle\langle 1|\hat{x}^2|0\rangle +$
$+\langle 0|\hat{x}^2|2\rangle\langle 2|\hat{x}^2|0\rangle + \langle 0|\hat{x}^2|3\rangle\langle 3|\hat{x}^2|0\rangle + \cdots. = x_0^4 +$
$+x_0^4\langle 0|(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)|1\rangle\langle 1|(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)|0\rangle +$
$+x_0^4\langle 0|(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)|2\rangle\langle 2|(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)|0\rangle +$
$+x_0^4\langle 0|(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)|3\rangle\langle 3|(\hat{a} + \hat{a}^+)(\hat{a} + \hat{a}^+)|0\rangle + \cdots. = x_0^4 + 0 +$
$+x_0^4\langle 1\big|\sqrt{2}\big|1\rangle\langle 1\big|\sqrt{2}\big|1\rangle + 0\ldots. = 3x_0^4$ .

## 8.15.11 Correlation Function

Consider a function, known as the correlation function, defined by

$C(t) = \langle \hat{x}(t)\hat{x}(0)\rangle$,

where $\hat{x}(t)$ is the position operator in the Heisenberg picture.

Evaluate the correlation function explicitly for the ground-state of the one-dimensional simple harmonic oscillator.

Reminder:

-the Schrödinger picture is about the dynamical variables(operators) remain fixed during a period of undisturbed motion, whereas the state vector evolves with time.

-the Heisenberg picture is about the dynamical variables(operators) depend on time , whereas the state vector does not evolve with time.

We evaluate the position operator in the Heisenberg representation.

$\hat{x}(t) = x_0[\hat{a}(t) + \hat{a}^+(t)]$,

and

$x_0 = \sqrt{\frac{\hbar}{2m\omega}}$.

Hence we have to find out about $\hat{a}(t)$.

We write, see section 6.7 The Heisenberg Picture, Eq.(6.137),

$\hat{a}(t) = e^{\frac{i\hat{H}t}{\hbar}}\hat{a}(0)e^{-\frac{i\hat{H}t}{\hbar}}$,

where

$\hat{H} = \hbar\omega\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)$, Eq.(8.356).

Use will be made of the Baker-Hausdorff Lemma:

$e^{\lambda G}Ae^{-\lambda G} = \sum_{k=0}^{\infty}\frac{\lambda^k}{k!}([G,)^k A(])^k$, See www.leennoordzij.me Quantum Mechanics in Texas Graduate Course.

The Baker-Hausdorff Lemma has been also been used in an earlier problem

$\hat{a}(t) = e^{\frac{i\hat{H}t}{\hbar}}\hat{a}(0)e^{-\frac{i\hat{H}t}{\hbar}} = \hat{a} + \frac{it}{\hbar}[\hat{H},\hat{a}] + \frac{1}{2}\left(\frac{it}{\hbar}\right)^2\left[\hat{H},[\hat{H},\hat{a}]\right] + \frac{1}{3!}[\hat{H},\left[\hat{H},[\hat{H},\hat{a}]\right] + \cdots$.

With $\hat{H} = \hbar\omega\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)$,

$[\hat{H},\hat{a}] = \hbar\omega\left(\hat{a}^+\hat{a}\hat{a} + \frac{1}{2}\hat{a} - \hat{a}\hat{a}^+\hat{a} - \frac{1}{2}\hat{a}\right) = \hbar\omega(\hat{a}^+\hat{a}\hat{a} - \hat{a}\hat{a}^+\hat{a}) = -\hbar\omega\hat{a}$,

where use has been made of $[\hat{a}^+,\hat{a}] = -1$.

$\left[\hat{H},[\hat{H},\hat{a}]\right] = -\hbar\omega[\hat{H},\hat{a}] = (\hbar\omega)^2\hat{a}$ .

Then,

$[\hat{H},\left[\hat{H},[\hat{H},\hat{a}]\right] = -(\hbar\omega)^3\hat{a}$.

So,

$\hat{a}(t) = e^{\frac{i\hat{H}t}{\hbar}}\hat{a}e^{-\frac{i\hat{H}t}{\hbar}} = \hat{a} - it\omega\hat{a} + \frac{1}{2}(it\omega)^2\hat{a} - \frac{1}{3!}(it\omega)^3\hat{a} + \cdots = e^{-i\omega t}\hat{a}(0)$.

Similarly, we find for $\hat{a}^+(t)$, with $[\hat{H},\hat{a}^+] = \hbar\omega(\hat{a}^+\hat{a}\hat{a}^+ - \hat{a}^+\hat{a}^+\hat{a}) = \hbar\omega\hat{a}^+$,

$\hat{a}^+(t) = e^{i\omega t}\hat{a}^+(0)$ .

We have

$\hat{x}(t) = x_0[\hat{a}(t) + \hat{a}^+(t)] = x_0\left[e^{-i\omega t}\hat{a}(0) + e^{i\omega t}\hat{a}^+(0)\right]$.

The momentum operator, see problem 8.15.9,

With $\hat{p}(t) = -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^+) \rightarrow$

$\hat{p}(t) = ix_0 m\omega[\hat{a}^+(t) - \hat{a}(t)] = ix_0 m\omega\left[e^{i\omega t}\hat{a}^+(0) - e^{-i\omega t}\hat{a}(0)\right]$.
Next, we express the raising and lowering operators into the position operator and momentum operator:
$\hat{x}(0) = x_0[\hat{a}(0) + \hat{a}^+(0)]$,
and
$\hat{p}(0) = ix_0 m\omega[\hat{a}^+(0) - \hat{a}(0)] \Longrightarrow$
$\Longrightarrow$
$\hat{a}(0) = \frac{1}{2x_0}\left[\hat{x}(0) - \frac{i}{m\omega}\,\hat{p}(0)\right]$,
and .
$\hat{a}^+(0) = \frac{1}{2x_0}\left[\hat{x}(0) + \frac{i}{m\omega}\,\hat{p}(0)\right]$.
Then
$\hat{x}(t) = x_0[\hat{a}(t) + \hat{a}^+(t)] = x_0\left[e^{-i\omega t}\hat{a}(0) + e^{i\omega t}\hat{a}^+(0)\right] =$
$= \frac{1}{2}\left\{e^{-i\omega t}\left[\hat{x}(0) - \frac{i}{m\omega}\,\hat{p}(0)\right] + e^{i\omega t}\left[\hat{x}(0) + \frac{i}{m\omega}\,\hat{p}(0)\right]\right\}$.
Plug the following expressions into $\hat{x}(t)$
$e^{i\omega t} = \cos\omega t + i\sin\omega t$ ,
and
$e^{-i\omega t} = \cos\omega t - i\sin\omega t \Longrightarrow$
$\Longrightarrow \hat{x}(t) = \hat{x}(0)\cos\omega t - \frac{\hat{p}(0)}{m\omega}\sin\omega t$.
Back to the correlation function
$C(t) = \langle\hat{x}(t)\hat{x}(0)\rangle$.
It is about the ground-state $|0\rangle$.
Hence
$C(t) = \langle\hat{x}(t)\hat{x}(0)\rangle = \langle 0|\hat{x}(t)\hat{x}(0)|0\rangle$.
$C(t) = \langle 0|x_0[\hat{a}(t) + \hat{a}^+(t)]x_0[\hat{a}(0) + \hat{a}^+(0)]|0\rangle =$
$= x_0^2\langle 0|\left[e^{i\omega t}\hat{a}^+(0) + e^{-i\omega t}\hat{a}(0)\right][\hat{a}(0) + \hat{a}^+(0)]|0\rangle$.
Make use of the raising and lowering operators, operating on the ground state.
This results into:
$C(t) = x_0^2 e^{-i\omega t}\langle 0|\hat{a}(0)\hat{a}^+(0)|0\rangle = x_0^2 e^{-i\omega t}\langle 0|0\rangle = x_0^2 e^{-i\omega t}$.

### 8.15.12 Instantaneous Force

Consider a simple harmonic oscillator in its ground-state.
An instantaneous force imparts momentum $p_0$ to the system such that the new state vector is given by
$|\psi\rangle = e^{-ip_0\hat{x}/\hbar}|0\rangle$,
where $|0\rangle$ is the ground-state of the original oscillator.
What is the probability $P(0)$ the system will stay in the ground-state?
The probability
$P(0) = |\langle 0|\psi\rangle|^2 = |\langle 0|e^{-ip_0\hat{x}/\hbar}|0\rangle|^2$.
We learned the identity for operators, real and complex numbers(a c-number), the GlauberÕs theorem Eq.(8.409),
$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-[\hat{A},\hat{B}]/2}$ ,
which holds for $[\hat{A},\hat{B}]$ represents a real or complex number(c-number).
We have
$\hat{x} = x_0[\hat{a} + \hat{a}^+]$,

and $[\hat{a}, \hat{a}^{+}] = 1$.
Then, with $[\hat{a}^{+}, \hat{a}] = -1$, and $\left[\hat{A}, \hat{B}\right] = [-\frac{ip_0 x_0 \hat{a}^{+}}{\hbar}, -\frac{ip_0 x_0 \hat{a}}{\hbar}] = (\frac{p_0 x_0}{\hbar})^2$

$e^{-ip_0\hat{x}/\hbar} = e^{-ip_0 x_0[\hat{a}+\hat{a}^{+}]/\hbar} = e^{-ip_0 x_0\hat{a}^{+}/\hbar} e^{-ip_0 x_0 \hat{a}/\hbar} e^{-\left(\frac{p_0 x_0}{\hbar}\right)^2/2}$.

Hence

$P(0) = e^{-\left(\frac{p_0 x_0}{\hbar}\right)^2} |\langle 0|e^{-ip_0 x_0\hat{a}^{+}/\hbar} e^{-ip_0 x_0 \hat{a}/\hbar}|0\rangle|^2 = e^{-\left(\frac{p_0 x_0}{\hbar}\right)^2} |\langle 0|0\rangle|^2 = e^{-\left(\frac{p_0 x_0}{\hbar}\right)^2}$,

with $x_0 = \sqrt{\frac{\hbar}{2m\omega}}$.

Reminder: the first term in the series expansion of, i.e., contributes, Eq.(8.412):

$e^{-ip_0 x_0 \hat{a}/\hbar}|0\rangle = \left[\hat{I} + \left(-\frac{ip_0 x_0 \hat{a}}{\hbar}\right) + \frac{1}{2}\left(-\frac{ip_0 x_0 \hat{a}}{\hbar}\right)^2 + \cdots.\right]|0\rangle = |0\rangle$.

Furthermore, $\hat{a}^{+} = \hat{a}^{\dagger}$.

### 8.15.13 Coherent States

Coherent states are defined to be eigenstates of the annihilation or lowering operator in the harmonic oscillator potential. Each coherent state has a complex label and is given by $|z\rangle = e^{z\hat{a}^{+}}|0\rangle$.

**a)** Show that $\hat{a}|z\rangle = z|z\rangle$.

$\hat{a}|z\rangle = \hat{a}e^{z\hat{a}^{+}}|0\rangle$:

use series expansion of the exponential and using $\hat{a}^{n}|n\rangle = \sqrt{n+1}|n+1\rangle$,

$\hat{a}|z\rangle = \hat{a}e^{z\hat{a}^{+}}|0\rangle = \sum_{n=0}^{\infty}\frac{z^n}{n!}\hat{a}(\hat{a}^{+})^n|0\rangle = \sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\hat{a}\frac{(\hat{a}^{+})^n}{\sqrt{n!}}|0\rangle$.

Then:

$\frac{(\hat{a}^{+})^n}{\sqrt{n!}}|0\rangle = \frac{(\hat{a}^{+})^{n-1}}{\sqrt{n!}}|1\rangle = \frac{(\hat{a}^{+})^{n-2}}{\sqrt{n!}}\sqrt{2}|2\rangle = \frac{(\hat{a}^{+})^{n-3}}{\sqrt{n!}}\sqrt{3\cdot 2}|3\rangle = \cdots. = |n\rangle$, see Eq.(8.372).

So,

$\hat{a}|z\rangle = \sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\hat{a}|n\rangle = \sum_{n=1}^{\infty}\frac{z^n}{\sqrt{n!}}\sqrt{n}|n-1\rangle = z\sum_{n=1}^{\infty}\frac{z^{n-1}}{\sqrt{(n-1)!}}|n-1\rangle$.

With a "new" $n$ :

$\hat{a}|z\rangle = z\sum_{n=1}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle$.

As derived above, Eq.(8.372)

$|n\rangle = \frac{(\hat{a}^{+})^n}{\sqrt{n!}}|0\rangle$ .

Hence

$\hat{a}|z\rangle = z\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\frac{(\hat{a}^{+})^n}{\sqrt{n!}}|0\rangle = z\sum_{n=0}^{\infty}\frac{z^n}{n!}(\hat{a}^{+})^n|0\rangle = ze^{z\hat{a}^{+}}|0\rangle$.

Each coherent state is given by

$|z\rangle = e^{z\hat{a}^{+}}|0\rangle$.

Consequently

$\hat{a}|z\rangle = ze^{z\hat{a}^{+}}|0\rangle = z|z\rangle$.

**b)** Show that $\langle z_1|z_2\rangle = e^{z_1^* z_2}$.

With $|z\rangle = e^{z\hat{a}^{+}}|0\rangle$ and $\langle z| = \langle 0|e^{z^*\hat{a}}$, we have

$\langle z_1|z_2\rangle = \langle 0|e^{z_1^*\hat{a}}e^{z_2\hat{a}^{+}}|0\rangle$ .

With the series expansion of the exponential, and the results under a):

$\langle z_1|z_2\rangle = \left[\sum_{m=0}^{\infty}\frac{(z_1^*)^m}{\sqrt{m!}}\langle m|\right]\left[\sum_{n=0}^{\infty}\frac{(z_2)^n}{\sqrt{n!}}|n\rangle\right] = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{(z_1^*)^m}{\sqrt{m!}}\frac{(z_2)^n}{\sqrt{n!}}\delta_{mn} =$

$= \sum_{n=0}^{\infty}\frac{(z_1^*)^n}{\sqrt{n!}}\frac{(z_2)^n}{\sqrt{n!}} = \sum_{n=0}^{\infty}\frac{(z_1^* z_2)^n}{n!} = e^{z_1^* z_2}$ ,

where use has been made of $\langle n-1|\hat{a} = \sqrt{n}\langle n|$, Eq.(8.365).

**c)** Show that the completeness relation takes the form:
$\frac{1}{\pi}\int dxdy\,|z\rangle\langle z|e^{-z^*z} = \frac{1}{\pi}\int dxdy\, e^{z\hat{a}^+}|0\rangle\langle 0|e^{z^*\hat{a}}e^{-z^*z} =$
$= \sum_{m,n}\frac{1}{\pi}\int dxdy\frac{z^m}{m!}(\hat{a}^+)^m|0\rangle\langle 0|\frac{(z^*)^n}{n!}(\hat{a})^n e^{-z^*z}.$
Now , change to polar coordinates:
$z = re^{i\varphi}, z = x + iy, r = \sqrt{x^2 + y^2}$, and $\tan\varphi = \frac{y}{x}$.
The summation over the integral becomes:
$\frac{1}{\pi}\int dxdy\,|z\rangle\langle z|e^{-z^*z} = \sum_{m,n}\frac{1}{\pi}\int_0^{2\pi}d\varphi\int_0^{\infty}rdr\frac{r^m}{m!}e^{mi\varphi}(\hat{a}^+)^m|0\rangle\left\langle 0\right|\frac{r^n}{n!}e^{-ni\varphi}(\hat{a})^n e^{-r^2}.$
We make use of Dirac delta function, in general:
$\delta(q) = \frac{1}{2\pi}\int_0^{2\pi}e^{ikq}dk.$
So,
$\frac{1}{2\pi}\int_0^{2\pi}e^{(m-n)i\varphi}\,d\varphi = \delta(m-n) = \delta_{mn}.$
Plugging the delta function into
$\frac{1}{\pi}\int dxdy\,|z\rangle\langle z|e^{-z^*z} =$
$= 2\delta_{mn}\int_0^{\infty}r\,e^{-r^2}dr\left[\sum_m\frac{r^m}{m!}(\hat{a}^+)^m|0\rangle\right]\left[\langle 0|\sum_n\frac{r^n}{n!}(\hat{a})^n\right].$
Due to the delta function, the cross products are 0, resulting into
$\frac{1}{\pi}\int dxdy\,|z\rangle\langle z|e^{-z^*z} = \sum_n\int_0^{\infty}rr^{2n}e^{-r^2}dr\frac{(\hat{a}^+)^n}{n!}|0\rangle\langle 0|\frac{(\hat{a})^n}{n!}.$
Making use of $|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle$, the integral becomes:
$\frac{1}{\pi}\int dxdy\,|z\rangle\langle z|e^{-z^*z} = \sum_n\frac{1}{n!}\int_0^{\infty}rr^{2n}e^{-r^2}dr\,|n\rangle\langle n|.$
The integral
$\int_0^{\infty}rr^{2n}e^{-r^2}dr,$
with substitution $r^2 = p \rightarrow \int_0^{\infty}rr^{2n}e^{-r^2}dr = \int_0^{\infty}p^n e^{-p}dp = n!,$
where use has been made of integration by parts.
Hence
$\frac{1}{\pi}\int dxdy\,|z\rangle\langle z|e^{-z^*z} = \sum_n\frac{1}{n!}\int_0^{\infty}rr^{2n}e^{-r^2}dr\,|n\rangle\langle n| = \sum_n|n\rangle\langle n| = \hat{I}.$

### 8.15.14 Oscillator with Delta Function

Consider a harmonic oscillator potential with an extra delta function term at the origin, that is,
$V(x) = \frac{1}{2}m\omega^2x^2 + \frac{\hbar^2 g}{2m}\delta(x).$
**a)** Using the parity invariance of the Hamiltonian, show that the energy eigenfunctions are even and odd functions and that the simple harmonic oscillator odd-parity eigenstates are still eigenstates of the system Hamiltonian, with the same eigen values.
Since $V(x) = V(-x)$[9], we have parity conservation and thus only even and odd eigenfunctions. The delta function term in Schrödinger's equation is proportional to $\psi(0)\delta(x)$ , which vanishes for any odd function that satisfies the rest of the equation, such as harmonic oscillator odd eigenfunctions.

[9] $\delta(x) = \delta(-x)$, Dirac, page 60

Thus, the odd eigenfunction of the harmonic oscillator alone are still eigenfunctions of the new Hamiltonian.

**b)** Expand the even-parity eigenstates of the new system in terms of the even-parity harmonic oscillator eigenfunctions and determine the expansion coefficients.

We have

$\psi_E(x) = \sum_{\nu=0}^{\infty} C_{2\nu}\, \psi_{2\nu}(x),$

where $\psi_{2\nu}(x)$ represents the even eigenfunctions of the harmonic oscillator which satisfy

$-\frac{\hbar^2}{2m}\frac{d^2\psi_{2\nu}(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi_{2\nu}(x) = E_{2\nu}\psi_{2\nu}(x) = \hbar\omega(2\nu + \frac{1}{2})\psi_{2\nu}(x).$

The Schrödinger including the delta function potential reads

$-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi_E(x) - E\psi_E(x) = -\frac{\hbar^2 g}{2m}\delta(x)\psi_E(x).$

With the above series expansion of eigenfunctions:

$\sum_{\nu=0}^{\infty} C_{2\nu}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 - E\right)\psi_{2\nu}(x) = -\frac{\hbar^2 g}{2m}\delta(x)\psi_E(x).$

Multiply the preceding expression with $\psi_{2\mu}(x)$, integrate over $x$ and use orthogonality

$\int dx \sum_{\nu=0}^{\infty} C_{2\nu}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 - E\right)\psi_{2\nu}(x)\psi_{2\mu}(x) = -\int dx \frac{\hbar^2 g}{2m}\delta(x)\psi_E(x)\psi_{2\mu}(x).$

Then,

with $-\frac{\hbar^2}{2m}\frac{d^2\psi_{2\nu}(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi_{2\nu}(x) = \hbar\omega(2\nu + \frac{1}{2})\psi_{2\nu}(x)$, we have

$\left[\hbar\omega\left(2\nu + \frac{1}{2}\right) - E\right]C_{2\nu} = -\frac{\hbar^2 g}{2m}\psi_E(0)\psi_{2\nu}(0) \rightarrow$

$\rightarrow C_{2\nu} = -\frac{\hbar^2 g}{2m}\frac{\psi_E(0)\psi_{2\nu}(0)}{\hbar\omega\left(2\nu+\frac{1}{2}\right)-E}.$

**c)** Show that the energy eigenvalues that correspond to even eigenstates are solutions of the equation

$\frac{2}{g} = -\sqrt{\frac{\hbar}{m\pi\omega}}\sum_{k=0}^{\infty}\frac{(2k)!}{2^{2k}(k!)^2}(2k + \frac{1}{2} - \frac{E}{\hbar\omega})^{-1}.$

We use the expansion of the wave function in Hermite polynomials, $H_n$ where:

$\psi_n(0) = \left[\sqrt{\pi}(n!)2^n\right]^{-\frac{1}{2}}H_n(0).$

So

$\psi_{2k}(0) = (\frac{m\omega}{\pi\hbar})^{1/4}\frac{\sqrt{(2k)!}}{2^k k!}.$

With the series expansion $\psi_E(x) = \sum_{\nu=0}^{\infty} C_{2\nu}\,\psi_{2\nu}(x)$ and $C_{2\nu} = -\frac{\hbar^2 g}{2m}\frac{\psi_E(0)\psi_{2\nu}(0)}{\hbar\omega\left(2\nu+\frac{1}{2}\right)-E}$:

$\psi_E(x) = -\frac{\hbar^2 g}{2m}\psi_E(0)\sum_{\nu=0}^{\infty}\frac{\psi_{2\nu}(0)}{\hbar\omega\left(2\nu+\frac{1}{2}\right)-E}\psi_{2\nu}(x).$

At $x = 0$, we have

$\psi_E(0) = -\frac{\hbar^2 g}{2m}\psi_E(0)\sum_{\nu=0}^{\infty}\frac{\psi_{2\nu}(0)}{\hbar\omega\left(2\nu+\frac{1}{2}\right)-E}\psi_{2\nu}(0).$

Consequently,

$1 = -\frac{\hbar^2 g}{2m}\sum_{\nu=0}^{\infty}\frac{\psi_{2\nu}(0)}{\hbar\omega\left(2\nu+\frac{1}{2}\right)-E}\psi_{2\nu}(0).$

Furthermore, using the Hermite polynomial expansion

$\psi_{2\nu}(0) = (\frac{m\omega}{\pi\hbar})^{1/4}\frac{\sqrt{(2\nu)!}}{2^\nu \nu!}.$

Plug the preceding result into

$1 = -\frac{\hbar^2 g}{2m}\sum_{\nu=0}^{\infty}\frac{\psi_{2\nu}(0)}{\hbar\omega\left(2\nu+\frac{1}{2}\right)-E}\psi_{2\nu}(0) \Rightarrow \frac{2}{g} = -\sqrt{\frac{\hbar}{m\pi\omega}}\sum_{k=0}^{\infty}\frac{(2k)!}{2^{2k}(k!)^2}(2k + \frac{1}{2} - \frac{E}{\hbar\omega})^{-1}.$

**d)** Using the given gamma function expression we get the following cases:
(1) $g > 0, E > 0$ ,
(2) $g < 0, E > 0$ ,
(3) $g < 0, E < 0$ .

The given gamma function expression?
In problem 8.15.7:
$\Gamma(k) = \int_0^\infty x^{k-1} e^{-x} dx$,
or as indicated by Boccio
$\sum_{k=0}^\infty \frac{(2k)!}{4^k (k!)^2} \frac{1}{2k+1-x} = \frac{\sqrt{\pi}}{2} \frac{\Gamma\left(\frac{1}{2}-\frac{x}{2}\right)}{\Gamma\left(1-\frac{x}{2}\right)}$.
See for gamma functions: Abramowitz, M., and I. A. Stegun Chapter 6.
Also,
$\Gamma\left(n+\frac{1}{2}\right) = \frac{(2n)!}{n! \cdot 2^{2n}}$,
for $n \in \mathbb{N}$ .
furthermore,
$\Gamma(z+1) = z\Gamma(z) = z! = z(z-1)!$
See for gamma functions: Abramowitz, M., and I. A. Stegun Chapter 6., and
www.nl.wikipedia.org

Show that for
(1) $g > 0, E > 0$ ,
(2) $g < 0, E > 0$ ,
there are an infinite number of energy eigenvalues.
We have
$\frac{2}{g} = -\sqrt{\frac{\hbar}{m\pi\omega}} \sum_{k=0}^\infty \frac{(2k)!}{2^{2k}(k!)^2} \left(2k + \frac{1}{2} - \frac{E}{\hbar\omega}\right)^{-1}$ .
Then with
$\sum_{k=0}^\infty \frac{(2k)!}{4^k (k!)^2} \frac{1}{2k+1-x} = \frac{\sqrt{\pi}}{2} \frac{\Gamma\left(\frac{1}{2}-\frac{x}{2}\right)}{\Gamma\left(1-\frac{x}{2}\right)}$
$\frac{4}{g} = -\sqrt{\frac{\hbar}{m\omega}} \frac{\Gamma\left(\frac{1}{4}-\frac{E}{2\hbar\omega}\right)}{\Gamma\left(\frac{3}{4}-\frac{E}{2\hbar\omega}\right)}$.
The right-hand side of the preceding expression has poles at
$\frac{1}{4} - \frac{E}{2\hbar\omega} = n,\ n = 0,1,2, \dots . \Longrightarrow E = \hbar\omega(2n + \frac{1}{2})$,
and zero's at the points
$\frac{3}{4} - \frac{E}{2\hbar\omega} = n,\ n = 0,1,2, \dots . \Longrightarrow E = \hbar\omega(2n + \frac{3}{2})$.
We use
$\Gamma(z+1) = z\Gamma(z)$, and $z = -\varepsilon$, with $\varepsilon > 0$
$\Gamma(1-\varepsilon) = -\varepsilon\Gamma(-\varepsilon) \Longrightarrow \Gamma(-\varepsilon) = -\frac{\Gamma(1-\varepsilon)}{\varepsilon} < 0$ .
Using a plot of
$\frac{\Gamma\left(\frac{1}{4}-\frac{E}{2\hbar\omega}\right)}{\Gamma\left(\frac{3}{4}-\frac{E}{2\hbar\omega}\right)}$,
shows for $g > 0$ an infinite number of points $E_n < \hbar\omega(2n + \frac{1}{2})$.
Conclusion

The positive energy eigenvalues are in correspondence with those of the even harmonic oscillator eigenfunctions, lying lower or higher than those in the repulsive or attractive delta function.

For $g < 0$

$\frac{4}{g} = -\sqrt{\frac{\hbar}{m\omega}} \frac{\Gamma\left(\frac{1}{4}+\frac{|E|}{2\hbar\omega}\right)}{\Gamma\left(\frac{3}{4}+\frac{|E|}{2\hbar\omega}\right)}$ or

$-\frac{4}{g}\sqrt{\frac{m\omega}{\hbar}} = \frac{\Gamma\left(\frac{1}{4}+\frac{|E|}{2\hbar\omega}\right)}{\Gamma\left(\frac{3}{4}+\frac{|E|}{2\hbar\omega}\right)}$,

is a monotonic function of $|E|$ that starts from the value

$\frac{\Gamma(\frac{1}{4})}{\Gamma(\frac{3}{4})} \approx 2.96$ ,

at $E = 0$ and decreases to 1 at $|E| \to \infty$.

The left hand side of $-\frac{4}{g}\sqrt{\frac{m\omega}{\hbar}} = \frac{\Gamma\left(\frac{1}{4}+\frac{|E|}{2\hbar\omega}\right)}{\Gamma\left(\frac{3}{4}+\frac{|E|}{2\hbar\omega}\right)}$ , is a horizontal line.

There is a single solution for

$[\frac{\Gamma(\frac{1}{4})}{\Gamma(\frac{3}{4})}]^{-2} < \frac{g^2\hbar}{16m\omega} < 1.$

### 8.15.15 Measurement on a Particle in a Box.

Consider a particle in a box of width $a$, prepared in the ground state.

I assume the configuration:

$\psi \neq 0, 0 < x < a,$

and

$\psi = 0, |x| \geq a.$

Another possible configuration:

$\psi \neq 0 , |x| \leq \frac{a}{2},$

and

$\psi = 0, |x| \geq \frac{a}{2}$

What are then the possible values one can measure for:

**a)** and **b)**

- energy,
- position,
- momentum?

The system is prepared in the ground state.

The boundary conditions for the wave function are: $\psi(x = 0) = 0 = \psi(x = a)$. A particle in an infinite well.

The wave function for this system is:

$\psi(x) = \sqrt{\frac{2}{a}} \sin\frac{\pi x}{a}$ .

Note the wave function for the other configuration and the particle prepared in the ground state is

$\psi(x) = \sqrt{\frac{2}{a}} \cos\frac{\pi x}{a}$ ,

with $n = 1$.

The possible values one can measure for any observable are its eigenvalues,

With the probability
$P = |\langle\psi_E|\psi\rangle|^2$.
- the energy
$\psi(x) = \sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}$,
is the energy eigenfunction in the ground state.
The energy measured in the ground state is:
$E_1 = \frac{\hbar^2 k_1^2}{2m} = \frac{\hbar^2\pi^2}{2ma^2}$,
$k_1$ is the ground state wave number.
There is just one value of the energy. Consequently, the probability to measure this observable is equal to one.
- the position
The probability density $P(x) = |\psi(x)|^2$.
Remark: I continue with the ground state
$\psi(x) = \sqrt{\frac{2}{a}}\cos\frac{\pi x}{a}$,
the second configuration.
The probability is
$P(x) = \frac{2}{a}\cos^2\frac{\pi x}{a}$.
- momentum
For a particle in a well, the eigenfunctions are plane waves.
Momentum
$p = \hbar k$.
So, we express the wave function in wavenumbers. We use Fourier transform for transformation of the position into $p$ or $k$.
The plane wave function in position representation
$u_k(x) = \frac{1}{\sqrt{2\pi}}e^{ikx}$.
The Fourier transform of the plane wave function
$\tilde{\psi}(k) = \langle u_k|\psi\rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x)\,e^{-ikx}dx$.
The probability density
$P(k) = |\tilde{\psi}(k)|^2$.
The momentum space wave function, $\tilde{\varphi}(p)$ , is the wave number wave function times a constant:
$\tilde{\varphi}(p) = \frac{1}{\sqrt{\hbar}}\tilde{\psi}(k)$ .
Next, we evaluate
$\tilde{\psi}(k) = \langle u_k|\psi\rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x)\,e^{-ikx}dx$.
Plug the expression for $\psi(x) = \sqrt{\frac{2}{a}}\cos\frac{\pi x}{a}$ into the preceding integral:
$$\tilde{\psi}(k) = \frac{1}{2}\sqrt{\frac{2}{a}}\int_{-\frac{a}{2}}^{\frac{a}{2}}\left[e^{i\left(\frac{\pi}{a}-k\right)x} + e^{-i\left(\frac{\pi}{a}+k\right)x}\right]dx = \sqrt{\frac{2}{a}}\left[\frac{\sin\left(\frac{\pi}{2}-\frac{ka}{2}\right)}{\frac{\pi}{2}-\frac{ka}{2}} + \frac{\sin\left(\frac{\pi}{2}+\frac{ka}{2}\right)}{\frac{\pi}{2}+\frac{ka}{2}}\right] =$$
$$= \sqrt{\frac{2}{a}}\left[\operatorname{sinc}\left(\frac{\pi}{2}-\frac{ka}{2}\right) + \operatorname{sinc}\left(\frac{\pi}{2}+\frac{ka}{2}\right)\right],$$
where
$\operatorname{sinc} x = \frac{\sin x}{x}$.

The momentum space wave function becomes

$\tilde{\varphi}(p) = \frac{1}{\sqrt{\hbar}}\tilde{\psi}(k) = \sqrt{\frac{2}{a\hbar}}\left[\mathrm{sinc}\left(\frac{\pi}{2} - \frac{ka}{2}\right) + \mathrm{sinc}\left(\frac{\pi}{2} + \frac{ka}{2}\right)\right],$

and

$P(p) = |\tilde{\varphi}(p)|^2$ .

**c)** At some time (call it $t = 0$) we perform a measurement on position. However, our detector has only finite resolution. We find that the particle is in de middle of the box(call it the origin) with an uncertainty of $\Delta x = \frac{a}{2}$, that is, we know the position is, for sure, in the range $-\frac{a}{4} < x < \frac{a}{4}$, but we are completely unsure where it is within this range. What is the (normalized) post-measurement state?

The particle is in the range $-\frac{a}{4} < x < \frac{a}{4}$ with 100% certainty. Meaning, there is a homogeneous distribution for the probability density. And with probability equal to $\frac{a}{2} \cdot \frac{2}{a} = 1$.

So, the height of the probability density is $\frac{2}{a}$ over the interval $-\frac{a}{4} < x < \frac{a}{4}$

$P(x) = |\psi(x)|^2 = \frac{2}{a} \Longrightarrow \psi(x) = \sqrt{\frac{2}{a}}\, , -\frac{a}{4} < x < \frac{a}{4}\, ,$

and

$\psi(x) = 0\, , -\frac{a}{2} < x < -\frac{a}{4}$, and $\frac{a}{4} < x < \frac{a}{2}$.

**d)** Immediately after the position measurement what are the possible values for the energy, position and momentum with what probabilities?

-energy eigenfunctions

In general

$\psi(x) = \sum_n c_n u_n(x)$.

Then, mathematically we are expanding the "hat function" in its Fourier transform:

- $u_n(x) = \sqrt{\frac{2}{a}}\cos\frac{n\pi x}{a}$ , $n$ is odd,

- $u_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$ , $n$ is even .

The coefficients $c_n$

$c_n = \int u_n^* \,\psi dx$ .

Since the hatfunction is even, only the cos terms contribute to the integral:

$c_n = \frac{2}{a}\int_{-a/4}^{a/4}\cos\frac{n\pi x}{a}dx = \mathrm{sinc}\frac{n\pi}{4}$, $n$ is odd.

The energies are the same as found under a) and with the odd value of $n$

$E_n = \frac{\hbar^2}{2m}(\frac{n\pi}{a})^2$.

The probability is, for the odd values of $n$

$|c_n|^2 = \mathrm{sinc}^2\frac{n\pi}{4} = \frac{8}{n^2\pi^2}$,

using $\sin^2\frac{n\pi}{4} = \frac{1}{2}$.

- possible positions

With the uniform probability distribution

$P(x) = \frac{2}{a}$.

- momentum

With Fourier transform

$\tilde{\psi}(k) = \langle u_k|\psi\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ikx} dx,$
with $p = \hbar k$

$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ipx/\hbar} dx = \sqrt{\frac{1}{a\pi\hbar}} \int_{-a/4}^{a/4} e^{-ipx/\hbar} dx = \frac{1}{2}\sqrt{\frac{a}{\pi\hbar}} \operatorname{sinc}\frac{pa}{4\hbar}.$

With this Fourier transform the probability density is:

$|\tilde{\psi}(p)|^2 = \frac{a}{4\pi\hbar} \operatorname{sinc}^2 \frac{pa}{4\hbar}.$

**e)** What we found at $t = 0$, we will find at any later time, since there is nothing special choosing $t = 0$.

### 8.15.16 Aharonov-Bohm Experiment

Consider an infinitely long solenoid which carries a current $I$ sothat there is a constant magnetic field inside the solenoid, Figure 8.5, Boccio.

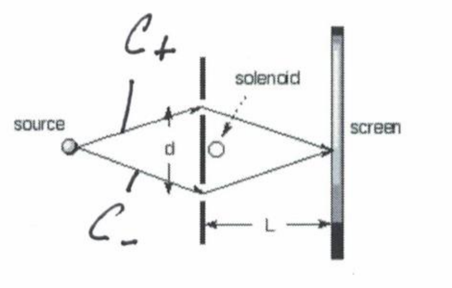



Figure 8.5: Aharonov-Bohm Setup

Suppose that in the region outside the solenoid the motion of a particle with charge $e$ and mass $m$ is described by the Schrödinger equation.
Assume that for $I = 0$ the solution of the Schrödinger equation is given by

$\psi_0(\vec{r}, t) = e^{iE_0 t/\hbar} \psi_0(\vec{r}).$

**a)** Write down and solve the Schrödinger equation in the region outside the solenoid in the case of $I \neq 0$.

There is a magnetic field and we use the vector potential $\vec{A}$ and minimal coupling(nonrelativistic), so momentum is written as:

$\vec{p} - \frac{e}{c}\vec{A},$

where $\nabla \times \vec{A} = \vec{B}.$

The Schrödinger equation reads in this case

$i\hbar \frac{\partial \psi_0(\vec{r},t)}{\partial t} = [\frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + V(\vec{r})]\, \psi_0(\vec{r}, t).$

Let us try the following approximation for the wave function

$\psi(\vec{r}, t) = e^{iE_0 t/\hbar} \psi_0(\vec{r}) e^{\frac{i}{\hbar}\int \frac{e}{c}\vec{A}\cdot d\vec{r}}.$

**b)** Consider the two-slit diffraction experiment for the particles described by $\psi(\vec{r}, t)$ shown in Figure 8.5 above. Assume that the distance d, Figure 8.5, is large compared to the diameter of the solenoid.

Compare the shift $\Delta S$ of the diffraction pattern on the screen due to the presence of the solenoid($I \neq 0$). Assume L, Figure 8.5, much larger than $\Delta S$.

For $I = 0$, for any point onthe screen, the probability amplitude is

$f = f_+ + f_-,$

where
$f_+$ is the probability amplitude from the upper slit path,
$f_-$ is the probability amplitude from the lower slit path.
When $I \neq 0$
$f' = f'_+ + f'_-$.
Using $\psi(\vec{r},t) = e^{iE_0 t/\hbar}\psi_0(\vec{r})e^{\frac{i}{\hbar}\int \frac{e}{c}\vec{A}\cdot d\vec{r}}$:
$f' = f'_+ + f'_- = f_+ e^{\frac{i}{\hbar}\int_{C_+}^{-} \int \frac{e}{c}\vec{A}\cdot d\vec{r}} + f_- e^{\frac{i}{\hbar}\int_{C_-}^{-} \int \frac{e}{c}\vec{A}\cdot d\vec{r}}$.
In the first term on the right hand side of the preceding expression, the integral is along the upper path, $C_+$. In the second term, the integral is along the lower path $C_-$. See the Figure above.
Next rewrite the preceding expression:
$f' = f'_+ + f'_- = (f_+ + f_- e^{\frac{i}{\hbar}\oint \frac{e}{c}\vec{A}\cdot d\vec{r}})e^{\frac{i}{\hbar}\int_{C_+}^{-} \int \frac{e}{c}\vec{A}\cdot d\vec{r}} \propto (f_+ + f_- e^{\frac{i}{\hbar}\oint \frac{e}{c}\vec{A}\cdot d\vec{r}})$.
The upper path and the lower path together represents a closed path integral surrounding the solenoid: $\oint \frac{e}{c}\vec{A}\cdot d\vec{r} = \int_{C_-}^{-} \int \frac{e}{c}\vec{A}\cdot d\vec{r} - \int_{C_+}^{-} \int \frac{e}{c}\vec{A}\cdot d\vec{r}$.
This results into a phase factor
$\frac{e\varphi}{\hbar c} = \frac{e\oint \vec{A}\cdot d\vec{r}}{\hbar c}$, remind Stokes Theorem.
We worked on a problem of Young's interference (in optics) we get the interference pattern be shifted by $\Delta S$ and L≫d and L≫ $\Delta S$,
$\Delta S \frac{d}{L} k = \frac{e\varphi}{\hbar c}$,
or,
$\Delta S = \frac{e\varphi L}{\hbar c d k}$.
Then, with $E_0 = \frac{\hbar^2 k^2}{2m} \Longrightarrow k = \sqrt{\frac{2mE_0}{\hbar^2}}$,
$\Delta S = \frac{e\varphi L}{\hbar c d k} = \frac{e\varphi L}{cd\sqrt{2mE_0}}$.

### 8.15.17 A Josephson Junction

**Introduction**
A Josephson junction is formed when two superconducting wires are separated by an insulating gap of capacitance $C$. The quantum states $\psi_i$ , $i = 1,2$ of the two wires can be characterized by the numbers $n_i$ of Cooper pairs (charge$= -2e$) and phase $\theta_i$, such that $\psi_i = \sqrt{n_i}e^{i\theta_i}$ (Ginzburg-Landau approximation).
The small amplitude that a pair tunnel across a narrow insulating barrier is $-E_J/n_o$ where $n_0 = n_1 + n_2$ and $E_J$ is the so-called Josephson energy.
The interesting physics is expressed in the differences
$n = n_1 - n_2$ , $\varphi = \theta_2 - \theta_1$.
We consider a junction where
$n_1 \approx n_2 \approx n_0/2$.
When there exists a nonzero difference $n$ between the numbers of pairs of charge $-2e$, where $e > 0$, on the two sides of the junction, there is a net charge $-ne$ on side 2 and a net charge $+ne$ on side 1. Hence a voltage difference $ne/C$ arises, where the voltage on side 1 is higher tah that onside 2 if $n_2 - n_1 > 0$. Taking the zero of the voltage to be at the center

of the junction, the electrostatic energy of the Cooper pair of charge $-2e$ on side 2 is $\frac{ne^2}{C}$, and that of a pair onside 1 is $-ne^2/C$ . The total electrostatic energy is $\frac{C(\Delta V)^2}{2} = \frac{Q^2}{2C} = \frac{ne^2}{2C}$ .

The equations of motion for a pair in the two-state system (1,2) are

$i\hbar \frac{d\psi_1}{dt} = U_1\psi_1 - \frac{E_J}{n_o}\psi_2 = -\frac{ne^2}{C}\psi_1 - \frac{E_J}{n_o}\psi_2$ ,

and

$i\hbar \frac{d\psi_2}{dt} = U_2\psi_2 - \frac{E_J}{n_o}\psi_1 = \frac{ne^2}{C}\psi_2 - \frac{E_J}{n_o}\psi_1$.

**a)** Discuss the physics of the term in both equations.

- $U_1\psi_1$, and $U_2\psi_2$ :

these two terms give the usual solutions of the form $e^{i\omega t}$ representing steady-state behaviour of the probability amplitude on side 1 and side 2.

- $\frac{E_J}{n_o}\psi_2$ , and $\frac{E_J}{n_o}\psi_1$:

These two terms represent the tunneling. A probability current flow across the boundary between regions, i.e., change in region 1 due to a current proportional to the amplitude on side 2 and vice versa.

**b)** Using $\psi_i = \sqrt{n_i}e^{i\theta_i}$, show that the equations of motion for $n$ and $\varphi$ are given by

$\dot{\varphi} = \dot{\theta}_2 - \dot{\theta}_1 \approx -\frac{2ne^2}{\hbar C}$ ,

and

$\dot{n} = \dot{n}_2 - \dot{n}_1 \approx \frac{E_J}{\hbar}\sin\varphi$.

With $\psi_i = \sqrt{n_i}e^{i\theta_i}$,

and $i\hbar \frac{d\psi_1}{dt} = U_1\psi_1 - \frac{E_J}{n_o}\psi_2 = -\frac{ne^2}{C}\psi_1 - \frac{E_J}{n_o}\psi_2$:

$i\hbar\left(\frac{\dot{n}_1}{2\sqrt{n_1}}e^{i\theta_1} + i\dot{\theta}_1\sqrt{n_1}e^{i\theta_1}\right) = U_1\sqrt{n_1}e^{i\theta_1} - \frac{E_J}{n_o}\sqrt{n_2}e^{i\theta_2}$,

and

$i\hbar \frac{d\psi_2}{dt} = U_2\psi_2 - \frac{E_J}{n_o}\psi_1 = \frac{ne^2}{C}\psi_2 - \frac{E_J}{n_o}\psi_1$:

$i\hbar\left(\frac{\dot{n}_2}{2\sqrt{n_2}}e^{i\theta_2} + i\dot{\theta}_2\sqrt{n_2}e^{i\theta_2}\right) = U_2\sqrt{n_2}e^{i\theta_2} - \frac{E_J}{n_o}\sqrt{n_1}e^{i\theta_1}$.

Multiply $i\hbar\left(\frac{\dot{n}_1}{2\sqrt{n_1}}e^{i\theta_1} + i\dot{\theta}_1\sqrt{n_1}e^{i\theta_1}\right) = U_1\sqrt{n_1}e^{i\theta_1} - \frac{E_J}{n_o}\sqrt{n_2}e^{i\theta_2}$, with$\sqrt{n_1}$ and divide by $e^{i\theta_1}$, giving

$i\hbar\frac{\dot{n}_1}{2} - \hbar n_1\dot{\theta}_1 = U_1 n_1 - \frac{E_J}{n_o}\sqrt{n_1 n_2}e^{i(\theta_2-\theta_1)} = U_1 n_1 - \frac{E_J}{n_o}\sqrt{n_1 n_2}e^{i\varphi}$.

Similar for the other differential equation

$i\hbar\frac{\dot{n}_2}{2} - \hbar n_2\dot{\theta}_2 = U_2 n_2 - \frac{E_J}{n_o}\sqrt{n_1 n_2}e^{-i(\theta_2-\theta_1)} = U_2 n_2 - \frac{E_J}{n_o}\sqrt{n_1 n_2}e^{-i\varphi}$.

Let us present these two differential equations in their real and imaginary partsand use the expression for $U_1$ and $U_2$

$i\hbar\frac{\dot{n}_1}{2} - \hbar n_1\dot{\theta}_1 = U_1 n_1 - \frac{E_J}{n_o}\sqrt{n_1 n_2}(\cos\varphi + i\sin\varphi)$,

$i\hbar\frac{\dot{n}_2}{2} - \hbar n_2\dot{\theta}_2 = U_2 n_2 - \frac{E_J}{n_o}\sqrt{n_1 n_2}(\cos\varphi - i\sin\varphi)$.

The real part

$\dot{\theta}_1 = \frac{ne^2}{\hbar C} + \frac{E_J}{\hbar n_o}\sqrt{\frac{n_2}{n_1}}\cos\varphi$ , $\dot{\theta}_2 = -\frac{ne^2}{\hbar C} + \frac{E_J}{\hbar n_o}\sqrt{\frac{n_1}{n_2}}\cos\varphi$ ,

and the imaginary part

$\dot{n}_1 = -\frac{E_J}{\hbar n_o}\sqrt{n_1 n_2}\sin\varphi$ , $\dot{n}_2 = \frac{E_J}{\hbar n_o}\sqrt{n_1 n_2}\sin\varphi$ .

The four preceding equations can be written as:

$\dot{\varphi} = \dot{\theta}_2 - \dot{\theta}_1 = -\frac{2ne^2}{\hbar C} - \frac{E_J}{\hbar n_o}\left(\sqrt{\frac{n_2}{n_1}} - \sqrt{\frac{n_1}{n_2}}\right)\cos\varphi$ .

$\dot{n} = \dot{n}_2 - \dot{n}_1 = \frac{2E_J}{\hbar n_o}\sqrt{n_1 n_2}\sin\varphi$ .

With $n_1 \approx n_2 \approx n_0/2$ , both preceding equations can be approximated by

$\dot{\varphi} \approx -\frac{2ne^2}{\hbar C}$ ,

and

$\dot{n} = \frac{E_J}{\hbar}\sin\varphi \ = 0$

**c)** Show that the pair (electric current) from side 1 to side 2 is given by

$J_S = J_0 \sin\varphi$ ,

with $J_0 = \frac{\pi E_J}{\phi_0}$ .

We identify a pair(electrical current) from side 1 to side 2, with the results under b)

$J_S = -2e\frac{\dot{n}}{2} = -\frac{2e\frac{E_J}{\hbar}\sin\varphi}{2} \equiv J_0 \sin\varphi$.

So, the maximum current is

$J_0 = e\frac{E_J}{\hbar} = \frac{\pi E_J}{\phi_0}$ ,

where $\phi_0 = \frac{\pi\hbar}{e}$

**d)** Show that

$\ddot{\varphi} \approx -\frac{2e^2}{\hbar C}\frac{E_J}{\hbar}\sin\varphi$ .

$\dot{\varphi} = -\frac{2ne^2}{\hbar C} \Longrightarrow \ddot{\varphi} = -\frac{2\dot{n}e^2}{\hbar C} = -\frac{2e^2}{\hbar C}\frac{E_J}{\hbar}\sin\varphi$ .

For $E_J$, positive show that $\ddot{\varphi} \approx -\frac{2e^2}{\hbar C}\frac{E_J}{\hbar}\sin\varphi$ implies there are oscillations about $\varphi = 0$ , whose angular frequency ( called the Josephson plasma frequency) is given by

$\omega_J = \sqrt{\frac{2e^2}{\hbar C}\frac{E_J}{\hbar}} = \sqrt{\frac{2e^2 E_J}{\hbar^2 C}}$

for small amplitudes.

We have the differential equation:

$\ddot{\varphi} + \frac{2e^2}{\hbar C}\frac{E_J}{\hbar}\sin\varphi \ = 0.$

For small amplitudes the preceding equation becomes

$\ddot{\varphi} + \frac{2e^2}{\hbar C}\frac{E_J}{\hbar}\varphi = 0.$

Hence the frequency of the oscillations is, for $E_J$ positive,

$\omega_J = \sqrt{\frac{2e^2 E_J}{\hbar^2 C}}$ .

When $E_J$ is negative , the small oscillations are near $\varphi = \pi$, with the same frequency.

So, $\pi - \varphi$ is the small amplitude.
**e)** If a voltage $V = V_1 - V_2$ is applied across the junction(by a battery), a charge $Q_1 = VC = (-2e)\left(-\frac{n}{2}\right) = e \cdot n$, is held on side 1, and the negative of this on side 2, then show we have

$$\dot{\varphi} \approx -\frac{2eV}{\hbar} \equiv -\omega.$$

with the result under b)

$$\dot{\varphi} \approx -\frac{2ne^2}{\hbar C} = -2\frac{(-2e)\left(-\frac{n}{2}\right)e}{\hbar C} = -2\frac{VCe}{\hbar C} = -\frac{2Ve}{\hbar} \equiv -\omega,$$

which gives $\varphi = -\omega t$ .
The battery holds the charge difference across the junction fixed at $VC = e \cdot n$ , but can be a source or sink of charge such that the current can flow in the circuit. In this case, the current is given by

$$J_S = -2e\frac{\dot{n}}{2} = -\frac{2e\frac{E_J}{\hbar}\sin\varphi}{2} \equiv J_0 \sin\varphi = -J_0 \sin\omega t,$$

where use has been made of the results under b) and c).

### 8.15.18 Eigenstates using Coherent States

Obtain eigenstates of the following Hamiltonian

$$\hat{H} = \hbar\omega\hat{a}^+\hat{a} + V\hat{a} + V^*\hat{a}^+$$

for a complex $V$ using coherent states.
A new set operators

$\hat{a} = \hat{b} + \alpha$ ,  $\hat{a}^+ = \hat{b}^+ + \alpha^*$, see page 601, the harmonic oscillator.
The new set of operators has the same commutation relations:

$$[\hat{a}, \hat{a}^+] = [\hat{b} + \alpha, \hat{b}^+ + \alpha^*] = (\hat{b} + \alpha)(\hat{b}^+ + \alpha^*) - (\hat{b}^+ + \alpha^*)(\hat{b} + \alpha) =$$
$$\hat{b}\hat{b}^+ - \hat{b}^+\hat{b} + \hat{b}\alpha^* - \alpha^*\hat{b} + \alpha\,\hat{b}^+ - \hat{b}^+\alpha + \alpha\alpha^* - \alpha^*\alpha.$$

Since $\alpha$ is a complex number, the preceding expression reduces into

$$[\hat{a}, \hat{a}^+] = \hat{b}\hat{b}^+ - \hat{b}^+\hat{b} = [\hat{b}, \hat{b}^+] = 1.$$

Since the operators cummute, they have the same eigenvalues and eigenvectors:

$$\hat{a}^+\hat{a}|n\rangle_a = \hat{a}^+\sqrt{n}|n-1\rangle = \sqrt{n}\hat{a}^+|n-1\rangle = \sqrt{n}\sqrt{n}|n\rangle = n|n\rangle_a \text{ , } n = 1,2,3, \ldots$$

and

$$\hat{b}^+\hat{b}|n\rangle_b = n|n\rangle_b, n = 1,2,3, \ldots$$

Substitute the new operators into the Hamiltonian

$$\hat{H} = \hbar\omega(\hat{b}^+ + \alpha^*)(\hat{b} + \alpha) + V(\hat{b} + \alpha) + V^*(\hat{b}^+ + \alpha^*) =$$
$$= \hbar\omega\hat{b}^+\hat{b} + \hbar\omega(\hat{b}^+\alpha + \alpha^*\hat{b} + \alpha^*\alpha) + V(\hat{b} + \alpha) + V^*(\hat{b}^+ + \alpha^*) =$$
$$= \hbar\omega\hat{b}^+\hat{b} + \hbar\omega(\hat{b}^+\alpha + \alpha^*\hat{b} + \alpha^*\alpha) + V\hat{b} + V^*\hat{b}^+ + V\alpha + V^*\alpha^* =$$
$$= \hbar\omega\hat{b}^+\hat{b} + (\hbar\omega\alpha^* + V)\hat{b} + \hbar\omega(\hat{b}^+\alpha + \alpha^*\alpha) + V^*\hat{b}^+ + V\alpha + V^*\alpha^*.$$

Her I used the procedure used by Boccio on page 601 for a new set of raising and lowering operators.
When I choose

$$\hbar\omega\alpha = -V^*,$$

the Hamiltonian becomes:

$$\hat{H} = \hbar\omega\hat{b}^+\hat{b}.$$

Therefore

$\hat{H}|n\rangle_b = \hbar\omega\hat{b}^+\hat{b}|n\rangle_b = \hbar\omega n|n\rangle_n.$
Thus the energy eigenvalues are
$E_n = \hbar\omega n$ , $n = 0,1,2, \ldots$
The ground state of the system corresponds to $E_0 = 0$.
In addition:
$\hat{b}|0\rangle_b = 0 = (\hat{a} - \alpha)|0\rangle_b = -\alpha|0\rangle_b = \frac{V^*}{\hbar\omega}|0\rangle_b.$
The groundstate is a coherent state.

### 8.15.19 Bogliubov Transformation

Suppose annilation and creation operators satisfy the standard commutation relations
$[\hat{a}, \hat{a}^+] = 1.$
Show that the Bogliubov transformation
$\hat{b} = \hat{a}\cosh\eta + \hat{a}^+\sinh\eta,$
preserves the commutation relation of the creation and annihilation operators, i.e.,
$\left[\hat{b}, \hat{b}^+\right] = 1.$
Use this fact to obtain eigenvalues of the following Hamiltonian
$\hat{H} = \hbar\omega\hat{a}^+\hat{a} + \frac{1}{2}V(\hat{a}\hat{a} + \hat{a}^+\hat{a}^+).$
There is an upper limit on $V$ for which this can be done.
Also show that the unitary operator
$\hat{U} = e^{\frac{(\hat{a}\hat{a}+\hat{a}^+\hat{a}^+)\eta}{2}}$
can relate the two sets of operators $\hat{a}, \hat{a}^+$ and $\hat{b}, \hat{b}^+$, as
$\hat{b} = \hat{U}\hat{a}\hat{U}^{-1}.$
We have
$\hat{b} = \hat{a}\cosh\eta + \hat{a}^+\sinh\eta,$
so,
$\hat{b}^+ = \hat{a}^+\cosh\eta + \hat{a}\sinh\eta.$
The, multiply $\hat{b}$ with $\cosh\eta$ and $\hat{b}^+$with $\sinh\eta$, respectively subtract the resulting equations, giving,
$\hat{a} = \hat{b}\cosh\eta - \hat{b}^+\sinh\eta.$
Similarly
$\hat{a}^+ = \hat{b}^+\cosh\eta - \hat{b}\sinh\eta,$
where use has been made of $\cosh^2\eta - \sinh^2\eta = 1.$
Furthermore
$\cosh 2\eta = \cosh^2\eta + \sinh^2\eta,$
and
$\sinh 2\eta = 2\sinh\eta\cosh\eta.$
I suppose $\eta$ to be a number.

- With $[\hat{a}, \hat{a}^+] = 1$, $\left[\hat{b}, \hat{b}^+\right] = 1$?
$\left[\hat{b}, \hat{b}^+\right] = [\hat{a}\cosh\eta + \hat{a}^+\sinh\eta\,, \hat{a}^+\cosh\eta + \hat{a}\sinh\eta] =$
$= \hat{a}\hat{a}^+\cosh^2\eta + \hat{a}\hat{a}\cosh\eta\sinh\eta + \hat{a}^+\hat{a}^+\sinh\eta\cosh\eta + \hat{a}^+\hat{a}\sinh^2\eta +$
$- \hat{a}^+\hat{a}\cosh^2\eta - \hat{a}^+\hat{a}^+\sinh\eta\cosh\eta - \hat{a}\hat{a}\sinh\eta\cosh\eta - \hat{a}\,\hat{a}^+\sinh^2\eta =$

$= \hat{a}\hat{a}^+ \cosh^2\eta + \hat{a}^+\hat{a}\sinh^2\eta - \hat{a}^+\hat{a}\cosh^2\eta - \hat{a}\,\hat{a}^+\sinh^2\eta =$
$= (\hat{a}\hat{a}^+ - \hat{a}^+\hat{a})\cosh^2\eta - (\hat{a}\,\hat{a}^+ - \hat{a}^+\hat{a})\sinh^2\eta =$
$= [\hat{a},\hat{a}^+](\cosh^2\eta - \sinh^2\eta) = [\hat{a},\hat{a}^+] = 1.$
The commutation relations are preserved.

- The eigenvalues of the Hamiltonian?
$\hat{H} = \hbar\omega\hat{a}^+\hat{a} + \frac{1}{2}V(\hat{a}\hat{a} + \hat{a}^+\hat{a}^+) = \hbar\omega(\hat{b}^+\cosh\eta - \hat{b}\sinh\eta)(\hat{b}\cosh\eta - \hat{b}^+\sinh\eta) +$
$+\frac{V}{2}[(\hat{b}\cosh\eta - \hat{b}^+\sinh\eta)^2 + (\hat{b}^+\cosh\eta - \hat{b}\sinh\eta)^2 =$
$= \hbar\omega\left[\hat{b}^+\hat{b}\cosh^2\eta - (\hat{b}^+)^2\cosh\eta\sinh\eta - (\hat{b})^2\sinh\eta\cosh\eta + \hat{b}\hat{b}^+\sinh^2\eta\right] +$
$+\frac{V}{2}\left[\left(\hat{b}^2 + \hat{b}^{+2}\right)(\cosh^2\eta + \sinh^2\eta) - 2(\hat{b}\hat{b}^+ + \hat{b}^+\hat{b})\sinh\eta\cosh\eta\right].$
Now use the hyperbolic relations and the commutator:
$\hat{H} = \hbar\omega(\hat{b}^+\hat{b}\cosh 2\eta + \sinh^2\eta) - \frac{\hbar\omega}{2}\left(\hat{b}^2 + \hat{b}^{+2}\right)\sinh 2\eta + \frac{V}{2}\left(\hat{b}^2 + \hat{b}^{+2}\right)\cosh 2\eta +$
$-\frac{V}{2}(\hat{b}\hat{b}^+ + \hat{b}^+\hat{b})\sinh 2\eta.$
How to proceed?
In problem 8.15.18 we have chosen a relation between $V^*, \alpha$ and $\hbar\omega$.
Inspecting the Hamiltonian of this problem 8.15.19 suggests to get rid of the squared operators. To this end we use:
$\tanh x = \frac{\sinh x}{\cosh x}.$
Hence, choose
$V = \hbar\omega\tanh 2\eta.$
Then, the Hamiltonian becomes
$\hat{H} = \hbar\omega(\hat{b}^+\hat{b}\cosh 2\eta + \sinh^2\eta) - \frac{V}{2}(\hat{b}\hat{b}^+ + \hat{b}^+\hat{b})\sinh 2\eta =$
$= \hbar\omega(\hat{b}^+\hat{b}\cosh 2\eta + \sinh^2\eta) - \frac{V}{2}(1 + 2\hat{b}^+\hat{b})\sinh 2\eta.$
Rearrange the operatorterms
$\hat{H} = \hat{b}^+\hat{b}(\hbar\omega\cosh 2\eta - V\sinh 2\eta) + \hbar\omega\sinh^2\eta - V\sinh\eta\cosh\eta.$
Use the usual expressions "Capital $\omega$" $= \Omega = (\hbar\omega\cosh 2\eta - V\sinh 2\eta)$
and the potential
$V' = \hbar\omega\sinh^2\eta - V\sinh\eta\cosh\eta,$
we have
$\hat{H} = \Omega\hat{b}^+\hat{b} + V'.$
Compare this with the eigenvalues of the harmonic oscillator and keep in mind
$[\hat{b},\hat{b}^+]$commutes with $[\hat{a},\hat{a}^+]$, the energy eigenvalues are:
$E_n = \Omega n + V',\ n = 0,1,2,3,..$
This leads to the conclusion, using the expression for $\Omega$
$\Omega > 0 \Longrightarrow (\hbar\omega\cosh 2\eta - V\sinh 2\eta) > 0 \Longrightarrow V < \frac{\hbar\omega}{\tanh 2\eta}.$
Next, plug $V = \hbar\omega\tanh 2\eta$ into $V < \frac{\hbar\omega}{\tanh 2\eta} \Longrightarrow V < \hbar\omega.$
- Show that the unitary operator
$\hat{U} = e^{\frac{(\hat{a}\hat{a}+\hat{a}^+\hat{a}^+)\eta}{2}}$

can relate the two sets of operators $\hat{a}, \hat{a}^+$ and $\hat{b}, \hat{b}^+$, as
$\hat{b} = \hat{U}\hat{a}\hat{U}^{-1}$.
We use
$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}\big[A, [A, B]\big] + \cdots$.
In addition we make use of:
$[\hat{a}^+\hat{a}^+, \hat{a}] = \hat{a}^+\hat{a}^+\hat{a} - \hat{a}\hat{a}^+\hat{a}^+ = \hat{a}^+\hat{a}^+\hat{a} - \hat{a}^+\hat{a}\hat{a}^+ + \hat{a}^+\hat{a}\hat{a}^+ - \hat{a}\hat{a}^+\hat{a}^+ =$
$= \hat{a}^+(\hat{a}^+\hat{a} - \hat{a}\hat{a}^+) + (\hat{a}^+\hat{a} - \hat{a}\hat{a}^+)\hat{a}^+ = -2\hat{a}^+$.
Similarly
$[\hat{a}\hat{a}, \hat{a}^+] = 2\hat{a}$.
Substitute
$A = \frac{(\hat{a}\hat{a} + \hat{a}^+\hat{a}^+)\eta}{2}$ into the Baker-Hausdorff expression:
$\hat{b} = \hat{U}\hat{a}\hat{U}^{-1} = \hat{a}\left(1 + \frac{\eta^2}{2!} + \cdots\right) + \hat{a}^+\left(\eta + \frac{\eta^3}{3!} + \cdots\right) = \hat{a}\cosh\eta + \hat{a}^+\sinh\eta$.

### 8.15.20 Harmonic Oscillator

Consider a particle in a 1-dimensional harmonic oscillator potential. Suppose at time $t = 0$, the state vector is
$|\psi(0)\rangle = e^{-i\hat{p}\alpha/\hbar}|0\rangle$,
where $\hat{p}$ is the momentum operator and $\alpha$ is a real number.
**a)** Use the equation of motion in the Heisenberg picture to find the operator $\hat{x}(t)$.
The equation of motion
$\frac{dx}{dt} = \frac{i}{\hbar}[H, x]$,
this equation is shorthand for
$\left\langle\psi\middle|\frac{d\hat{x}}{dt}\middle|\psi\right\rangle = \frac{i}{\hbar}\langle\psi|[\hat{H}, \hat{x}]|\psi\rangle$.
The operators are time dependent, i.e., the Heisenberg picture.
- $\frac{dx}{dt} = \frac{i}{\hbar}\left[\frac{p^2}{2m}, x\right] = \frac{i}{2m\hbar}(ppx - xpp) = \frac{i}{2m\hbar}(ppx - pxp + pxp - xpp) =$
$= \frac{i}{2m\hbar}(p(px - xp) + (px - xp)p) = \frac{i}{2m\hbar}(p[p, x] + [p, x]p) = \frac{i}{2m\hbar}(-2i\hbar p) = \frac{p(t)}{m}$.
- $\frac{dp}{dt} = \frac{i}{\hbar}[H, p]$.
For completeness, the Hamiltonian of the harmonic oscillator is
$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$.
So
$\frac{dp}{dt} = \frac{i}{\hbar}[H, p] = \frac{im\omega^2}{2\hbar}(xxp - pxx) = \frac{im\omega^2}{2\hbar}(xxp - xpx + xpx - pxx) =$
$= \frac{im\omega^2}{2\hbar}(x(xp - px) + (xp - px)x) = \frac{im\omega^2}{2\hbar}(x[x, p] + [x, p]x) = \frac{im\omega^2}{2\hbar}2i\hbar x =$
$= -m\omega^2 x(t)$.
The two equations of motion are:
- $\frac{dx}{dt} = \frac{p(t)}{m}$,
- $\frac{dp}{dt} = -m\omega^2 x(t)$.
Solutions of this set of equations are:
$x(t) = c_1\cos\omega t + c_2\sin\omega t$.

At $t = 0$,
$x(t) = x$ , and
$x(t) = x\cos\omega t + c_2\sin\omega t$ .
Furthermore at $t = 0$
$\frac{dx}{dt} = c_2\omega = \frac{p(0)}{m} \equiv \frac{p}{m}$ .
So, we have
$\hat{x}(t) = x\cos\omega t + \frac{p}{m\omega}\sin\omega t,$
and similarly
$\hat{p}(t) = p\cos\omega t - m\omega x\sin\omega t$ .

**b)** Show that $e^{-i\hat{p}\alpha/\hbar}$ is the translation operator.
See also problem 6.19.12:
*The last step to prove the operator*
$\hat{U}(a) = e^{i\hat{p}a/\hbar}$
*is a translation operator.*
*Now* $A = e^{ipa/\hbar}$ .
*So we have:*
$e^{ipa/\hbar}xe^{-ipa/\hbar} = \sum_{n=0}^{\infty}\frac{a^n}{n!}(\frac{i}{\hbar})^n[p,p,\dots[p,x]\dots]].$
*Let us demonstrate what will happen by looking at the first three terms:*
$x + \frac{ia}{\hbar}[p,x] + \frac{(ia)^2}{2!}[p,[p,x]] + \cdots = x + \frac{ia}{\hbar}(-i\hbar) + \frac{(ia)^2}{2!}[p,-i\hbar] + \cdots = x + a + 0 + \cdots =$
$= x + a.$

The translation operator $T(a) = e^{-i\hat{p}\alpha/\hbar}$. (See also Fitzpatrick, Graduate Course Chapter 2.8, *Displacement Operators*).
Then,
$T(a)|x\rangle = e^{-i\hat{p}\alpha/\hbar}|x\rangle = |x + a\rangle$ .

**c)** In the Heisenberg picture calculate the expectation value $\langle x\rangle$ for $t \geq 0$.
We have, with the translation operator and the identity operator,
$\langle\hat{x}\rangle = \langle\psi(0)|\hat{x}(t)|\psi(0)\rangle = \left\langle 0\middle|e^{\frac{i\hat{p}\alpha}{\hbar}}\hat{x}(t)e^{-\frac{i\hat{p}\alpha}{\hbar}}\middle|0\right\rangle = \left\langle 0\middle|\hat{I}e^{\frac{i\hat{p}\alpha}{\hbar}}\hat{x}(t)e^{-\frac{i\hat{p}\alpha}{\hbar}}\hat{I}\middle|0\right\rangle.$
Now we use the continuum representation:
$\langle\hat{x}\rangle = \int dx' \int dx''\,\langle 0|x'\rangle\langle x'|e^{\frac{i\hat{p}\alpha}{\hbar}}\hat{x}(t)e^{-\frac{i\hat{p}\alpha}{\hbar}}|x''\rangle\langle x''|0\rangle.$
With $\hat{x}(t) = x\cos\omega t + \frac{p}{m\omega}\sin\omega t$
$\langle x\rangle = \int dx' \int dx''\,\langle 0|x'\rangle\langle x' + a|(x\cos\omega t + \frac{p}{m\omega}\sin\omega t)|x'' + a\rangle\langle x''|0\rangle.$
We make use of:
$\langle\psi(0)|\hat{p}|\psi(0)\rangle = \left\langle 0\middle|e^{\frac{i\hat{p}\alpha}{\hbar}}\hat{p}e^{-\frac{i\hat{p}\alpha}{\hbar}}\middle|0\right\rangle = \langle 0|\hat{p}|0\rangle = 0$ ,
and
$\hat{x}(0)\cos\omega t\,|x'' + a\rangle = \cos\omega t\,(x'' + a)|x'' + a\rangle \equiv (x'' + a)\cos\omega t\,|x'' + a\rangle.$
Then,
$\langle\hat{x}(t)\rangle = \int dx' \int dx''\,\langle 0|x'\rangle\langle x' + a|(x'' + a)\cos\omega t\,|x'' + a\rangle\langle x''|0\rangle.$
Using

$\int dx' \langle x' + a | x'' + a \rangle = \delta_{x'x''}$,
and dropping the prime
$\langle \hat{x}(t) \rangle = \int dx \langle 0|x\rangle (x+a) \cos\omega t \langle x|0\rangle =$
$= \cos\omega t \int dx \langle 0|x\rangle \hat{x}(0) \langle x|0\rangle + a\cos\omega t \int dx \langle 0|0\rangle = a\cos\omega t.$

### 8.15.21 Another Oscillator

A 1-dimensional harmonic oscillator is , at time $t = 0$, in the state
$|\psi(t=0)\rangle = \frac{1}{\sqrt{3}}(|0\rangle + |1\rangle + |2\rangle),$
where $|n\rangle$ the $n^{th}$ energy eigenstate. Find the expectation value of position and energy at time $t$.
- The expectation value of energy:
With the results of chapter 6, we have for the state vector at time $t$ :
$|\psi(t)\rangle = \frac{1}{\sqrt{3}}\left(e^{-\frac{iE_0 t}{\hbar}}|0\rangle + e^{-\frac{iE_1 t}{\hbar}}|1\rangle + e^{-\frac{iE_2 t}{\hbar}}|2\rangle\right),$
where for the harmonic oscillator we have
$E_n = \hbar\omega\left(n + \frac{1}{2}\right).$
Energy at time $t$
$\langle\psi(t)|E(t)|\psi(t)\rangle = \langle\psi(t)|(E_0 + E_1 + E_2)|\psi(t)\rangle = (E_0 + E_1 + E_2)\langle\psi(t)|\psi(t)\rangle =$
$= \frac{9}{2}\frac{\hbar\omega}{3} = \frac{3}{2}\hbar\omega,$
where use have been made of $\langle i|j\rangle = \delta_{ij}$.
- The expectation value of position:
we know the state vector , so it is helpful to express the position operator in raising and lowering operators:
$\hat{x} = x_0[\hat{a} + \hat{a}^+]$ , and $x_0 = \sqrt{\frac{\hbar}{2m\omega}}$.
Then
$\langle\hat{x}\rangle = x_0\langle\psi(t)|\hat{a} + \hat{a}^+|\psi(t)\rangle =$
$= \frac{x_0}{3}\left(e^{\frac{iE_0 t}{\hbar}}\langle 0| + e^{\frac{iE_1 t}{\hbar}}\langle 1| + e^{\frac{iE_2 t}{\hbar}}\langle 2|\right)(\hat{a} + \hat{a}^+)\left(e^{-\frac{iE_0 t}{\hbar}}|0\rangle + e^{-\frac{iE_1 t}{\hbar}}|1\rangle + e^{-\frac{iE_2 t}{\hbar}}|2\rangle\right) =$
$= \frac{x_0}{3}\left(e^{\frac{iE_1 t}{\hbar}}\langle 0| + \sqrt{2}\cdot e^{\frac{iE_2 t}{\hbar}}\langle 1|\right)\left(e^{-\frac{iE_0 t}{\hbar}}|1\rangle + \sqrt{2}\cdot e^{-\frac{iE_1 t}{\hbar}}|2\rangle\right) =$
$= \frac{x_0}{3}\left(e^{\frac{i(E_1 - E_0 t)}{\hbar}}\langle 0|1\rangle + \sqrt{2}\cdot e^{\frac{i(E_1 - E_1 t)}{\hbar}}\langle 0|2\rangle + \sqrt{2}\cdot e^{\frac{i(E_2 - E_0 t)}{\hbar}}\langle 1|1\rangle + 2\cdot e^{\frac{i(E_2 - E_1 t)}{\hbar}}\langle 1|2\rangle\right) =$
$= \frac{x_0}{3}\sqrt{2}\cdot e^{\frac{i(E_2 - E_0 t)}{\hbar}}\langle 1|1\rangle = \frac{x_0}{3}\sqrt{2}\cdot e^{i2\omega t}.$
Consequently, the real part of $e^{i2\omega t}$
$\langle\hat{x}\rangle = \frac{x_0}{3}\sqrt{2}\cos 2\omega t.$
Next, let $(\hat{a} + \hat{a}^+)$ operate both on $\left(e^{-\frac{iE_0 t}{\hbar}}|0\rangle + e^{-\frac{iE_1 t}{\hbar}}|1\rangle + e^{-\frac{iE_2 t}{\hbar}}|2\rangle\right)$.
We obtain for $\langle\hat{x}\rangle$
$\langle\hat{x}\rangle = \frac{x_0}{3}\left(e^{\frac{i(E_0 - E_1 t)}{\hbar}}\langle 0|0\rangle + e^{\frac{i(E_1 - E_0 t)}{\hbar}}\langle 1|1\rangle + \sqrt{2}\cdot e^{\frac{i(E_1 - E_2 t)}{\hbar}}\langle 1|1\rangle + \sqrt{2}\cdot e^{\frac{i(E_2 - E_1 t)}{\hbar}}\langle 2|2\rangle\right) =$

$= \frac{x_0}{3}\left(2\cos\omega t + 2\sqrt{2}\cos\omega t\right) = \frac{1}{3}\sqrt{\frac{2\hbar}{m\omega}}(1+\sqrt{2})\cos\omega t,$

where use have been made of $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$.

## 8.15.22 The Coherent State

Consider a particle of mass $m$ in a harmonic oscillator potential of frequency $\omega$.
Suppose the particle is in the state

$|\alpha\rangle = \sum_{n=0}^{\infty} c_n\,|n\rangle$ ,

where

$c_n = \frac{\alpha^n}{\sqrt{n!}} e^{-|\alpha|^2/2}$.

As has been discussed this is a coherent state or alternatively a quasi-classical state.

**a)** Show that $|\alpha\rangle$ is an eigenstate of the annihilation operator, i.e.,

$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle$.

We have

$\hat{a}\,|\alpha\rangle = \sum_{n=0}^{\infty} c_n\,\hat{a}|n\rangle = \sum_{n=0}^{\infty} c_n\sqrt{n}|n-1\rangle = \sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}|n\rangle$.

Furthermore, with $c_n = \frac{\alpha^n}{\sqrt{n!}} e^{-|\alpha|^2/2}$

$c_{n+1}\sqrt{n+1} = \frac{\alpha^{n+1}}{\sqrt{(n+1)!}} e^{-|\alpha|^2/2}\sqrt{n+1} = \alpha\frac{\alpha^n}{\sqrt{n!}} e^{-|\alpha|^2/2} = \alpha c_n$.

We finally obtain

$\hat{a}\,|\alpha\rangle = \sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}|n\rangle = \sum_{n=0}^{\infty} \alpha c_n|n\rangle = \alpha\,|\alpha\rangle$.

**b)** Show that in this state, $|\alpha\rangle$,

$\langle\hat{x}\rangle = x_c\mathrm{Re}(\alpha)$,

and

$\langle\hat{p}\rangle = p_c\mathrm{Im}(\alpha)$.

With the raising and lowering operators

$\hat{x} = x_c\frac{\hat{a}+\hat{a}^+}{2}$ , and $x_c = \sqrt{\frac{2\hbar}{m\omega}}$,

$\hat{p} = p_c\frac{\hat{a}-\hat{a}^+}{2i}$ , and $p_c = \sqrt{2m\omega\hbar}$ .

Furthermore

$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle \Longrightarrow \langle\alpha|\hat{a}^+ = \alpha^*\langle\alpha|$.

From this we conclude

$\langle\alpha|\hat{a}|\alpha\rangle = \alpha\langle\alpha|\alpha\rangle = \alpha$ ,

and

$\langle\alpha|\hat{a}^+|\alpha\rangle = \alpha^*\langle\alpha|\alpha\rangle = \alpha^*$.

With respect to the expectation values, we than find:

$\langle\alpha|\hat{x}|\alpha\rangle = \left\langle\alpha\middle|x_c\frac{\hat{a}+\hat{a}^+}{2}\middle|\alpha\right\rangle = x_c\frac{\alpha^*+\alpha}{2} = x_c\mathrm{Re}(\alpha)$.

Just for completeness, with $\alpha$ a complex number, $a+ib$ say, we have

$\frac{\alpha^*+\alpha}{2} = \frac{(a-ib+a+ib)}{2} = a \Longrightarrow \mathrm{Re}(\alpha)$

Similarly

$\langle\alpha|\hat{p}|\alpha\rangle = \left\langle\alpha\middle|p_c\frac{\hat{a}-\hat{a}^+}{2i}\middle|\alpha\right\rangle = p_c\mathrm{Im}(\alpha)$.

**c)** Show that, in position space, the wave function for this state is

$\psi_\alpha = e^{\frac{ip_0x}{\hbar}} u_0(x - x_0)$ ,

where $u_0(x)$ is the ground state gaussian function and $\langle\hat{x}\rangle = x_0$ and $\langle\hat{p}\rangle = p_0$.

We have with $\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle$ and $\hat{a} = \frac{\hat{x}}{x_c} + \frac{i\hat{p}}{p_c}$

$\alpha\langle x|\alpha\rangle = \langle x|\hat{a}|\alpha\rangle = \left\langle x\left|\frac{\hat{x}}{x_c} + \frac{i\hat{p}}{p_c}\right|\alpha\right\rangle = \frac{x}{x_c}\langle x|\alpha\rangle + \frac{\hbar}{p_c}\frac{d}{dx}\langle x|\alpha\rangle.$

With $\langle x|\alpha\rangle = \psi_\alpha(x)$ , we obtain the differential equation:

$\alpha\psi_\alpha = \frac{x}{x_c}\psi_\alpha + \frac{\hbar}{p_c}\frac{d\psi_\alpha}{dx} \Rightarrow \frac{d\psi_\alpha}{\psi_\alpha} = \frac{p_c}{\hbar}\left(\alpha - \frac{x}{x_c}\right)dx \Rightarrow \ln\psi_\alpha = \frac{p_c}{\hbar}\left(\alpha x - \frac{x^2}{2x_c}\right) + constant \Rightarrow$

$\Rightarrow \ln\frac{\psi_\alpha}{\psi_0} = \frac{p_c}{\hbar}\left(\alpha x - \frac{x^2}{2x_c}\right) \Rightarrow \psi_\alpha = \psi_0 e^{\frac{p_c}{\hbar}\left(\alpha x - \frac{x^2}{2x_c}\right)}.$

Now, let us use the imaginary part of $\alpha$ and the real part of $\alpha$ :

$\psi_\alpha = \psi_0 e^{\frac{p_c}{\hbar}\left(\alpha x - \frac{x^2}{x_c}\right)} = \psi_0 e^{\frac{ip_cx}{\hbar}Im(\alpha)} e^{\frac{p_c}{\hbar}(xRe(\alpha) - \frac{x^2}{2x_c})}$ .

Use

Re$(\alpha) = \frac{\langle\hat{x}\rangle}{x_c} = \frac{x_0}{x_c}$ , and Im$(\alpha) = \frac{\langle\hat{p}\rangle}{p_c} = \frac{p_0}{p_c}$ :

$\psi_\alpha = \psi_0 e^{\frac{ip_0x}{\hbar}} e^{\frac{p_c}{\hbar}(x\frac{x_0}{x_c} - \frac{x^2}{2x_c})} \Rightarrow \psi_\alpha = \psi_0 e^{\frac{ip_0x}{\hbar}} e^{\frac{p_c}{2\hbar x_c}[(x-x_0)^2 - x_0^2]} = \psi_0 e^{\frac{ip_0x}{\hbar}} e^{\frac{p_c}{2\hbar x_c}(x-x_0)^2} e^{-\frac{p_c}{2\hbar x_c}x_0^2}$ .

Hence

$\psi_\alpha = \psi_0 e^{\frac{ip_0x}{\hbar}} u_0(x - x_0).$

**d)** What is the wave function in momentum space? Interpret $x_0$ and $p_0$.

Summarize some results, we have,

$\langle\hat{x}\rangle = x_0 = x_c\text{Re}(\alpha) \Rightarrow \text{Re}(\alpha) = \frac{x_0}{x_c}$,

and

$\langle\hat{p}\rangle = p_0 = p_c\text{Im}(\alpha) = \frac{p_0}{p_c}$.

Consequently

$\alpha = \frac{x_0}{x_c} + i\frac{p_0}{p_c}$,

and $x_0$ and $p_0$ are the mean position and momentum respectively.

$\psi_\alpha(x) = \psi_0 e^{\frac{ip_0x}{\hbar}} u_0(x - x_0)$ is the wave packet, Gaussian, centered at $x = x_0$ with carrier wave momentum $p_0$.

The momentum space wave function is the Fourier transform of $\psi_\alpha(x)$

$\mathcal{F}(\psi_\alpha(x)) = \tilde{\psi}_a(p) = \frac{1}{\sqrt{2\pi\hbar}}\int dx\,\psi_\alpha(x)e^{-ipx/\hbar}.$

Now we will use the convolution theorem

$\tilde{\psi}_a(p) = \mathcal{F}(e^{\frac{ip_0x}{\hbar}}) \circledast \mathcal{F}(u_0(x - x_0)).$

The delta function:

$\mathcal{F}\left(e^{\frac{ip_0x}{\hbar}}\right) = \delta(p - p_0).$

The shift property

$\mathcal{F}(u_0(x - x_0)) = e^{\frac{-ix_0(p-p_0)}{\hbar}}\tilde{u}_0(p - p_0).$

Then

$\tilde{\psi}_a(p) = e^{\frac{ip_0x_0}{\hbar}} e^{\frac{-ix_0p}{\hbar}}\tilde{u}_0(p - p_0).$

In momentum space $\tilde{u}_0$ is centered at $p_0$.
The mean position $x_0$ appears as a phase in momentum space.

**e)** Explicitly show $\psi_\alpha(x)$ is an eigenstate of the annihilation operator using the position space representation of the annihilation operator.
This is demonstrated under c).

**f)** Show that the coherent state is a minimum uncertainty state. With equal uncertainties in $x$ and $p$, in characteristic dimensionless units.
We know, some ingredients,

$\Delta x = \sqrt{\Delta x^2}$, $\Delta p = \sqrt{\Delta p^2}$,

where

$(\Delta x)^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$ , $(\Delta p)^2 = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$.

$\langle \hat{x} \rangle = x_0 = x_c \mathrm{Re}(\alpha)$, and $\langle \hat{p} \rangle = p_0 = p_c \mathrm{Im}(\alpha)$.

Furthermore

$\hat{x} = x_c \frac{\hat{a}+\hat{a}^+}{2}$ , and $x_c = \sqrt{\frac{2\hbar}{m\omega}}$,

$\hat{p} = p_c \frac{\hat{a}-\hat{a}^+}{2i}$ , and $p_c = \sqrt{2m\omega\hbar}$ .

Then,

$$\langle \hat{x}^2 \rangle = \frac{x_c^2}{4} \langle \alpha | \hat{a}^2 + \hat{a}\hat{a}^+ + \hat{a}^+\hat{a} + (\hat{a}^+)^2 | \alpha \rangle.$$

In addition we use in the preceding expression

$$\hat{a}\, |\alpha\rangle = \alpha\, |\alpha\rangle \Longrightarrow \langle \alpha | \hat{a}^+ = \alpha^* \langle \alpha |.$$

$$\langle \hat{x}^2 \rangle = \frac{x_c^2}{4} [\langle \alpha | \hat{a}^2 | \alpha \rangle + \langle \alpha | \hat{a}\hat{a}^+ | \alpha \rangle + \langle \alpha | \hat{a}^+\hat{a} | \alpha \rangle + \langle \alpha | (\hat{a}^+)^2 | \alpha \rangle].$$

In the above expression we use the commutator $[\hat{a}\hat{a}^+, \hat{a}^+\hat{a}] = 1 \Longrightarrow \hat{a}\hat{a}^+ = 1 + \hat{a}^+\hat{a}$.
So,

$$\langle \hat{x}^2 \rangle = \frac{x_c^2}{4} [\langle \alpha | \hat{a}^2 | \alpha \rangle + \langle \alpha | 1 + \hat{a}^+\hat{a} | \alpha \rangle + \langle \alpha | \hat{a}^+\hat{a} | \alpha \rangle + \langle \alpha | (\hat{a}^+)^2 | \alpha \rangle] =$$

$$= \frac{x_c^2}{4} [\langle \alpha | \hat{a}^2 | \alpha \rangle + \langle \alpha | \alpha \rangle + 2\langle \alpha | \hat{a}^+\hat{a} | \alpha \rangle + \langle \alpha | (\hat{a}^+)^2 | \alpha \rangle] = \frac{x_c^2}{4} [\alpha^2 + 1 + 2\alpha^*\alpha + (\alpha^*)^2] =$$

$$= \frac{x_c^2}{4} (\alpha + \alpha^*)^2 + \frac{x_c^2}{4} = [x_c \mathrm{Re}(\alpha)]^2 + \frac{x_c^2}{4} = \langle \hat{x} \rangle^2 + \frac{x_c^2}{4} ,$$

where use has been made of

$$\mathrm{Re}(\alpha) = \frac{1}{2}(\alpha + \alpha^*).$$

We have

$$(\Delta x)^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2 = \langle \hat{x} \rangle^2 + \frac{x_c^2}{4} - \langle \hat{x} \rangle^2 = \frac{x_c^2}{4} .$$

Hence,

$$\Delta x = \frac{x_c}{2} = \sqrt{\frac{\hbar}{2m\omega}} .$$

Similarly we obtain:

$$\Delta p = \frac{p_c}{2} = \sqrt{\frac{m\omega\hbar}{2}} .$$

Finally, we obtain for the uncertainty

$\Delta x \Delta p = \sqrt{\frac{\hbar}{2m\omega}} \cdot \sqrt{\frac{m\omega\hbar}{2}} = \frac{\hbar}{2}$.

We conclude the coherent state to be a minimum uncertainty state.

**g)** If at time $t = 0$ , the state $|\psi(0)\rangle = |\alpha\rangle$ , show that at a later time,

$|\psi(t)\rangle = e^{-i\omega t/2}|\alpha e^{-i\omega t}\rangle$.

what does it mean?

At $t = 0$ , the state $|\psi(0)\rangle = |\alpha\rangle$.

Then, with the time development operator $\hat{U}(t)$:

$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle = \sum_{n=0}^{\infty} c_n \, \hat{U}(t)|n\rangle$.

It is still about the harmonic oscillator, with $E_n = \hbar\omega(n + \frac{1}{2})$

$|\psi(t)\rangle = \sum_{n=0}^{\infty} c_n \, \hat{U}(t)|n\rangle = \sum_{n=0}^{\infty} c_n \, e^{-iE_n t/\hbar}|n\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} c_n \, e^{-in\omega t}|n\rangle$ ,

where $c_n = \frac{\alpha^n}{\sqrt{n!}} e^{-|\alpha|^2/2}$.

So,

$|\psi(t)\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} e^{-|\alpha|^2/2} \, (\alpha e^{-i\omega t})^n |n\rangle$.

Now we use the results obtained under a):

$\sum_{n=0}^{\infty} \alpha c_n |n\rangle = \alpha \, |\alpha\rangle$,

$\alpha \frac{\alpha^n}{\sqrt{n!}} e^{-|\alpha|^2/2} = \alpha c_n$ ,

and denote $\alpha(t)$ to be $\alpha e^{-i\omega t}$,

we finally obtain

$|\psi(t)\rangle = e^{-i\omega t/2}|\alpha(t)\rangle$ .

At every time, the state is a coherent state with eigenvalue that evolves in time as the classical complex variable of the harmonic oscillator.

**h)** Show that, as a function of time, $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$ follow the classical trajectory of the harmonic oscillator, hence the name *quasi-classical* state.

We have

$|\psi(t)\rangle = e^{-i\omega t/2}|\alpha(t)\rangle$.

So, $\hat{x} = x_c \frac{\hat{a}+\hat{a}^+}{2}$ , and $\langle \alpha|\hat{x}|\alpha\rangle = \left\langle \alpha \middle| x_c \frac{\hat{a}+\hat{a}^+}{2} \middle| \alpha \right\rangle = x_c \frac{\alpha^* + \alpha}{2} = x_c \mathrm{Re}(\alpha)$, see b),

$\langle \psi(t)|\hat{x}|\psi(t)\rangle = \langle \alpha(t)|\hat{x}|\alpha(t)\rangle = x_c \mathrm{Re}[\alpha(t)] = x_c \mathrm{Re}[\alpha e^{-i\omega t}]$.

Similarly

$\langle \psi(t)|\hat{p}|\psi(t)\rangle = \langle \alpha(t)|\hat{p}|\alpha(t)\rangle = p_c \mathrm{Im}[\alpha(t)] = p_c \mathrm{Im}\left[\alpha e^{-i\omega t}\right]$.

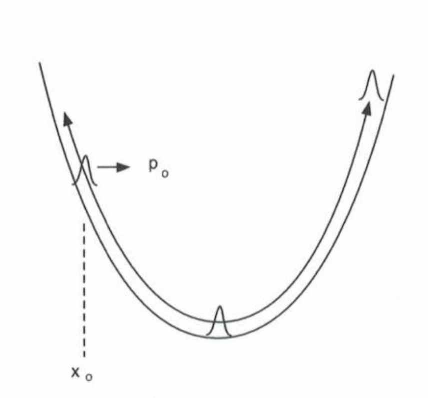
The preceding two equations are the classical equations of motion: $x_c \alpha \cos \omega t$ and $p_c \alpha \sin \omega t$.

**i)** Write the wave function as a function of time, $\psi_\alpha(x, t)$. Sketch the time evolving probability density.

The wave function is, see c),

$\psi_{\alpha(t)}(x, t) = e^{\frac{ip(t)x}{\hbar}} u_0[x - x(t)]$,

where $x(t)$ and $p(t)$ are the classical trajectories. This is an oscillating wave packet, i.e., a gaussian oscillating like a classical simple harmonic oscillator. A sketch:




**j)** Show that in the classical limit

$$\lim_{|\alpha|\to\infty} \frac{\Delta\hat{N}}{\hat{N}} \to 0 \;.$$

The operator $\hat{N} = \hat{a}^{+}\hat{a}$ .

The expectation value of $\hat{N}$

$$\langle\hat{N}\rangle = \langle\alpha|\hat{a}^{+}\hat{a}|\alpha\rangle = \alpha^{*}\alpha\langle\alpha|\alpha\rangle = |\alpha|^2.$$

The definition

$$\Delta\hat{N} = \sqrt{\langle\hat{N}^2\rangle - \langle\hat{N}\rangle^2}.$$

$$\langle\hat{N}^2\rangle = \langle\alpha|(\hat{a}^{+}\hat{a})^2|\alpha\rangle = \langle\alpha|(\hat{a}^{+}\hat{a})(\hat{a}^{+}\hat{a})|\alpha\rangle = \alpha^{*}\alpha\langle\alpha|\hat{a}\hat{a}^{+}|\alpha\rangle = \alpha^{*}\alpha\langle\alpha|1 + \hat{a}^{+}\hat{a}|\alpha\rangle =$$
$$= \alpha^{*}\alpha + (\alpha^{*}\alpha)^2 = |\alpha|^2 + |\alpha|^4,$$

where use has been made of the commutator $[\hat{a}, a^{+}] = 1$.

So, we have the ingredients for

$$\Delta\hat{N} = \sqrt{\langle\hat{N}^2\rangle - \langle\hat{N}\rangle^2} = \sqrt{|\alpha|^2 + |\alpha|^4 - |\alpha|^4} = |\alpha|.$$

From this result we conclude:

$$\Delta\hat{N} = \sqrt{\langle\hat{N}\rangle}\;.$$

Then,

$$\lim_{|\alpha|\to\infty} \frac{\Delta\hat{N}}{\hat{N}} \to \lim_{|\alpha|\to\infty} \frac{1}{\sqrt{\langle\hat{N}\rangle}} \to \lim_{|\alpha|\to\infty} \frac{1}{|\alpha|} = 0\;.$$

**k)** Show that the probability distribution in $n$ is Poissonian, with the appropriate parameters.

The probability for finding the particle in the $n^{th}$ excited state is given by

$$P_n = |\langle n|\alpha\rangle|^2.$$

Then, with $|\alpha\rangle = \sum_{n=0}^{\infty} c_n\,|n\rangle$ ,

where

$$c_n = \frac{\alpha^n}{\sqrt{n!}} e^{-|\alpha|^2/2},$$

$$P_n = |\langle n|\alpha\rangle|^2 = |c_n|^2 = |\frac{\alpha^n}{\sqrt{n!}} e^{-|\alpha|^2/2}|^2 = \frac{(\langle n\rangle)^n}{n!} e^{-\langle n\rangle}$$ → The Poisson Distribution.

**l)** Use a rough time-energy uncertainty principle, $\Delta E\Delta t > \hbar$, to find an uncertainty principle between the number and phase of a quantum oscillator.

For the oscillator we have $Et{\sim}n\hbar\omega t$ .

The phase of the oscillator $\phi = \omega t$.

Then we can write
$Et \sim n\hbar\omega t \rightarrow \Delta E\Delta t \sim \hbar\Delta n\Delta\phi \rightarrow \Delta n\Delta\phi \sim \Delta E\Delta t/\hbar > 1 \rightarrow \Delta n\Delta\phi \geq 1.$

### 8.15.23 Neutrino Oscillations

It is generally recognized that there are at least three different kinds of neutrinos. They can be distinguished by the reactions in which the neutrinos are created or absorbed. Let us call these three types of neutrinos $\nu_e$ , $\nu_\mu$ and $\nu_\tau$. It has been speculated that each of these neutrinos has a small but finite rest mass, possibly different for each type. Let us suppose, that there is a small perturbing interaction between these neutrino types, in the absence of which all three types of neutrinos have the same rest mass $M_0$. The Hamiltonian of the system can be written as
$\hat{H} = \hat{H}_0 + \hat{H}_1,$
where
$$\hat{H}_0 = \begin{pmatrix} M_0 & 0 & 0 \\ 0 & M_0 & 0 \\ 0 & 0 & M_0 \end{pmatrix} \rightarrow \text{no interaction present} \quad \hbar\omega_1$$
and
$$\hat{H}_1 = \begin{pmatrix} 0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & 0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & 0 \end{pmatrix} \rightarrow \text{effect of interactions}$$
where we use as basis
$|\nu_e\rangle = |1\rangle$ , $|\nu_\mu\rangle = |2\rangle$, and $|\nu_\tau\rangle = |3\rangle$.
The Hamiltonian
$$\hat{H} = \hat{H}_0 + \hat{H}_1 = \begin{pmatrix} M_0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 \end{pmatrix}.$$

**a)** We first assume that $\omega_1 = 0$, i.e., no interaction. What is the time development operator? What happens if the neutrino initially was in the state
$$|\psi(0)\rangle = |\nu_e\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \text{ or } \ |\psi(0)\rangle = |\nu_\mu\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \ \text{ or } \ |\psi(0)\rangle = |\nu_\tau\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$
What is happening physically in this case?
There are two methods to solve the problem:
- differential equation method,
- linear algebraic method.

**First: the differential equation method**.
The Schrödinger equation:
$\frac{\hbar}{i}\frac{\partial\psi}{\partial t} + \hat{H}\psi = 0$ .
We expand $\psi$ in the "neutrino base" :
$$\psi = a_1\,|\nu_e\rangle + a_2|\nu_\mu\rangle + a_3|\nu_\tau\rangle = a_1\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + a_2\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + a_3\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}.$$
We rewrite the neutrino states for obvious reason,
$\psi = a_1\,|\nu_1\rangle + a_2|\nu_2\rangle + a_3|\nu_3\rangle,$

and $\alpha_i$ is the probability amplitude to have $|\nu_i\rangle$.
In the Schrödinger representation the differential equation is:

$$i\hbar\begin{pmatrix}\dot{a}_1\\ \dot{a}_2\\ \dot{a}_3\end{pmatrix}=\begin{pmatrix}M_0 & \hbar\omega_1 & \hbar\omega_1\\ \hbar\omega_1 & M_0 & \hbar\omega_1\\ \hbar\omega_1 & \hbar\omega_1 & M_0\end{pmatrix}\begin{pmatrix}a_1\\ a_2\\ a_3\end{pmatrix}.$$

Let $\omega_1 = 0$.
Then, the time dependency of the vector elements is[10]:

$$a_1(t) = a_1(0)e^{-iM_0t/\hbar},$$
$$a_2(t) = a_2(0)e^{-iM_0t/\hbar},$$
$$a_3(t) = a_3(0)e^{-iM_0t/\hbar}\ .$$

Or with the time development operator

$$\begin{pmatrix}a_1(t)\\ a_2(t)\\ a_3(t)\end{pmatrix}=\widehat{U}(t)\begin{pmatrix}a_1(0)\\ a_2(0)\\ a_3(0)\end{pmatrix}=e^{-iM_0t/\hbar}\begin{pmatrix}a_1(0)\\ a_2(0)\\ a_3(0)\end{pmatrix}.$$

If the neutrino is in one of the basis states, say $|\nu_1\rangle$ ,

$$\begin{pmatrix}a_1(t)\\ a_2(t)\\ a_3(t)\end{pmatrix}=e^{-iM_0t/\hbar}\begin{pmatrix}1\\ 0\\ 0\end{pmatrix}=|\nu_1\rangle.$$

The neutrino stays in the state $|\nu_1\rangle$ .

**b)** Next we assume $\omega_1 \neq 0$ . We assume the neutrino is initially in one of the basis states, say, $|\nu_1\rangle$. Also assume that at $t = 0$, the neutrino is in the state

$$|\psi(0)\rangle = |\nu_e\rangle \equiv |\nu_1\rangle = \begin{pmatrix}1\\ 0\\ 0\end{pmatrix}.$$

What is the probability as a function of time, that the neutrino will be in each of the other two states?
We have

$$i\hbar\begin{pmatrix}\dot{a}_1\\ \dot{a}_2\\ \dot{a}_3\end{pmatrix}=\begin{pmatrix}M_0 & \hbar\omega_1 & \hbar\omega_1\\ \hbar\omega_1 & M_0 & \hbar\omega_1\\ \hbar\omega_1 & \hbar\omega_1 & M_0\end{pmatrix}\begin{pmatrix}a_1\\ a_2\\ a_3\end{pmatrix}.$$

At $t = 0$ ,

$$a_1(0) = 1 \quad , a_2(0) = 0 \quad , \ a_3(0) = 0.$$

Let

$$a_1(t) = e^{-\frac{iM_0t}{\hbar}}b_1(t) \to b_1(0) = 1,$$
$$a_2(t) = e^{-\frac{iM_0t}{\hbar}}b_2(t) \to b_2(0) = 0,$$
$$a_3(t) = e^{-\frac{iM_0t}{\hbar}}b_3(t) \to b_3(0) = 0.$$

With $a_1(t) = e^{-\frac{iM_0t}{\hbar}}b_1(t) \to \dot{a}_1 = -\frac{iM_0}{\hbar}e^{-\frac{iM_0t}{\hbar}}b_1(t) + e^{-\frac{iM_0t}{\hbar}}\dot{b}_1 = -\frac{iM_0}{\hbar}a_1(t) + e^{-\frac{iM_0t}{\hbar}}\dot{b}_1 \to$

$\to \dot{a}_1 + \frac{iM_0}{\hbar}a_1(t) = e^{-\frac{iM_0t}{\hbar}}\dot{b}_1$, **Eq.(1)**.

The above matrix multiplication gives:

[10] Notice: the time dependency in general reads $e^{-iEt/\hbar}$. With $E = M_0c^2$, and $c = 1$, we can replace $e^{-iEt/\hbar}$ through $e^{-iM_0t/\hbar}$

$i\hbar\dot{a}_1 = M_0 a_1 + \hbar\omega_1(a_2 + a_3) \rightarrow i\hbar\dot{a}_1 - M_0 a_1 = \hbar\omega_1 e^{-\frac{iM_0 t}{\hbar}}[b_2(t) + b_3(t)] \rightarrow$
$\rightarrow \dot{a}_1 + \frac{iM_0}{\hbar} a_1(t) = -i\omega_1 e^{-\frac{iM_0 t}{\hbar}}[b_2(t) + b_3(t)]$, **Eq.(2)**.
Equate Eqs.(1) and (2):
$\dot{b}_1 = -i\omega_1[b_2(t) + b_3(t)]$.
Similarly we obtain
$\dot{b}_2 = -i\omega_1[b_1(t) + b_3(t)]$,
$\dot{b}_3 = -i\omega_1[b_1(t) + b_2(t)]$.
There is no way to distinguish between $b_2(t)$ and $b_3(t)$ due to initial state
we have
$\dot{b}_1 = -2i\omega_1 b_2(t)$,
$\dot{b}_2 = -i\omega_1[b_1(t) + b_2(t)]$.
Differentiate the preceding expression for $\dot{b}_2$ with respect to time and use the expression for $\dot{b}_1$, we obtain
$\ddot{b}_2 + i\omega_1\dot{b}_2 + 2\omega_1^2 b_2 = 0$ .
Assume $b_2 = e^{i\alpha t}$ and the preceding equation changes into an algebraic expression:
$-\alpha^2 + \omega_1\alpha + 2\omega_1^2 = 0 \rightarrow \alpha = -2\omega_1, \omega_1$.
The solution for $b_2$ is
$b_2(t) = Ae^{i\omega_1 t} + Be^{-2i\omega_1 t}$.
The initial condition $b_2(0) = 0 \rightarrow b_2(t) = A\left(e^{i\omega_1 t} - e^{-2i\omega_1 t}\right) = b_3(t)$.
We have for $b_1(t)$
$\dot{b}_1 = -2i\omega_1 b_2(t) = -2i\omega_1 A(e^{i\omega_1 t} - e^{-2i\omega_1 t})$.
Integrating gives
$b_1(t) = -2i\omega_1 A\left(\frac{1}{i\omega_1}e^{i\omega_1 t} + \frac{1}{2i\omega_1}e^{-2i\omega_1 t}\right) = -2A\left(e^{i\omega_1 t} + \frac{1}{2}e^{-2i\omega_1 t}\right)$.
Hence
$b_1(0) = 1 = -3A \rightarrow A = -\frac{1}{3}$.
Consequently
$b_1(t) = \frac{2}{3}\left(e^{i\omega_1 t} + \frac{1}{2}e^{-2i\omega_1 t}\right)$,

and
$b_2(t) = -\frac{1}{3}\left(e^{i\omega_1 t} - e^{-2i\omega_1 t}\right) = b_3(t)$.
The probability to find te neutrino in state $|\nu_2\rangle$ or $|\nu_3\rangle$
$P\left(|\nu_e\rangle \rightarrow |\nu_\mu\rangle, t\right) = |a_2(t)|^2 = |b_2(t)|^2 = |-\frac{1}{3}\left(e^{i\omega_1 t} - e^{-2i\omega_1 t}\right)|^2 = \frac{2}{9}(1 - \cos 3\,\omega_1 t)$.

**c)** An experiment to detect the neutrino oscillations is being performed. The flight path of the neutrinos is 2000 meters. Their energy is $100GeV$. The sensitivity of the experiment is such that the presence of 1% of neutrinos different from those present at the start of the flight can be measured with confidence. Let $M_0 = 20eV$, what is the smallest value of $\hbar\omega_1$ that can be detected? How does this depend on $M_0$? Do not ignore special relativity.

The time of flight of the $\nu_e$ neutrino is $\Delta t = l/v$ in laboratory time.
Since we have to deal with special relativity, we need to obtain proper flight time

$\Delta\tau = \frac{\Delta t}{\gamma} = \Delta t\sqrt{1-\frac{v^2}{c^2}} = \frac{l}{v}\sqrt{1-\frac{v^2}{c^2}}$ .

The energy is

$E = \gamma mc^2 \to \gamma = \frac{M_0}{E}$

Again I assume Boccio meant $M_0$ to be $mc^2$ and $v \approx c$ , then

$\Delta\tau \approx \frac{l}{c}\frac{M_0}{E}$ .

We obtained , b),

$P(|\nu_e\rangle \to |\nu_\mu\rangle, t) = \frac{2}{9}(1 - \cos 3\,\omega_1 t)$.

With the 1% condition:

$P(|\nu_e\rangle \to |\nu_\mu\rangle, t) \geq 0.01$,

or with $t = \Delta\tau$

$\frac{2}{9}(1 - \cos 3\,\omega_1\Delta\tau) \geq 0.01 \to 1 - \cos 3\,\omega_1\Delta\tau \geq 0.045$.

Since $\cos 3\,\omega_1\Delta\tau$ is close to 1, we can expand $\cos 3\,\omega_1\Delta\tau$

$\cos 3\,\omega_1\Delta\tau \approx 1 - \frac{1}{2}(3\omega_1\Delta\tau)^2 \to \frac{9}{2}(\omega_1\Delta\tau)^2 \geq 0.045 \to \omega_1 \geq \frac{0.1}{\Delta\tau} \approx 0.1\frac{c\cdot E}{l\cdot M_0}$ .

Plug into the preceding expression the given numbers and the value of Planck's constant in $eVs$, we obtain

$\hbar\omega_1 \geq 0.05eV$.

**Next: the linear algebra method**.

**a)** and **b)** In this case we look for the eigenvalues of the determinant of the Hamiltonian

$$\begin{vmatrix} M_0 - E & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 - E & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 - E \end{vmatrix} = 0 = (M_0 - E)\begin{vmatrix} M_0 - E & \hbar\omega_1 \\ \hbar\omega_1 & M_0 - E \end{vmatrix} +$$

$$-\hbar\omega_1\begin{vmatrix} \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 - E \end{vmatrix} + \hbar\omega_1\begin{vmatrix} \hbar\omega_1 & M_0 - E \\ \hbar\omega_1 & \hbar\omega_1 \end{vmatrix} = (M_0 - E)^3 - (M_0 - E)(\hbar\omega_1)^2 +$$

$$-(M_0 - E)(\hbar\omega_1)^2 + (\hbar\omega_1)^3 + (\hbar\omega_1)^3 - (M_0 - E)(\hbar\omega_1)^2 =$$

$$= (M_0 - E)^3 - 3(M_0 - E)(\hbar\omega_1)^2 + 2(\hbar\omega_1)^3.$$

For convenience set

$M_0 - E = \alpha$ and $\hbar\omega_1 = \beta$ , we obtain for the eigenvalue equation

$\alpha^3 - 3\beta^2\alpha + 2\beta^3 = 0$.

This cubic equation has all roots real and at least two are equal(Abramowitz and Stegun).

Rewrite $\alpha^3 - 3\beta^2\alpha + 2\beta^3 = 0 = \alpha^3 - 2\alpha^2\beta + \alpha\beta^2 + 2\alpha^2\beta - 4\alpha\beta^2 + 2\beta^3 =$

$= \alpha(\alpha^2 - 2\alpha\beta + \beta^2) + 2\beta(\alpha^2 - 2\alpha\beta + \beta^2) = (\alpha + 2\beta)(\alpha - \beta)^2$.

Hence, $\alpha = \beta$ (twice) and $\alpha = -2\beta$.

The three eigen values:

$\alpha = -2\beta \to M_0 - E = -2\hbar\omega_1 \to E_1 = M_0 + 2\hbar\omega_1$,

and

$\alpha = \beta \to E_2 = E_3 = M_0 - \hbar\omega_1$ (degeneracy).

The eigenvectors:

- with the eigenvalue $E_1 = M_0 + 2\hbar\omega_1$

$$\hat{H}|E_1\rangle = (M_0 + 2\hbar\omega_1)|E_1\rangle \to \begin{pmatrix} M_0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 \end{pmatrix}|E_1\rangle = (M_0 + 2\hbar\omega_1)|E_1\rangle.$$

$|E_1\rangle$ in vector representation with elements which I assume to be real $\begin{pmatrix} a \\ b \\ c \end{pmatrix}$:

$$\begin{pmatrix} M_0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = (M_0 + 2\hbar\omega_1)\begin{pmatrix} a \\ b \\ c \end{pmatrix}.$$

Then

$M_0 a + \hbar\omega_1 b + \hbar\omega_1 c = M_0 a + 2\hbar\omega_1 a \to -2a + b + c = 0,$

$\hbar\omega_1 a + M_0 b + \hbar\omega_1 c = M_0 b + 2\hbar\omega_1 b \to a - 2b + c = 0,$

$\hbar\omega_1 a + \hbar\omega_1 b + M_0 c = M_0 c + 2\hbar\omega_1 c \to a + b - 2c = 0.$

These three equations give: $a = b = c$.

With normalization $3a^2 = 1$.

So

$$|E_1\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

Next $|E_2\rangle$, similarly with the unknown vector elements:

$$\begin{pmatrix} M_0 & \hbar\omega_1 & \hbar\omega_1 \\ \hbar\omega_1 & M_0 & \hbar\omega_1 \\ \hbar\omega_1 & \hbar\omega_1 & M_0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = (M_0 - \hbar\omega_1)\begin{pmatrix} a \\ b \\ c \end{pmatrix}.$$

Then, the eigenvalue equation:

$M_0 a + \hbar\omega_1 b + \hbar\omega_1 c = M_0 a - \hbar\omega_1 a \to a + b + c = 0$

Assuming the elements are real, at least 1 must be negative.

$\langle E_1 | E_2 \rangle = 0$, does not create new information.

So,

$a = -(b + c).$

Plug the preceding expression into the normalization equation:

$$a^2 + b^2 + c^2 = 1 \to b^2 + bc + c^2 = \frac{1}{2} \to b = -\frac{1}{2}c \pm \sqrt{\frac{1}{2} - \frac{3}{4}c^2}.$$

With $a + b + c = 0$

$$a - \frac{1}{2}c + \left(\pm\sqrt{\frac{1}{2} - \frac{3}{4}c^2}\right) + c = 0 \to a + \frac{1}{2}c = \left(\pm\sqrt{\frac{1}{2} - \frac{3}{4}c^2}\right) \to$$

$$\to a^2 + ac + \frac{1}{4}c^2 = \frac{1}{2} - \frac{3}{4}c^2 \to a^2 + ac + c^2 = \frac{1}{2}.$$

We have:

$a^2 + ac + c^2 = \frac{1}{2}$, and $b^2 + bc + c^2 = \frac{1}{2}$.

Hence

$a = b$.

Then, with $a + b + c = 0$

$c = -2a$.

Normalization: $a^2 + b^2 + c^2 = 1$

$$a^2 + a^2 + 4a^2 = 1 \to a = \sqrt{\frac{1}{6}}.$$

Note: we could have done the following:
Choose $\sqrt{\frac{1}{2}-\frac{3}{4}c^2}=0 \to c=\pm\sqrt{\frac{2}{3}} \to b=\pm\frac{1}{2}c=\pm\sqrt{\frac{1}{6}}$,
and $a=-(b+c)=\pm\frac{1}{2}c=\pm\sqrt{\frac{1}{6}}$.

Hence

$$|E_2\rangle=\sqrt{\frac{1}{6}}\begin{pmatrix}1\\1\\-2\end{pmatrix}.$$

Finally $|E_3\rangle$, similarly with the unknown vector elements:
the eigenvalue equation $M_0a+\hbar\omega_1 b+\hbar\omega_1 c=M_0a-\hbar\omega_1 a \to a+b+c=0$.
Orthogonality

$$\langle E_2|E_3\rangle=0 \to \sqrt{\frac{1}{6}}(1\ \ 1\ \ -2)\begin{pmatrix}a\\b\\c\end{pmatrix}=a+b-2c=0.$$

With $a+b+c=0$, and $a+b-2c=0$ ,
we find $a=-b$, and $c=0$.

Normalization: $a^2+b^2+c^2=1 \to 2a^2=1 \to a=\sqrt{\frac{1}{2}}$.

Hence

$$|E_3\rangle=\sqrt{\frac{1}{2}}\begin{pmatrix}1\\-1\\0\end{pmatrix}.$$

The initial state of the neutrino

$$|\psi(0)\rangle=|\nu_e\rangle=\begin{pmatrix}1\\0\\0\end{pmatrix}.$$

Then, with the projection operator

$$|\psi(0)\rangle=\begin{pmatrix}1\\0\\0\end{pmatrix}=\sum_n |E_n\rangle\langle E_n|\psi(0)\rangle=|E_1\rangle\sqrt{\frac{1}{3}}+|E_2\rangle\sqrt{\frac{1}{6}}+|E_3\rangle\sqrt{\frac{1}{2}}.$$

For the time development operator we have

$$\hat{U}(t)=e^{-i\hat{H}t/\hbar}.$$

So,

$$|\psi(t)\rangle=e^{-i\hat{H}t/\hbar}|\psi(0)\rangle=\sqrt{\frac{1}{3}}e^{-iE_1t/\hbar}|E_1\rangle+\sqrt{\frac{1}{6}}e^{-\frac{iE_2t}{\hbar}}|E_2\rangle+\sqrt{\frac{1}{2}}e^{-iE_3t/\hbar}|E_3\rangle.$$ [11]

$$P(|\nu_e\rangle\to|\nu_\mu\rangle,t)=|\langle\nu_\mu|\psi(t)\rangle|^2,$$

where

$$|\nu_\mu\rangle=\begin{pmatrix}0\\1\\0\end{pmatrix}.$$

Then,

$$P(|\nu_e\rangle\to|\nu_\mu\rangle,t)=|\langle\nu_\mu|\psi(t)\rangle|^2.$$

$$\langle\nu_\mu|\psi(t)\rangle=\frac{1}{3}e^{-2i\omega_1t}+\frac{1}{6}e^{i\omega_1t}-\frac{1}{2}e^{i\omega_1t}.$$

[11] $e$^$(-iM_0\,t/\hbar)$ does not contribute in the probability.

So

$|\langle \nu_\mu|\psi(t)\rangle|^2 = \left(\frac{1}{3}e^{2i\omega_1 t} - \frac{1}{3}e^{-i\omega_1 t}\right)\left(\frac{1}{3}e^{-2i\omega_1 t} - \frac{1}{3}e^{i\omega_1 t}\right) = \frac{2}{9}(1-\cos 3\omega_1 t).$

Consequently,

$P(|\nu_e\rangle \to |\nu_\mu\rangle, t) = \frac{2}{9}(1-\cos 3\omega_1 t).$

**c)** The same result as obtained with the differential equation method.
Hence, for the smallest possible value $\hbar\omega_1$, we obtain the same result:

$\hbar\omega_1 \geq 0.05eV.$

> Note : what about $P(|\nu_e\rangle \to |\nu_\tau\rangle, t) = |\langle \nu_\tau|\psi(t)\rangle|^2$?
> With $|\nu_\tau\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}$, and $|\psi(t)\rangle = \sqrt{\frac{1}{3}}e^{-iE_1 t/\hbar}|E_1\rangle + \sqrt{\frac{1}{6}}e^{-\frac{iE_2 t}{\hbar}}|E_2\rangle + \sqrt{\frac{1}{2}}e^{-iE_3 t/\hbar}|E_3\rangle$
> $\langle \nu_\tau|\psi(t)\rangle = \left(\frac{1}{3}e^{-2i\omega_1 t} - \frac{1}{3}e^{i\omega_1 t}\right).$
> Then
> $P(|\nu_e\rangle \to |\nu_\tau\rangle, t) = |\langle \nu_\tau|\psi(t)\rangle|^2 = \frac{2}{9}(1-\cos 3\omega_1 t).$
> As it should be.

### 8.15.24 Generating Function

Use te generating function for Hermite polynomials

$e^{2xt-t^2} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$, or $e^{2\alpha xt-t^2} = \sum_{n=0}^{\infty} H_n(\alpha x)\frac{t^n}{n!}$,

to work out the matrix elements of $x$ in the position representation, that is, compute

$\langle x\rangle_{nn'} = \int_{-\infty}^{\infty} \psi_n^*(x)x\psi_{n'}(x)dx$ , or $\langle \alpha x\rangle_{nn'} = \int_{-\infty}^{\infty} \psi_n^*(\alpha x)\alpha x\psi_{n'}(\alpha x)d\alpha x$,

where

$\psi_n(\alpha x) = N_n H_n(\alpha x)e^{-\frac{1}{2}\alpha^2 x^2}$ ,

and

$N_n = \left(\frac{\alpha}{2^n n!\sqrt{\pi}}\right)^{1/2}$ , $\alpha = \left(\frac{m\omega}{\hbar}\right)^{1/2}$, $[\alpha] = \left(\frac{kg/sec}{Joulesec}\right)^{1/2} = \left(\frac{kg/sec}{kgm^2sec^{-2}sec}\right)^{1/2} = \frac{1}{m}$,

$[N_n] = \left(\frac{1}{m}\right)^{1/2}$, $\alpha x$ is dimensionless when $[x] = m$.

Now we have the ingredients to calculate the matrix elements.

$\langle \alpha x\rangle_{nn'} = \int_{-\infty}^{\infty} \psi_n^*(\alpha x)\alpha x\psi_{n'}(\alpha x)dx = \int_{-\infty}^{\infty} N_n H_n(\alpha x)\alpha x N_{n'}H_{n'}(\alpha x)e^{-\alpha^2 x^2}dx.$

The generating function and the integral over two Hermite polynomials, for convenience $q = \alpha x$:

$$\int_{-\infty}^{\infty} e^{2qt-t^2}e^{2qs-s^2}q\,e^{-q^2}dq = \int_{-\infty}^{\infty}\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty} H_n(q)\frac{t^n}{n!}H_{n'}(q)\frac{s^{n'}}{n'!}qe^{-q^2}dq =$$

$$= \sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{t^n}{n!}\frac{s^{n'}}{n'!}\int_{-\infty}^{\infty} H_n(q)\,H_{n'}(q)qe^{-q^2}dq.$$

So,

$$\langle \alpha x\rangle_{nn'} = \frac{1}{\alpha}N_n N_{n'}\int_{-\infty}^{\infty} H_n(\alpha x)\,\alpha x H_{n'}(\alpha x)e^{-\alpha^2 x^2}d\alpha x =$$

$$= \frac{1}{\alpha}N_n N_{n'}\int_{-\infty}^{\infty} H_n(q)\,qH_{n'}(q)e^{-q^2}dq$$

$$\to \int_{-\infty}^{\infty} H_n(q)\,qH_{n'}(q)e^{-q^2}dq = \frac{\alpha}{N_n N_{n'}}\langle \alpha x\rangle_{nn'}.$$

$\frac{\alpha}{N_n N_{n'}}\langle \alpha x\rangle_{nn'} = \int_{-\infty}^{\infty} H_n(q)\, qH_{n'}(q)e^{-q^2}dq.$

Then,

$\int_{-\infty}^{\infty} e^{2qt-t^2}e^{2qs-s^2}q\, e^{-q^2}dq = \sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{t^n}{n!}\frac{s^{n'}}{n'!}\int_{-\infty}^{\infty} H_n(q)\, H_{n'}(q)qe^{-q^2}dq.$

Let us evaluate the integral, Gaussian,

$\int_{-\infty}^{\infty} e^{2qt-t^2}e^{2qs-s^2}q\, e^{-q^2}dq = \int_{-\infty}^{\infty} e^{-(q+s+t)^2+2st}(q+s+t)d(q+s+t) =$

$= (s+t)e^{2st}\int_{-\infty}^{\infty} e^{-(q+s+t)^2}d(q+s+t) + \int_{-\infty}^{\infty} e^{-(q+s+t)^2+2st}qdq = (s+t)\sqrt{\pi}e^{2st},$

since $\int_{-\infty}^{\infty} e^{-(q+s+t)^2+2st}qdq = 0$ →anti-symmetric.

Hence

$\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{t^n}{n!}\frac{s^{n'}}{n'!}\int_{-\infty}^{\infty} H_n(q)\, H_{n'}(q)qe^{-q^2}dq =$

$= (s+t)\sqrt{\pi}e^{2st} = \sqrt{\pi}\sum_{k=0}^{\infty}\frac{2^k}{k!}(s^{k+1}t^k + s^k t^{k+1}).$

How to derive the matrix elements from the preceding equation?
Let us pay some attention to(Mahan)

$\Longrightarrow \int_{-\infty}^{\infty} e^{2qt-t^2}e^{2qs-s^2}\, e^{-q^2}dq = \sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{t^n}{n!}\frac{s^{n'}}{n'!}\int_{-\infty}^{\infty} H_n(q)\, H_{n'}(q)e^{-q^2}dq.$

From the preceding analysis we have also

$\Longrightarrow \int_{-\infty}^{\infty} e^{2qt-t^2}e^{2qs-s^2}\, e^{-q^2}dq = \sqrt{\pi}e^{2st} = \sqrt{\pi}\sum_{k=0}^{\infty}\frac{(2st)^k}{k!}.$

Compare the series in the two preceding expressions(⟹):
These series must be equal. Consequently, $n = n'$. This is what we already obtained applying normalization:

$\int_{-\infty}^{\infty}\psi_n^*(x)\psi_{n'}(x)dx = \delta_{nn'}.$

So,

$\frac{t^n}{n!}\frac{s^{n'}}{n'!}\int_{-\infty}^{\infty} H_n(q)\, H_{n'}(q)e^{-q^2}dq = \sqrt{\pi}\delta_{nn'}\frac{(2st)^n}{n!} \to \int_{-\infty}^{\infty} H_n(q)\, H_{n'}(q)e^{-q^2}dq =$

$= \sqrt{\pi}2^n n!\,\delta_{nn'} = \frac{\alpha}{N_n^2}\delta_{nn'}.$

Back to the matrix elements of $x$ in position representation.
A matrix element: $\langle n|x|n'\rangle$, where $|n\rangle$ and $|n'\rangle$ represents two different eigenvectors or the eigenfunctions $\psi_n(x)$ and $\psi_{n'}(x)$.
Next we use a recursion relation for the Hermite polynomials:

$\frac{1}{2}H_{n+1} = qH_n - nH_{n-1} \to qH_n = \frac{1}{2}H_{n+1} + nH_{n-1}.$

With the eigenfunctions:

$\psi_n(\alpha x) = N_n H_n(\alpha x)e^{-\frac{1}{2}\alpha^2x^2} \to \psi_n(q) = N_n H_n(q)e^{-\frac{1}{2}q^2}.$

$qH_n = \frac{1}{2}H_{n+1} + nH_{n-1} \to qN_nH_ne^{-\frac{1}{2}q^2} = \frac{1}{2}N_nH_{n+1}e^{-\frac{1}{2}q^2} + nN_nH_{n-1}e^{-\frac{1}{2}q^2}.$

$N_{n+1} = (\frac{\alpha}{2^{n+1}(n+1)!\sqrt{\pi}})^{1/2} = \frac{1}{\sqrt{n+1}\sqrt{2}}N_n \to N_n = \sqrt{n+1}\sqrt{2}N_{n+1},$

$N_{n-1} = (\frac{\alpha}{2^{n-1}(n-1)!\sqrt{\pi}})^{1/2} = \sqrt{n}\sqrt{2}N_n \to N_n = \frac{1}{\sqrt{n}\sqrt{2}}N_{n-1}.$

Rewrite $N_nH_ne^{-\frac{1}{2}q^2} = \frac{1}{2}N_nH_{n+1}e^{-\frac{1}{2}q^2} + nN_nH_{n-1}e^{-\frac{1}{2}q^2}$ with the expressions of $N_n = \sqrt{n+1}\sqrt{2}N_{n+1}$ and $N_n = \frac{1}{\sqrt{n}\sqrt{2}}N_{n-1}$:

$qN_nH_ne^{-\frac{1}{2}q^2} = \frac{1}{2}N_nH_{n+1}e^{-\frac{1}{2}q^2} + nN_nH_{n-1}e^{-\frac{1}{2}q^2} \to$

$\to qN_nH_ne^{-\frac{1}{2}q^2} = \frac{1}{\sqrt{2}}(\sqrt{n+1}N_{n+1}H_{n+1}e^{-\frac{1}{2}q^2} + \sqrt{n}N_{n-1}H_{n-1}e^{-\frac{1}{2}q^2}) \to$

$\to q\psi_n(q) = \frac{1}{\sqrt{2}}[\sqrt{n+1}\psi_{n+1}(q) + \sqrt{n}\psi_{n-1}(q)].$

The matrix elements is about to calculate

$\langle x\rangle_{nn'} = \frac{1}{\alpha}\int_{-\infty}^{\infty}\psi_n^*(q)q\psi_{n'}(q)dq =$

$= \frac{1}{\alpha}\int_{-\infty}^{\infty}\psi_n^*(q)\frac{1}{\sqrt{2}}\left[\sqrt{n'+1}\psi_{n'+1}(q) + \sqrt{n'}\psi_{n'-1}(q)\right]dq =$

$= \frac{1}{\alpha}\frac{1}{\sqrt{2}}[\sqrt{n'+1}\delta_{nn'+1} + \sqrt{n'}\delta_{nn'-1}]$ .

Hence, the matrix elements are of the position representation between two harmonic oscillator states $n$ and $n'$ are non-zero when $n = n' \pm 1$ .

Note: when we make $x$ dimensionless→ $\alpha x$ the, the factor $\frac{1}{\alpha}$ disappears and $\sqrt{\alpha}$ is the normalization factor to normalize $\int_{-\infty}^{\infty} \psi_n^*(q)\psi_{n'}(q)dq$.

Furthermore, we did not derive the matrix element from

$\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{t^n}{n!}\frac{s^{n'}}{n'!}\int_{-\infty}^{\infty} H_n(q)\,H_{n'}(q)qe^{-q^2}dq = \sqrt{\pi}\sum_{k=0}^{\infty}\frac{2^k}{k!}(s^{k+1}t^k + s^k t^{k+1})$.

Next, find the matrix elements

$$\frac{\alpha}{N_n N_{n'}}\langle \alpha x\rangle_{nn'} = \int_{-\infty}^{\infty} H_n(q)\,qH_{n'}(q)e^{-q^2}dq.$$

So,

$$\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{t^n}{n!}\frac{s^{n'}}{n'!}\int_{-\infty}^{\infty} H_n(q)\,H_{n'}(q)qe^{-q^2}dq = \sqrt{\pi}\sum_{k=0}^{\infty}\frac{2^k}{k!}(s^{k+1}t^k + s^k t^{k+1}) \to$$

$$\to \sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{t^n}{n!}\frac{s^{n'}}{n'!}\frac{\alpha}{N_n N_{n'}}\langle \alpha x\rangle_{nn'} = \sqrt{\pi}\sum_{k=0}^{\infty}\frac{2^k}{k!}(s^{k+1}t^k + s^k t^{k+1}).$$

Equating the same powers of $s$ and $t$

$$\sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\frac{t^n}{n!}\frac{s^{n'}}{n'!}\frac{\alpha}{N_n N_{n'}}\langle \alpha x\rangle_{nn'} = \sqrt{\pi}\frac{2^n}{n!}(t^n s^{n+1} + t^{n+1}s^n).$$

Hence,

$s^{n'} \to s^{n+1}$: $n' = n+1 \to n = n'-1$

$$\frac{\alpha}{N_n N_{n+1}}\langle \alpha x\rangle_{n(n+1)} = \sqrt{\pi}\,(n+1)!\,2^n,$$

and

$s^{n'} \to s^n$: $n' = n$

$$\frac{\alpha}{N_{n+1}N_n}\langle \alpha x\rangle_{(n+1)n} = \sqrt{\pi}(n+1)!\,2^n.$$

Use $N_n = \left(\frac{\alpha}{2^n n!\sqrt{\pi}}\right)^{\frac{1}{2}}$:

with

$N_n N_{n+1} = \frac{\alpha}{2^n\sqrt{2}\pi}[\frac{1}{n!(n+1)!}]^{1/2}$, and

$$\langle \alpha x\rangle_{n(n+1)} = \frac{1}{\sqrt{2}}\sqrt{n+1} \to \frac{1}{\sqrt{2}}\sqrt{n'}\ ,$$

$$\langle \alpha x\rangle_{(n+1)n} = \frac{1}{\sqrt{2}}\sqrt{n+1} \to \frac{1}{\sqrt{2}}\sqrt{n'+1}.$$

How to interpret this result?

$$\langle x\rangle_{nn'} = \frac{1}{\alpha}\frac{1}{\sqrt{2}}\left[\sqrt{n'+1}\delta_{nn'+1} + \sqrt{n'}\delta_{nn'-1}\right]$$

The matrix elements are of the position representation between two harmonic oscillator states $n$ and $n'$ are non-zero when $n = n' \pm 1$.

### 8.15.25. Given the wave function .......

A particle of mass $m$ moves in one dimension under the influence of a potential $V(x)$. Suppose the particle is in an energy eigenstate

$$\psi(x) = (\frac{\gamma^2}{\pi})^{1/4}e^{-\gamma^2x^2/2},$$

with energy $E = \frac{\hbar^2\gamma^2}{2m}$ .

**a)** Find the mean position of the particle

$\langle x\rangle = \int_{-\infty}^{\infty}\psi^*(x)x\psi(x)dx = 0.$

$\int_{-\infty}^{\infty}\psi^*(x)x\psi(x)dx = \int_{-\infty}^{\infty}(\frac{\gamma^2}{\pi})^{1/2}xe^{-\gamma^2x^2}\,dx$ .

The function $xe^{-\gamma^2x^2}$ is anti-symmetric.

Consequently,

$\langle x\rangle = 0$ .

**b)** Find the momentum of the particle

$\langle p\rangle = \int_{-\infty}^{\infty}\psi^*(x)p\psi(x)dx = -i\hbar\int_{-\infty}^{\infty}\psi^*(x)\frac{d}{dx}\psi(x)dx =$

$= i\hbar\gamma^2\int_{-\infty}^{\infty}(\frac{\gamma^2}{\pi})^{1/2}xe^{-\gamma^2x^2}\,dx.$

Hence,

$\langle p\rangle = 0.$

**c)** Find $V(x)$.

We use the time independent Schrödinger equation, the energy operator,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - [E - V(x)]\psi(x) = 0 \to -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left[\left(\frac{\gamma^2}{\pi}\right)^{\frac{1}{4}}e^{-\frac{\gamma^2x^2}{2}}\right] =$$

$$= [E - V(x)]\left[\left(\frac{\gamma^2}{\pi}\right)^{\frac{1}{4}}e^{-\frac{\gamma^2x^2}{2}}\right] \to -\frac{\hbar^2}{2m}(-\gamma^2 + \gamma^4x^2) = E - V(x).$$

With $E = \frac{\hbar^2\gamma^2}{2m} \to$

$\to V(x) = \frac{\hbar^2\gamma^4}{2m}x^2.$

**d)** Find the probability $P(p)dp$ that the particle's momentum is between $p$ and $p + dp$.

Making use of the Fourier transform→ $\psi(p)$ is the Fourier transform of $\psi(x)$:

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int e^{-ipx/\hbar}\ \psi(x)dx = \frac{1}{\sqrt{2\pi\hbar}}\int e^{-ipx/\hbar}\,(\frac{\gamma^2}{\pi})^{1/4}e^{-\gamma^2x^2/2}\,dx =$$

$$= \frac{1}{\sqrt{2\pi\hbar}}(\frac{\gamma^2}{\pi})^{1/4}\int dx\text{exp}\left(-\frac{ipx}{\hbar} - \frac{\gamma^2x^2}{2}\right) = \frac{1}{\sqrt{2\pi\hbar}}(\frac{\gamma^2}{\pi})^{1/4}\int dx\text{exp}\left[\left(\frac{p}{\hbar\gamma\sqrt{2}} - \frac{i\gamma x}{\sqrt{2}}\right)^2 - \frac{1}{2}\left(\frac{p}{\hbar\gamma}\right)^2\right] =$$

$$= \frac{1}{\sqrt{2\pi\hbar}}(\frac{\gamma^2}{\pi})^{1/4}e^{-\frac{1}{2}\left(\frac{p}{\hbar\gamma}\right)^2}\int dx\ \text{exp}\left[-\left(\frac{p}{\hbar\gamma i\sqrt{2}} - \frac{\gamma x}{\sqrt{2}}\right)^2\right] =$$

$$= \frac{1}{\sqrt{2\pi\hbar}}(\frac{\gamma^2}{\pi})^{1/4}e^{-\frac{1}{2}\left(\frac{p}{\hbar\gamma}\right)^2}\frac{\sqrt{2}}{\gamma}\int d(-\frac{pi}{\hbar\gamma\sqrt{2}} + \frac{\gamma x}{\sqrt{2}})\ \text{exp}\left[-\left(-\frac{ip}{\hbar\gamma\sqrt{2}} + \frac{\gamma x}{\sqrt{2}}\right)^2\right] =$$

$$= \frac{1}{\sqrt{2\pi\hbar}}(\frac{\gamma^2}{\pi})^{1/4}\frac{\sqrt{2\pi}}{\gamma}e^{-\frac{1}{2}\left(\frac{p}{\hbar\gamma}\right)^2} = (\frac{1}{\pi\gamma^2\hbar^2})^{1/4}e^{-\frac{1}{2}\left(\frac{p}{\hbar\gamma}\right)^2}.$$

$$P(p)dp = |\psi(p)|^2dp = (\frac{1}{\pi\gamma^2\hbar^2})^{1/2}e^{-\left(\frac{p}{\hbar\gamma}\right)^2}\,dp.$$

### 8.15.26 What is the oscillator doing?

Consider a one dimensional simple harmonic oscillator. Use the number basis to do the following algebraically:

**a)** Construct a linear combination of $|0\rangle$ and $|1\rangle$ such that $\langle\hat{x}\rangle$is as large as possible.

With the basis vectors, we choose the combination

$|\alpha\rangle = a|0\rangle + b|1\rangle,$

with normalization $|a|^2 + |b|^2 = 1.$

Now

$\langle \hat{x} \rangle = (a^*\langle 0| + b^*\langle 1|)\hat{x}(a|0\rangle + b|1\rangle)$.
Then,
$\langle \hat{x} \rangle = x_c(a^*\langle 0| + b^*\langle 1|)\frac{\hat{a}+\hat{a}^+}{2}(a|0\rangle + b|1\rangle)$,
with $x_c = \sqrt{\frac{2\hbar}{m\omega}}$.
Sometimes use is made of
$\hat{x} = x_0(\hat{a} + \hat{a}^+)$, with $x_0 = \sqrt{\frac{\hbar}{2m\omega}}$ and $x_c = 2x_0$.
With $\langle \hat{x} \rangle = x_c(a^*\langle 0| + b^*\langle 1|)\frac{\hat{a}+\hat{a}^+}{2}(a|0\rangle + b|1\rangle)$:
$\langle \hat{x} \rangle = x_c \left[a^*a \left\langle 0\left|\frac{\hat{a}+\hat{a}^+}{2}\right|0\right\rangle + b^*b\left\langle 1\left|\frac{\hat{a}+\hat{a}^+}{2}\right|1\right\rangle + a^*b\left\langle 0\left|\frac{\hat{a}+\hat{a}^+}{2}\right|1\right\rangle + b^*a\left\langle 1\left|\frac{\hat{a}+\hat{a}^+}{2}\right|0\right\rangle\right]$.
With
$\left\langle 0\left|\frac{\hat{a}+\hat{a}^+}{2}\right|0\right\rangle = 0$, and $\left\langle 1\left|\frac{\hat{a}+\hat{a}^+}{2}\right|1\right\rangle = 0$, we have
$\langle \hat{x} \rangle = x_c\left[a^*b\left\langle 0\left|\frac{\hat{a}+\hat{a}^+}{2}\right|1\right\rangle + b^*a\left\langle 1\left|\frac{\hat{a}+\hat{a}^+}{2}\right|0\right\rangle\right] =$
$= x_c\left[a^*b\left(\left\langle 0\left|\frac{\hat{a}}{2}\right|1\right\rangle + \left\langle 0\left|\frac{\hat{a}^+}{2}\right|1\right\rangle\right) + b^*a\left(\left\langle 1\left|\frac{\hat{a}}{2}\right|0\right\rangle + \left\langle 1\left|\frac{\hat{a}^+}{2}\right|0\right\rangle\right)\right] =$
$= x_c\left[\frac{a^*b}{2}(\langle 0|0\rangle + \langle 1|1\rangle) + \frac{b^*a}{2}(\langle 0|0\rangle + \langle 1|1\rangle)\right]$.
Hence,
$\langle \hat{x} \rangle = \sqrt{\frac{2\hbar}{m\omega}}(a^*b + b^*a)$.
To find the maximum, we choose $a$ and $b$ to be real and with $|a|^2 + |b|^2 = 1$:
$\langle \hat{x} \rangle = \sqrt{\frac{2\hbar}{m\omega}}(a^*b + b^*a) = 2\sqrt{\frac{2\hbar}{m\omega}}a\sqrt{1-a^2}$.
With
$\frac{d}{dx}\langle \hat{x} \rangle = 0 \rightarrow a = \frac{1}{\sqrt{2}} \rightarrow b = \frac{1}{\sqrt{2}} \rightarrow \langle \hat{x} \rangle_{max} = \sqrt{\frac{2\hbar}{m\omega}}$.
The state vector $|\alpha\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ .

**b)** Suppose the oscillator is in the state constructed in **a)** at $t = 0$ .What is the state vector for $t > 0$? Evaluate $\langle \hat{x} \rangle$ as function of time for $t > 0$ using (i) the Schrödinger picture and (ii) the Heisenberg picture.
With the time development operator:
$|\alpha(t)\rangle = \hat{U}(t)|\alpha\rangle = e^{-i\hat{H}t/\hbar}|\alpha\rangle = \frac{1}{\sqrt{2}}(e^{-i\hat{H}t/\hbar}|0\rangle + e^{-i\hat{H}t/\hbar}|1\rangle)$.
With the ground state and the first excited state of the oscillator, $n = 0,1$ :
$|\alpha(t)\rangle = \frac{1}{\sqrt{2}}(e^{-i\omega t/2}|0\rangle + e^{-i3\omega t/2}|1\rangle)$.
- In the Schrödinger picture:
With $a = \frac{1}{\sqrt{2}}e^{-i\omega t/2}$, and $b = \frac{1}{\sqrt{2}}e^{-3i\omega t/2}$
$\langle \hat{x} \rangle = \sqrt{\frac{2\hbar}{m\omega}}(a^*b + b^*a) \rightarrow \langle \hat{x} \rangle = \sqrt{\frac{2\hbar}{m\omega}}\cos\omega t$,

- In the Heisenberg picture
With the results of Problem 8.15.20a , The Harmonic oscillator:
$\hat{x}(t) = \hat{x}(0)\cos\omega t + \frac{\hat{p}(0)}{m\omega}\sin\omega t$ , and $\hat{x} = x_c\frac{\hat{a}+\hat{a}^+}{2}$ , $x_c = \sqrt{\frac{2\hbar}{m\omega}}$ , $\hat{p}(0) = p_c\frac{\hat{a}-\hat{a}^+}{2i}$ , and $p_c = \sqrt{2m\omega\hbar}$ ,

$$\langle\hat{x}(t)\rangle = \langle\alpha|\hat{x}(t)|\alpha\rangle = \left\langle\alpha\middle|\hat{x}(0)\cos\omega t + \frac{\hat{p}(0)}{m\omega}\middle|\alpha\right\rangle =$$

$$= \frac{1}{2}[\cos\omega t\,\langle\alpha|\hat{x}(0)|\alpha\rangle + \frac{\sin\omega t}{m\omega}\langle\alpha|\hat{p}(0)|\alpha\rangle] =$$

$$= \frac{1}{2}\Big[\cos\omega t\,(\langle 0|\hat{x}(0)|0\rangle + \langle 1|\hat{x}(0)|1\rangle + \langle 1|\hat{x}(0)|0\rangle + \langle 0|\hat{x}(0)|1\rangle) + \frac{\sin\omega t}{m\omega}(\langle 0|\hat{p}(0)|0\rangle +$$
$$\langle 1|\hat{p}(0)|1\rangle) + \langle 1|\hat{p}(0)|0\rangle + \langle 0|\hat{p}(0)|1\rangle)\Big] =$$

$$= \frac{1}{2}\Big[x_c\cos\omega t\left(\left\langle 0\middle|\frac{\hat{a}+\hat{a}^+}{2}\middle|0\right\rangle + \left\langle 1\middle|\frac{\hat{a}+\hat{a}^+}{2}\middle|1\right\rangle + \left\langle 1\middle|\frac{\hat{a}+\hat{a}^+}{2}\middle|0\right\rangle + \left\langle 0\middle|\frac{\hat{a}+\hat{a}^+}{2}\middle|1\right\rangle\right) +$$
$$+ \frac{p_c\sin\omega t}{m\omega}\left(\left\langle 0\middle|\frac{\hat{a}-\hat{a}^+}{2i}\middle|0\right\rangle + \left\langle 1\middle|\frac{\hat{a}-\hat{a}^+}{2i}\middle|1\right\rangle + \left\langle 1\middle|\frac{\hat{a}-\hat{a}^+}{2i}\middle|0\right\rangle\right) + \left\langle 0\middle|\frac{\hat{a}-\hat{a}^+}{2i}\middle|1\right\rangle)\Big] =$$

$$= \frac{1}{2}\Big[x_c\cos\omega t\left(\left\langle 1\middle|\frac{\hat{a}+\hat{a}^+}{2}\middle|0\right\rangle + \left\langle 0\middle|\frac{\hat{a}+\hat{a}^+}{2}\middle|1\right\rangle\right) + \frac{p_c\sin\omega t}{m\omega}\left(\left\langle 1\middle|\frac{\hat{a}-\hat{a}^+}{2i}\middle|0\right\rangle + \left\langle 0\middle|\frac{\hat{a}-\hat{a}^+}{2i}\middle|1\right\rangle\right)\Big] =$$

$$= \frac{1}{2}[x_c\cos\omega t\,(\left\langle 1\middle|\frac{\hat{a}}{2}\middle|0\right\rangle + \left\langle 1\middle|\frac{\hat{a}^+}{2}\middle|0\right\rangle + \left\langle 0\middle|\frac{\hat{a}}{2}\middle|1\right\rangle + \left\langle 0\middle|\frac{\hat{a}^+}{2}\middle|1\right\rangle +$$
$$+ \frac{p_c\sin\omega t}{m\omega}(\left\langle 1\middle|\frac{\hat{a}}{2i}\middle|0\right\rangle - \left\langle 1\middle|\frac{\hat{a}^+}{2i}\middle|0\right\rangle + \left\langle 0\middle|\frac{\hat{a}}{2i}\middle|1\right\rangle - \left\langle 0\middle|\frac{\hat{a}^+}{2i}\middle|1\right\rangle)] =$$

$$= x_c\cos\omega t = \sqrt{\frac{2\hbar}{m\omega}}\cos\omega t,$$ see Problem 8.15.20.c

The Schrödinger picture:

$$\sqrt{\frac{2\hbar}{m\omega}}\cos\omega t\ .$$

**c)** Evaluate $\langle(\Delta x)^2\rangle$ as a function of time using the Schrödinger picture.

$\langle(\Delta x)^2\rangle = \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2$.

With $|\alpha(t)\rangle = \frac{1}{\sqrt{2}}(e^{-i\omega t/2}|0\rangle + e^{-i3\omega t/2}|1\rangle)$

$$\langle\hat{x}^2\rangle = \langle\alpha(t)|\hat{x}^2|\alpha(t)\rangle = \frac{1}{2}[\left(e^{\frac{i\omega t}{2}}\langle 0| + e^{\frac{i3\omega t}{2}}\langle 1|\right)\left(x_c\frac{\hat{a}+\hat{a}^+}{2}\right)^2(e^{-\frac{i\omega t}{2}}|0\rangle + e^{-\frac{i3\omega t}{2}}|1\rangle)] =$$

$$= \frac{1}{8}x_c^2\left[\left(e^{\frac{i\omega t}{2}}\langle 0| + e^{\frac{i3\omega t}{2}}\langle 1|\right)\hat{a}^2 + 1 + 2\hat{a}^+\hat{a} + (\hat{a}^+)^2\left(e^{-\frac{i\omega t}{2}}|0\rangle + e^{-\frac{i3\omega t}{2}}|1\rangle\right)\right] =$$

$$= \frac{1}{8}x_c^2[4+4] = x_c^2\ .$$

Note: keep in mind $\left(e^{\frac{i\omega t}{2}}\langle 0| + e^{\frac{i3\omega t}{2}}\langle 1|\right)\hat{a}^2\left(e^{-\frac{i\omega t}{2}}|0\rangle + e^{-\frac{i3\omega t}{2}}|1\rangle\right) =$

$$= \left(e^{\frac{i\omega t}{2}}\langle 0| + e^{\frac{i3\omega t}{2}}\langle 1|\right)\hat{a}\hat{a}\left(e^{-\frac{i\omega t}{2}}|0\rangle + e^{-\frac{i3\omega t}{2}}|1\rangle\right) = \langle 0|0\rangle\ .$$

With the result of b)

$\langle\hat{x}\rangle^2 = x_c^2\cos^2\omega t.$

Hence:

$\langle(\Delta x)^2\rangle = x_c^2(1-\cos^2\omega t).$

### 8.15.27 Coupled Oscillators

Two identical in one dimension each have a mass $m$ and frequency $\omega$. Let the two oscillators be coupled by an interaction term $C\hat{x}_1\hat{x}_2$ where $C$ is a constant and $x_1$ and $x_2$ are the

coordinates of the oscillators. Find the exact energy spectrum of eigenvalues for this coupled system.
We have for the Hamiltonian:
$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{int} = \frac{\hat{p}_1^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_1^2 + \frac{\hat{p}_2^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_2^2 + C\hat{x}_1\hat{x}_2.$
A shift to the centre of mass coordinates in order to reduce complexity
$\hat{X} = \hat{x}_1 - \hat{x}_2$ , $\hat{Y} = \frac{\hat{x}_1+\hat{x}_2}{2}$,
$\hat{P} = \frac{\hat{p}_1-\hat{p}_2}{2}$ , $\hat{\wp} = \hat{p}_1 + \hat{p}_2$.
With these four expression we find
$\hat{x}_1 = \frac{\hat{X}}{2} + \hat{Y}$ , $\hat{x}_2 = -\frac{\hat{X}}{2} + \hat{Y}$
$\hat{p}_1 = \hat{P} + \frac{\hat{\wp}}{2}$ , $\hat{p}_2 = -\hat{P} + \frac{\hat{\wp}}{2}$.
We plug these transformations into the Hamiltonian:
$\hat{H} = \frac{\hat{P}^2}{m} + \frac{m\hat{X}^2}{4}\left(\omega^2 - \frac{C}{m}\right) + \frac{\hat{\wp}^2}{4m} + m\hat{Y}^2\left(\omega^2 + \frac{C}{m}\right).$
Indeed, the preceding expression for the Hamiltonian is less complex: two uncoupled oscillators.
Hence, we use the results for a single simple harmonic oscillator.
The so-called $\hat{X}$-oscillator has frequency
$\omega_{\hat{X}} = \sqrt{\left(\omega^2 - \frac{C}{m}\right)}.$
The energy eigenvalues are
$E_{n_{\hat{X}}} = \hbar\omega_{\hat{X}}\left(n_{\hat{X}} + \frac{1}{2}\right), n_{\hat{X}} = 0,1,2,\ldots$
The so-called $\hat{Y}$-oscillator has frequency
$\omega_{\hat{Y}} = \sqrt{\left(\omega^2 + \frac{C}{m}\right)}.$
The energy eigenvalues are
$E_{n_{\hat{Y}}} = \hbar\omega_{\hat{Y}}\left(n_{\hat{Y}} + \frac{1}{2}\right), n_{\hat{Y}} = 0,1,2,\ldots$
The energy spectrum of eigenvalues for these coupled system is
$E_{n_{\hat{X}}n_{\hat{Y}}} = \hbar\omega_{\hat{X}}\left(n_{\hat{X}} + \frac{1}{2}\right) + \hbar\omega_{\hat{Y}}\left(n_{\hat{Y}} + \frac{1}{2}\right).$

### 8.15.28 Interesting Operators

The operator $\hat{c}$ is defined by the following relations
$\hat{c}^2 = 0$, and $\hat{c}\hat{c}^+ + \hat{c}^+\hat{c} = \{\hat{c}, \hat{c}^+\} = \hat{I}$ .
**a)**
- $\hat{c}^+\hat{c} \equiv \hat{M}$ is Hermitian $\rightarrow \hat{M}^\dagger = \hat{M}$ ?
$\hat{M}^\dagger = (\hat{c}^+\hat{c})^\dagger = \hat{c}^\dagger(\hat{c}^+)^\dagger = \hat{c}^+\hat{c} = \hat{M}.$
Hence,
$\hat{c}^+\hat{c} \equiv \hat{M}$ is Hermitian .
- $\hat{M}^2 = \hat{M}$ ?
$\hat{M}^2 = \hat{c}^+\hat{c}\hat{c}^+\hat{c} = \hat{c}^+\left(\hat{I} - \hat{c}^+\hat{c}\right)\hat{c} = \hat{c}^+\hat{I}\hat{c} - \hat{c}^+\hat{c}^+\hat{c}^2 = \hat{c}^+\hat{c} \equiv \hat{M}.$
- The eigenvalues of $\hat{M}$ are 0 and 1 (eigenstates $|0\rangle$ and $|1\rangle$ ).
Let $\hat{M}$ operate on $|\alpha\rangle$ and denote the eigenvalue to be $\alpha$:

$\widehat{M}|\alpha\rangle = \alpha|\alpha\rangle$.
Then, we also have
$\widehat{M}^2|\alpha\rangle = \widehat{M}\alpha|\alpha\rangle = \alpha^2|\alpha\rangle$ .
Consequently
$\left(\widehat{M}^2 - \widehat{M}\right)|\alpha\rangle = (\alpha^2 - \alpha)|\alpha\rangle = 0$,
for any $|\alpha\rangle$.
Hence
$(\alpha^2 - \alpha) = 0 \rightarrow \alpha = 0{,}1$ .
- $\hat{c}^+|0\rangle = |1\rangle$ , and $\hat{c}|1\rangle = 0$ ?
$\widehat{M}|1\rangle = 1|1\rangle \rightarrow \hat{c}^+\hat{c}|1\rangle = 1|1\rangle \rightarrow \left(\hat{I} - \hat{c}\hat{c}^+\right)|1\rangle = 1|1\rangle \rightarrow \hat{I}|1\rangle - \hat{c}\hat{c}^+|1\rangle = 1|1\rangle$,
and
$\hat{c}\hat{c}^+|1\rangle = 0$ .
$\widehat{M}|0\rangle = 0|0\rangle \rightarrow \hat{c}^+\hat{c}|0\rangle = 0|0\rangle \rightarrow \left(\hat{I} - \hat{c}\hat{c}^+\right)|0\rangle = 0|0\rangle \rightarrow \hat{I}|0\rangle - \hat{c}\hat{c}^+|0\rangle = 0|0\rangle$,
and
$\hat{c}\hat{c}^+|0\rangle = 0$
Now,
$\langle 1|\hat{c}\hat{c}^+|1\rangle = 0 \rightarrow \left\langle 1\middle|\hat{I}\middle|1\right\rangle - \langle 1|\hat{c}^+\hat{c}|1\rangle = 0 \rightarrow \langle 1|\hat{c}^+\hat{c}|1\rangle = 1$
and
$\langle 0|\hat{c}^+\hat{c}|0\rangle = 0 \rightarrow \left\langle 0\middle|\hat{I}\middle|0\right\rangle - \langle 0|\hat{c}\hat{c}^+|0\rangle = 0 \rightarrow \langle 0|\hat{c}\hat{c}^+|0\rangle = 1$.
With the preceding expressions. The only possible solutions are:
$\hat{c}|1\rangle = |0\rangle$, and $\hat{c}^+|0\rangle = |1\rangle$ .

**b)** Consider the Hamiltonian
$\widehat{H} = \hbar\omega_0(\widehat{M} + \frac{1}{2})$.
Denote the eigenstates of $\widehat{H}$ by $|n\rangle$, show that the only nonvanishing states are the states $|0\rangle$ and $|1\rangle$ . The eigenstates of $\widehat{M}$ with the eigenvalues given under a).
Now,
$\widehat{H}|n\rangle = E_n|n\rangle$ ,
and $|n\rangle$ expanded in the eigenstates of $\widehat{M}$ :
$|n\rangle = a_n|0\rangle + b_n|1\rangle$.
With the Hamiltonian operator
$\widehat{H}|n\rangle = \hbar\omega_0(\widehat{M} + \frac{1}{2})(\, a_n|0\rangle + b_n|1\rangle)$.
With $\widehat{M} = \hat{c}^+\hat{c}$, the time independent Schrödinger equation becomes:
$\widehat{H}|n\rangle = \hbar\omega_0 b_n|1\rangle + \frac{\hbar\omega_0}{2}|n\rangle$ .
With
$n = 0 \rightarrow a_0 = 1, b_0 = 0$ , and $E_0 = \frac{\hbar\omega_0}{2}$ ,
$n = 1 \rightarrow a_1 = 0, b_1 = 1$ , and $E_1 = \frac{3\hbar\omega_0}{2}$ .
It is about fermions.

### 8.15.29 What is the state?

A particle of mass $m$ in a one dimensional harmonic oscillator potential is in a state for which the measurement of the energy yields the values $\frac{\hbar\omega_0}{2}$ or $\frac{3\hbar\omega_0}{2}$ , each with a probability of one-half. The average value of the momentum $\langle \hat{p}_x \rangle$ at time $t = 0$ is $(\frac{m\omega\hbar}{2})^{1/2}$. This information specifies the state of the particle completely. What is the state and what is $\langle \hat{p}_x \rangle$ at time $t$?

We know the two base states and express the state of the particle at $t = 0$ into the two base states:

$|\psi(0)\rangle = a|0\rangle + b|1\rangle$.

We have $|a|^2 + |b|^2 = 0$.

So, with a probability of one-half for $|0\rangle$ and $|1\rangle$ respectively and take into a count a phase difference $\alpha$:

$|a|^2 = \frac{1}{2} \to a = \frac{1}{\sqrt{2}}$,

$|b|^2 = \frac{1}{2} \to b = \frac{1}{\sqrt{2}} e^{i\alpha}$.

The state at $t = 0$ :

$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i\alpha}|1\rangle\right)$.

$\langle \hat{p}_x \rangle$ at time $t = 0$ is $(\frac{m\omega\hbar}{2})^{1/2}$:

$\langle \hat{p}_x \rangle = \langle \psi(0)|\hat{p}_x|\psi(0)\rangle = (\frac{m\omega\hbar}{2})^{1/2}$.

With $\hat{p}_x = -i\left(\frac{m\omega\hbar}{2}\right)^{\frac{1}{2}}(\hat{a} - \hat{a}^+)$ :

$$\langle \hat{p}_x \rangle = \langle \psi(0)|\hat{p}_x|\psi(0)\rangle = -\frac{i\left(\frac{m\omega\hbar}{2}\right)^{\frac{1}{2}}}{2}[\left\langle 0\right| + e^{-i\alpha}\langle 1|](\hat{a} - \hat{a}^+)\left[|0\rangle + e^{i\alpha}|1\rangle\right] =$$

$$= \left(\frac{m\omega\hbar}{2}\right)^{\frac{1}{2}} \sin\alpha = (\frac{m\omega\hbar}{2})^{\frac{1}{2}} \to \alpha = \frac{\pi}{2}.$$

For the state of the particle at time $t = 0$ , we obtain

$|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$ .

Then, applying the time development operator, we have for the state at time $t$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(e^{-\frac{i\omega t}{2}}|0\rangle + ie^{-\frac{i3\omega t}{2}}|1\rangle\right).$$

$\langle \hat{p}_x \rangle$ at time $t$:

$$\langle \hat{p}_x \rangle_t = \langle \psi(t)|\hat{p}_x|\psi(t)\rangle =$$

$$= -\frac{i\left(\frac{m\omega\hbar}{2}\right)^{\frac{1}{2}}}{2}\left[e^{\frac{i\omega t}{2}}\left\langle 0\right| - ie^{\frac{i3\omega t}{2}}\langle 1|\right](\hat{a} - \hat{a}^+)\left[e^{-\frac{i\omega t}{2}}|0\rangle + ie^{-\frac{i3\omega t}{2}}|1\rangle\right] =$$

$$= \frac{i\left(\frac{m\omega\hbar}{2}\right)^{\frac{1}{2}}}{2}\left[e^{\frac{i\omega t}{2}}\left\langle 0\right| - ie^{\frac{i3\omega t}{2}}\langle 1|\right]\left[e^{-\frac{i\omega t}{2}}|1\rangle + ie^{-\frac{i3\omega t}{2}}|0\rangle\right] =$$

$$= (\frac{m\omega\hbar}{2})^{\frac{1}{2}} \cos\omega t.$$

### 8.15.30 Things about Particles in a Box.

A particle of mass $m$ moves in a one-dimensional infinite well of length $l$ with the potential

$$V(x) = \begin{cases} \infty & x < 0 \\ 0 & 0 < x < l \\ \infty & x > l \end{cases}$$

At $t = 0$ , the wave function of this particle is known to have the form

$\psi(x,0) = \sqrt{\frac{30}{l^5}}x(l-x)$, for $0 < x < l$ ,

and

$\psi(x,0) = 0$, otherwise.

**a)** The eigenfunctions of this particle in a box are given in Problem 8.15.15:

$\psi_n(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{\pi n x}{l}\right)$ , and the eigenvalues are $E_n = \frac{(n\pi\hbar)^2}{2ml^2}$ , $n = 1,2,3, \ldots$

We expand $\psi(x,0)$ in the eigenfunctions

$\psi(x,0) = \sum_n^\infty a_n\, \psi_n(x)$ .

Then,

$\int \psi_k^*(x)\, \psi(x,0)dx = \sum_n^\infty a_n \int \psi_k^*(x)\, \psi_n(x)dx = \sum_n^\infty a_n\, \delta_{nk} = a_k.$

So,

$$a_k = \int_0^l \sqrt{\frac{2}{l}}\sin\left(\frac{\pi k x}{l}\right)\sqrt{\frac{30}{l^5}}x(l-x)dx = \sqrt{\frac{60}{l^6}}\int_0^l x(l-x)\sin\left(\frac{\pi k x}{l}\right)dx.$$

Applying integration by parts:

$$a_k = 2\sqrt{\frac{60}{l^6}}\left(\frac{l}{\pi k}\right)^3(1-\cos\pi k) = \frac{4\sqrt{15}}{(\pi k)^3}(1-\cos\pi k) = \frac{8\sqrt{15}}{(\pi k)^3},\ \ k = 1,3,5, \ldots$$

The wave function

$$\psi(x,0) = \sum_k^\infty a_k\, \psi_k(x) = \sum_{k\ is\ odd}\frac{8\sqrt{15}}{(\pi k)^3}\psi_k(x).$$

**b)** What is the probability of measuring $E_k$ at $t = 0$?

$$P(E_k) = |a_k|^2 = \left(\frac{8\sqrt{15}}{(\pi k)^3}\right)^2,\ k = 1,3,5, \ldots$$

With help of this result an expression for an infinite sum can be obtained:

$$\sum_k P(E_k) = 1 \to \sum_{k\ is\ odd}\left(\frac{8\sqrt{15}}{(\pi k)^3}\right)^2 = 1 \to \sum_{k\ is\ odd}\frac{1}{k^6} = \frac{\pi^6}{960}.$$

Obviously, the same result is obtained with the box symmetrically positioned at $x = 0$ , and

$\psi(x,0) = \sqrt{\frac{30}{l^5}}\left(\frac{l}{2}+x\right)\left(\frac{l}{2}-x\right)$, for $-\frac{l}{2} < x < \frac{l}{2}$.

**c)** Using the time development operator, we find for the wave function at time $t$

$\psi(x,t) = \sum_k^\infty a_k\, \psi_k(x)e^{-iE_k t/\hbar}$ .

### 8.15.31 Handling Arbitrary Barriers ……

Electrons in a metal are bound by a potential that may be approximated by a finite square well. Electrons fill up the energy levels of this well to an energy called the Fermi energy as shown in the following figures below(Boccio):

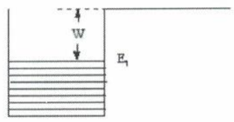



Figure 8.6: Finite Square Well

The difference between the Fermi energy and the top of the well is the *work function* $W$ of the metal. Photons with energies exceeding the work function can eject electrons from the metal - this is the so-called *photoelectric effect*.

Another way to pull out electrons is through application of an external uniform electric field $\vec{\mathcal{E}}$, which alters the potential energy as shown in the figure below:

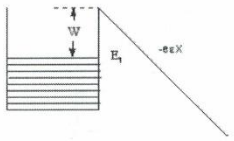



Figure 8.7: Finite Square Well + Electric Field

By approximating(see notes below) the linear part of the function by a series of square barriers, show that the transmission coefficient $T$ for electrons at the Fermi energy is given by

$T \approx \exp\left(\frac{-4\sqrt{2m}W^{\frac{3}{2}}}{3e|\vec{\mathcal{E}}|\hbar}\right)$.

**Note:**

*In Fitzpatrick Chapter 5, The Undergraduate Course, the tunneling through the barrier in Figure 8.7 has been derived using the WKB Approximation.*

*There, the ratio of the probability densities to the right and to the left of the potential barrier is interpreted as the probability, $|T|^2$, that a particle incident from the left will tunnel through the barrier and emerge at the other side: i.e.,*

$|T|^2 = \frac{|\psi_2|^2}{|\psi_1|^2} = exp\left(-\frac{2\sqrt{2}m}{\hbar}\int_{x_1}^{x_2}\sqrt{V(x) - E}\,dx\right)$*, Eqs.(5.49) and (5.50).*

*See also Mahan , Chapter 3 Approximate Methods, Section 3.3 Electron Tunneling, pages 76 and 77, Figure 3.6.*

How would you expect this field- or cold-emission current vary with the applied voltage?
This calculation also plays a role in the derivation of the current-voltage characteristic of a Schottky diode in semiconductor physics.

We have for the transmission coefficient

$T \approx \exp\left(-\frac{2\sqrt{2}m}{\hbar}\int_{x_1}^{x_2}\sqrt{V(x) - E}\,dx\right)$,

with $x$ is along the horizontal axis and at $x = 0$, $W$ the work function of the surface is 0.

In the absence of the electric field, the potential barrier just above the surface is

$V(x) - E_f = W$,

where $E_f$ is indicated in Figure 8.7.

The electric field modifies the barrier to

$V(x) - E_f = W - e\mathcal{E}x$.

At $x = L$, we have $V(x) - E_f = 0$,

and

$W = e\mathcal{E}L$.

Hence,

$$T \approx \exp\left(-\frac{2\sqrt{2m}}{\hbar}\int_0^L \sqrt{W - e\mathcal{E}x}\,dx\right) = \exp\left(-\frac{2\sqrt{2m}}{\hbar}\int_0^{W/e\mathcal{E}} \sqrt{W - e\mathcal{E}x}\,dx\right) =$$

$$= \exp\left(-\frac{2\sqrt{2m}W^{3/2}}{\hbar e\mathcal{E}}\int_0^1 \sqrt{1-y}\,dy\right) = \exp\left(\frac{-4\sqrt{2m}W^{\frac{3}{2}}}{3e|\vec{\mathcal{E}}|\hbar}\right).$$

**Approximating an Arbitrary Barrier**

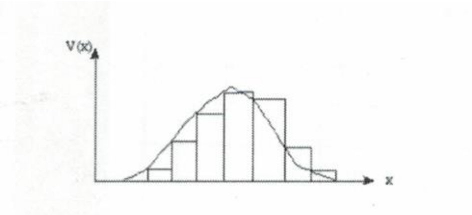


Figure 8.8: Arbitrary Barrier Potential

An example of an arbitrary potential barrier is shown in Figure 8.8 (Boccio).
For a rectangular barrier of width $a$ and height $V_0$, we found the transmission coefficient to be

$T = \frac{1}{1+\frac{V_0^2 \sinh^2 \gamma a}{4E(V_0-E)}}$ , $k^2 = \frac{2m}{\hbar^2}E$ , and $\gamma^2 = k^2(\frac{V_0}{E} - 1)$ .

See Section 8.5.2 *Tunneling* ,Eq.(8.187) page 565.

Boccio presented a useful limiting case for $\gamma a \gg 1 \rightarrow \sinh \gamma a \rightarrow \frac{e^{\gamma a}}{2}$.

$\frac{V_0^2}{E(V_0-E)} = \frac{1}{(\frac{\gamma E}{kV_0})^2}$,

and

$(\frac{V_0}{E})^2 = (\frac{\gamma^2+k^2}{k^2})^2$ .

Then with the preceding two expressions and $\gamma a \gg 1$

$T = \frac{1}{1+\frac{V_0^2 \sinh^2 \gamma a}{4E(V_0-E)}} \rightarrow \frac{1}{1+\frac{e^{2\gamma a}}{4}(\frac{\gamma^2+k^2}{2\gamma k})^2} \rightarrow (\frac{4\gamma k}{\gamma^2+k^2})^2 e^{-2\gamma a}$.

Boccio took the natural log of $T$ and approximated

$\ln(\frac{4\gamma k}{\gamma^2+k^2})^2 \rightarrow 0.$

So $(\frac{4\gamma k}{\gamma^2+k^2})^2 = 1,$

and

$\gamma^2 = k^2(7 \pm 4\sqrt{3}).$

With $\gamma^2 = k^2(\frac{V_0}{E} - 1),$

$V_0 = 4E(2 \pm \sqrt{3})$. Is this realistic?

Hence, with $\gamma a \gg 1$

$T = e^{-2\gamma a}$.

See Figure 8.8 . Now the probability of transmission through an arbitrary barrier is just the product of the individual transmission coefficients of a succession of rectangular barriers.

Thus, if the barrier is sufficiently smooth so that we can approximate it by a series of rectangular barriers (each of width $\Delta x$) that are not too thin for the condition $\gamma a \gg 1$ to hold, then for the barrier as a whole

$$\ln T \approx \ln \prod_i T_i = \sum_i \ln T_i = -2 \sum_i \gamma_i \Delta x$$

If we now assume that we can approximate this last term by an integral, we find

$$T \approx \exp\left(-2 \sum_i \gamma_i \Delta x\right) \approx \exp\left(-2 \int \sqrt{\frac{2m}{\hbar^2}} \sqrt{V(x) - E} dx\right)$$

where the integration is over the region for which the square root is real.

You may have a somewhat uneasy feeling about this crude derivation. Clearly, the approximations made break down near the turning points, where $E = V(x)$. Nevertheless, a more detailed treatment shows that it works amazingly well.

A detailed treatment is the WKB approximate method?

### 8.15.32 Deuteron Model

Consider the motion of a particle of mass $m = 0.8 \cdot 10^{-24}$ gm in the well shown below, Boccio:

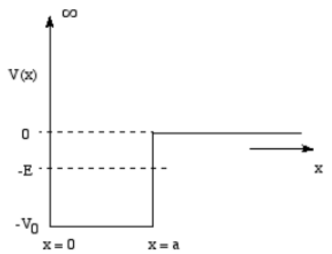



Figure 8.9: Deuteron Model

The size of the well(range of the potential) is $a = 1.4 \cdot 10^{-13}$ cm. If the binding energy of the system is 2.2 MeV, find the depth of the potential.
This is a model of the deuteron in one dimension.

*See also Mahan pages 17, 18 and 19, Chapter One Dimension section 2.2*

$$V(x) = \begin{cases} \infty & x < 0 \\ -V_0 & 0 < x < a \\ 0 & a < x \end{cases}$$

Bound states are defined as having an eigenvalue $E < 0$ and use $E = -|E|$.

The general solution of the Schrödinger equation for $0 < x < a$ and $k = \sqrt{\frac{2m(V_0 - |E|)}{\hbar^2}}$:

$\psi_1 = Ae^{ikx} + Be^{-ikx}$,
with the boundary condition at $x = 0 \rightarrow \psi_1 = 0 \rightarrow A = -B$.
So,
$\psi_1 = C \sin kx$.
The general solution for $x > a$ and $\gamma^2 = \frac{2m}{\hbar^2}|E|$ :
$\psi_2 = De^{-\gamma x} + Fe^{\gamma x}$ .
The eigenfunction vanishes for $x \rightarrow \infty \rightarrow F = 0$ >

At $x = a$

$\psi_1 = \psi_2 \to C \sin kx = De^{-\gamma a}$,

$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx} \to Ck \cos ka = -D\gamma e^{-\gamma a}$.

Dividing the two preceding equations, which cancels the two constants $C$ and $D$,

$\tan ka = -\frac{k}{\gamma}$.

$ka = a \cdot \sqrt{\frac{2m(V_0-|E|)}{\hbar^2}} = a \cdot \sqrt{\frac{2m|E|)}{\hbar^2}} \sqrt{\frac{V_0-|E|)}{|E|}} = a\gamma \sqrt{\frac{V_0-|E|)}{|E|}}$.

So,

$\frac{k}{\gamma} = \sqrt{\frac{V_0-|E|)}{|E|}}$.

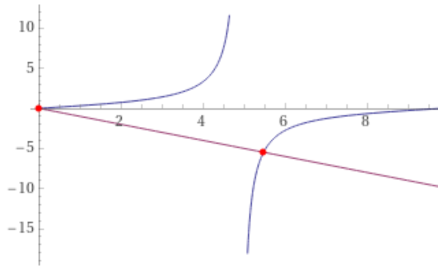
Then

$\tan\left[a\gamma\sqrt{\frac{V_0-|E|)}{|E|}}\right] = -\sqrt{\frac{V_0-|E|)}{|E|}}$.

Plug into the preceding expression the given numbers

$\tan[0.32 \cdot \sqrt{\frac{V_0-|E|)}{|E|}}] = -\sqrt{\frac{V_0-|E|)}{|E|}}$.

With the WolframAlpha app:




$\sqrt{\frac{V_0-|E|)}{|E|}} \approx 5.47$.

Hence

$V_0 = 66.55$ MeV

### 8.15.33 Use Matrix Methods(Matrix Algebra)

A one-dimensional potential barrier is shown in the figure below, Boccio:

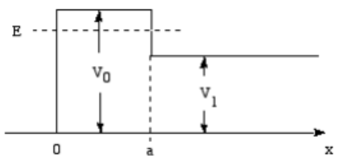



Figure 8.10: A Potential Barrier

Define and calculate the transmission probability for a particle of mass $m$ and energy $E$ ($V_1 < E < V_0$) incident on the barrier from the left. If you let $V_1 \to 0$ and $a \to 2a$, then you can compare your answer to other textbook results[12]. Develop matrix methods (as in the texts) to solve the boundary condition equations.

Figure 8.10 shows we have three regions to consider:

[12] I think if you let $V_1 \to 0$ and do not change $a$, you can still compare your answer with textbook results.

1) $x < 0$ , $\psi_1 = e^{ikx} + Re^{-ikx}$, and $E = \frac{\hbar^2 k^2}{2m}$ ,

2) $0 \le x \le a$ , tunneling $\psi_2 = Ae^{-\beta x} + Be^{\beta x}$ and $V_0 - E = \frac{\hbar^2 \beta^2}{2m}$ ,

3) $x \ge a$ , $\psi_3 = Te^{ik_1 x}$ , and $E - V_1 = \frac{\hbar^2 k_1^2}{2m}$ .

The boundary conditions result into four equations:

at $x = 0$

$\psi_1(x = 0) = \psi_2(x = 0) \rightarrow 1 + R = A + B,$

$\frac{d}{dx}\psi_1(x = 0) = \frac{d}{dx}\psi_2(x = 0) \rightarrow ik(1 - R) = -\beta(A - B),$

two equations represented in matrix form:

$\begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}\begin{pmatrix} 1 \\ R \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ -\beta & \beta \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix};$

at $x = a$

$\psi_2(x = a) = \psi_3(x = a) \rightarrow Ae^{-\beta a} + Be^{\beta a} = Te^{ik_1 a},$

$\frac{d}{dx}\psi_2(x = a) = \frac{d}{dx}\psi_3(x = a) \rightarrow -\beta\left(Ae^{-\beta a} - Be^{\beta a}\right) = ik_1 Te^{ik_1 a},$

two equations represented in matrix form:

$\begin{pmatrix} e^{-\beta a} & e^{\beta a} \\ -\beta e^{-\alpha a} & \beta e^{\beta a} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 \\ ik_1 \end{pmatrix} Te^{ik_1 a}.$

With matrix algebra we can obtain an expression for $T$:

$\begin{pmatrix} 1 \\ R \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}^{-1}\begin{pmatrix} 1 & 1 \\ -\beta & \beta \end{pmatrix}\begin{pmatrix} e^{-\beta a} & e^{\beta a} \\ -\beta e^{-\beta a} & \beta e^{\beta a} \end{pmatrix}^{-1}\begin{pmatrix} 1 \\ ik_1 \end{pmatrix} Te^{ik_1 a}.$

I will use old fashioned methods.

The first set of equations:

$1 + R = A + B$ ,

$ik(1 - R) = -\beta(A - B).$

Then,

$A = \frac{\beta - ik + R(\beta + ik)}{2\beta}$ ,

and

$B = \frac{\beta + ik + R(\beta - ik)}{2\beta}$ .

The second set of equations:

$Ae^{-\beta a} + Be^{\beta a} = Te^{ik_1 a},$

$-\beta\left(Ae^{-\beta a} - Be^{\beta a}\right) = ik_1 Te^{ik_1 a}.$

Then,

$A = \frac{T(\beta - ik_1)e^{a(ik_1 + \beta)}}{2\beta}$ ,

and

$B = \frac{T(\beta + ik_1)e^{a(ik_1 - \beta)}}{2\beta}$ .

With both expressions for $A$:

$\frac{T(\beta - ik_1)e^{a(ik_1 + \beta)}}{2\beta} = \frac{\beta - ik + R(\beta + ik)}{2\beta} \rightarrow R = \frac{T(\beta - ik_1)e^{a(ik_1 + \beta)}}{\beta + ik} - \frac{\beta - ik}{\beta + ik}$ .

With both expression for $B$:

$\frac{T(\beta + ik_1)e^{a(ik_1 - \beta)}}{2\beta} = \frac{\beta + ik + R(\beta - ik)}{2\beta} \rightarrow T(\beta + ik_1)e^{a(ik_1 - \beta)} = \beta + ik + R(\beta - ik).$

Plug into the latter expression, the expression we derived for $R$:

$$T(\beta+ik_1)e^{a(ik_1-\beta)}=\beta+ik+\frac{T(\beta-ik_1)e^{a(ik_1+\beta)}}{\beta+ik}(\beta-ik)-\frac{\beta-ik}{\beta+ik}(\beta-ik)\rightarrow$$

$$\rightarrow T[(\beta+ik_1)e^{a(ik_1-\beta)}-\frac{\beta-ik}{\beta+ik}(\beta-ik_1)e^{a(ik_1+\beta)}]=\beta+ik-\frac{\beta-ik}{\beta+ik}(\beta-ik).$$

Multiply the latter expression $\beta+ik$ :

$$T[(\beta+ik)(\beta+ik_1)e^{a(ik_1-\beta)}-(\beta-ik)(\beta-ik_1)e^{a(ik_1+\beta)}]=(\beta+ik)^2-(\beta-ik)^2\rightarrow$$

$$\rightarrow T\left[(\beta+ik)(\beta+ik_1)e^{-\beta a}-(\beta-ik)(\beta-ik_1)e^{\beta a}\right]=4i\beta ke^{-ik_1a}\rightarrow$$

$$\rightarrow T\left[\{\beta^2+i\beta(k+k_1)-kk_1\}e^{-\beta a}-\{\beta^2-i\beta(k+k_1)-kk_1\}e^{\beta a}\right]=4i\beta ke^{-ik_1a}\rightarrow$$

$$\rightarrow T\left[\left\{\frac{\beta}{k}+i\left(1+\frac{k_1}{k}\right)-\frac{k_1}{\beta}\right\}e^{-\beta a}-\left\{\frac{\beta}{k}-i\left(1+\frac{k_1}{k}\right)-\frac{k_1}{\beta}\right\}e^{\beta a}\right]=4ie^{-ik_1a}.$$

The latter expression can be written as:

$$T\left[i\left(1+\frac{k_1}{k}\right)\cosh\beta a-\left(\frac{\beta}{k}-\frac{k_1}{\beta}\right)\sinh\beta a\right]=2ie^{-ik_1a}.$$

So,

$$T=\frac{2ie^{-ik_1a}}{i\left(1+\frac{k_1}{k}\right)\cosh\beta a-\left(\frac{\beta}{k}-\frac{k_1}{\beta}\right)\sinh\beta a}.$$

The limit case is a single barrier of width $a$ .

For a rectangular barrier of width $a$ and height $V_0$, we found the transmission coefficient to be

$$T=\frac{1}{1+\frac{V_0^2\sinh^2\gamma a}{4E(V_0-E)}}\ ,\ k^2=\frac{2m}{\hbar^2}E\ \text{, and }\ \gamma^2=k^2(\frac{V_0}{E}-1)\text{ , Problem 8.15.31.}$$

See Section 8.5.2 *Tunneling* ,Eq.(8.187) page 565.

What we are looking for is $|T|^2$, Problem 8.15.31 *Handling arbitrary barriers*.

We have for the limit case:

$$(\frac{\beta}{k})^2=\frac{V_0}{E}-1\rightarrow\frac{V_0}{E}=1+(\frac{\beta}{k})^2\text{, and }1+\left(\frac{k}{\beta}\right)^2=\frac{V_0}{V_0-E}.$$

Then

$$T=\frac{2ie^{-ika}}{2i\cosh\beta a-\left(\frac{\beta}{k}-\frac{k}{\beta}\right)\sinh\beta a}=\frac{2ie^{-ika}[-2i\cosh\beta a-\left(\frac{\beta}{k}-\frac{k}{\beta}\right)\sinh\beta a]}{4\cosh^2\beta a+(\frac{\beta}{k}-\frac{k}{\beta})^2\sinh^2\beta a}.$$

Hence,

$$|T|^2=\frac{4}{4\cosh^2\beta a+(\frac{\beta}{k}-\frac{k}{\beta})^2\sinh^2\beta a}=\frac{1}{1+\sinh^2\beta a+\frac{1}{4}(\frac{\beta}{k}-\frac{k}{\beta})^2\sinh^2\beta a}=\frac{1}{1+\frac{1}{4}[2+\left(\frac{\beta}{k}\right)^2+\left(\frac{k}{\beta}\right)^2]\sinh^2\beta a}\rightarrow$$

$$\rightarrow\ |T|^2=\frac{1}{1+\frac{V_0^2\sinh^2\beta a}{4E(V_0-E)}},$$

where use has been made of: $\cosh^2\beta a-\sinh^2\beta a=1$.

## 8.15.34 Finite Square Well Encore.

Consider the symmetric finite square well of depth $V_0$ and width $a$ , page 570 Course.

**a)** Let $k=\sqrt{\frac{2mV_0}{\hbar^2}}$. Sketch the bound states for the following choices of $\frac{ka}{2}$ :

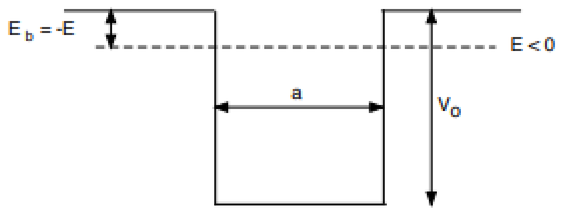
i) $\frac{ka}{2}=1$ , ii) $\frac{ka}{2}=1.6$ , iii) $\frac{ka}{2}=5$ .

Symmetric square potential well

$$V(x) = \begin{cases} -V_0 & -\frac{a}{2} \le x \le \frac{a}{2} \\ 0 & otherwise \end{cases} ,$$

where $V_0 > 0$ .

The issue of parity is discussed on the pages 572-574.
The finite symmetrical square well potential:




Even parity: $y = x \tan x$ , $x^2 + y^2 = r^2$.
*Pages 571-572, **Even Parity Results**:*

$$p \tan pa/2\hbar = \hbar k$$

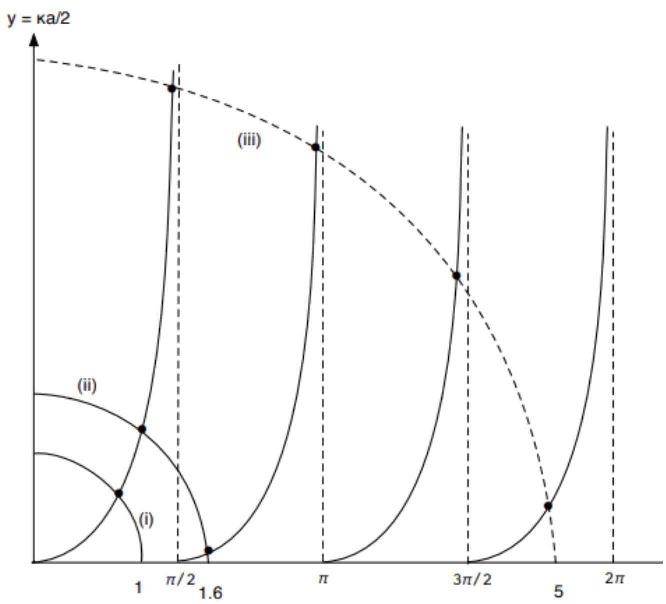
$p^2 = 2m(V_0 - |E|)$ *, and for* $|x| > \frac{a}{2}$, $k^2 = \frac{2m|E|}{\hbar^2}$
*See also Fitzpatrick page 77, Undergraduate Course.*

Odd parity: $y = -x \cot x$ , $x^2 + y^2 = r^2$.
With

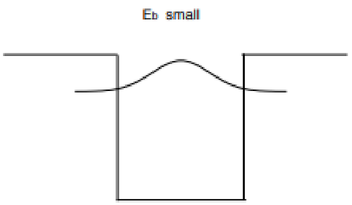
$y = \frac{\kappa a}{2}$ , $x = \frac{ka}{2}$,

$\kappa = \sqrt{\frac{2mE_b}{\hbar^2}}$ , $k = \sqrt{\frac{2m(V_0 - E_b)}{\hbar^2}}$,

and $x, y > 0$ , $r = \frac{k_0 a}{2} > 0$.
In the figure below the solutions for the three cases are shown

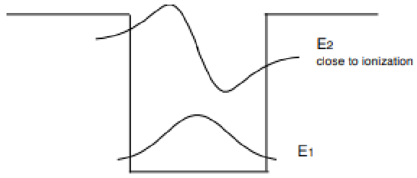



**Case i)** $\frac{ka}{2} = 1$.
We have one bound state with the following wave function:



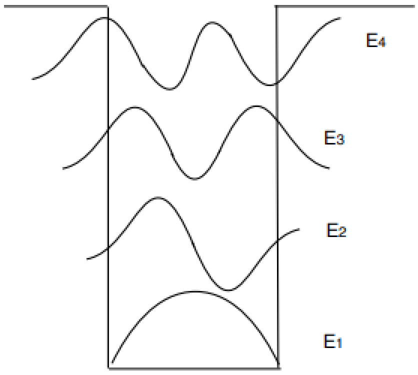

**Case ii)** $\frac{ka}{2} = 1.6$ .

We have two bound states with wave functions shown below:




**Case iii)** $\frac{ka}{2} = 5$ .

There are four bound states with wave functions shown below:




**b)** Show, no matter how shallow the well, there is at least one bound state of this potential. Describe it.

As the well becomes deeper and deeper, increasing $V_0$, there are more and more bound states. Inspecting the solutions on the foregoing page, with decreasing $\frac{ka}{2}$ and the well becomes more shallow, there is still one solution.

**c)** Let us re-derive the bound state energy for the delta function potential(see page 583) directly from the limit of the finite potential well. We use again the graphical solution discussed in the text. Take the limit as $a \to 0$ , $V_0 \to \infty$, but $aV_0$ to be a constant, say $U_0$. Show the binding energy to be $E_b = \frac{mU_0^2}{2\hbar^2}$ .

With the above information:

$$ka = \sqrt{\frac{2mV_0}{\hbar^2}}a = \sqrt{\frac{2m}{\hbar^2 V_0}} \cdot V_0 a = \sqrt{\frac{2m}{\hbar^2}} \cdot \frac{U_0}{\sqrt{V_0}} .$$

Hence

$$\lim_{V_0 \to \infty} ka = 0 ,$$

Consequently,

$$\lim_{V_0 \to \infty} \kappa a = 0.$$

Then, expand the tangent function for $a \to 0$

$$\frac{ka}{2}\tan\frac{ka}{2} = \frac{\kappa a}{2} \to \frac{(ka)^2}{4} = \frac{\kappa a}{2} \to \kappa = \frac{k^2 a}{2} = \frac{a}{2}\frac{2m(V_0 - E_b)}{\hbar^2} .$$

Then, with $aV_0 = U_0$

$\kappa = \frac{k^2 a}{2} = \frac{m(U_0 - aE_b)}{\hbar^2}$, using $a \to 0 \to \kappa = \frac{mU_0}{\hbar^2}$.

$\kappa = \sqrt{\frac{2mE_b}{\hbar^2}} \to \sqrt{\frac{2mE_b}{\hbar^2}} = \frac{mU_0}{\hbar^2} \to E_b = \frac{mU_0^2}{2\hbar^2}$.

The bound energy for the delta potential well with strength $U_0$.

**d)** Consider now the half-infinite well, half-finite potential well as shown in the figure below:

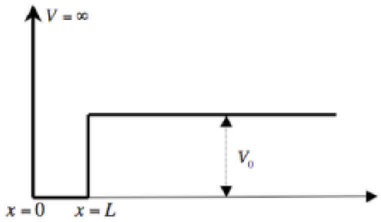



Figure 8.11: Half-Infinite, Half-Finite Well

Without doing any calculation, show that there are no bound states unless $kL > \frac{\pi}{2}$.

Think about erecting an infinite wall down the center of a symmetric finite well of width $a = 2L$. Also think about parity.

For the above potential we have

$\psi(0) = 0.$

The above "geometry" is equivalent to a symmetric square well of width $2L$ and $\psi(0) = 0$.

This implies odd-parity of the wave function.

As we learned, a), the odd-parity solution is

$-x \cot x.$

Then we know the preceding function to be positive for $x > \pi/2$.

Hence,

$\frac{ka}{2} > \pi/2 \to kL > \pi/2$ .

**e)** Show that in general, the binding energy eigenvalues satisfy the eigenvalue equation

$\kappa = -k \cot kL.$

For the potential well shown in Figure 8.11, we have for the eigenfunction:

$$\psi(x) \begin{cases} 0 & x < 0 \\ A_1 \sin(kx) & 0 < x < L \\ A_2 e^{-\kappa x} & x > a \end{cases}$$

where

$k^2 = \frac{2m(V_0 - E_b)}{\hbar^2}$, and $\kappa^2 = \frac{2mE_b}{\hbar^2}$.

Now, match the eigenfunction and its derivative at $x = L$:

$A_1 \sin ka = A_2 e^{-\kappa L}$,

$kA_1 \cos ka = -\kappa A_2 e^{-\kappa L}$.

Dividing the preceding two expressions:

$\tan ka = -\frac{k}{\kappa} \to \kappa = -k \cot kL$ .

### 8.15.35 Half-Infinite Half-Finite Square Well Encore

Consider the unbound case eigenstate of the potential below:

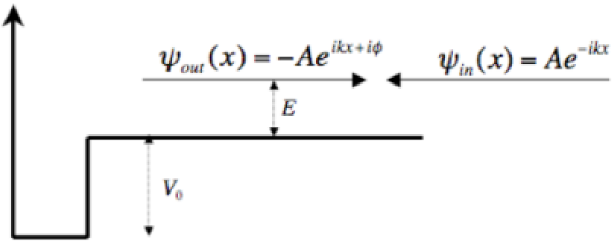



Figure 8.12: Half-Infinite, Half-Finite Well Again

We assume the "bottom" of the well to be at $-V_0$, and $E > 0$ . The width of the well is $L$.
First, some observations.
Consider a free particle $x > 0$ and an infinite potential wall at $x = 0$.
An incoming wave from the right and a reflected wave.
The general solution of the time independent Schrödinger's equation:

$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$ and $k^2 = \frac{2m}{\hbar^2}E \rightarrow$

$\rightarrow \psi(x) = Be^{ikx} + Ae^{-ikx}$.

At $x = 0 \rightarrow \psi(x) = 0 \rightarrow B = -A \rightarrow \psi(x) = 2Ae^{-i\pi/2}\sin(kx)$.
This illustrates the odd parity situation.
Next $V_0 < E$. Continuous states are analysed
$0 < x < L$ :
The time independent Schrödinger's equation:

$\frac{d^2\psi(x)}{dx^2} + p^2\psi(x) = 0$ and $p^2 = \frac{2m}{\hbar^2}(E_k + V_0)$.

Unlike the potentials with finite wall, the scattering in this case is reflection from the infinite wall potential. If we send a plane wave towards the potential, Figure 8.12 above,

$\psi_{in}(x) = Ae^{-ikx}$,

where the particle has energy $E = \frac{(\hbar k)^2}{2m}$,

the refelcted wave will emerge from the potential with a phase shift

$\psi_{out}(x) = -Ae^{ikx+\phi}$.

**a)** Calculate the phase shift.
The time independent Schrödinger equation:
for $0 < x < L$

$\frac{d^2\psi(x)}{dx^2} + q^2\psi(x) = 0$, and $q^2 = \frac{2m}{\hbar^2}(E + V_0) = k^2 + k_0^2$,

$E$ is the energy of the free particle.
We have odd parity:

$\psi(x) = C\sin(qx)$.

For $x > L$, the general solution is :

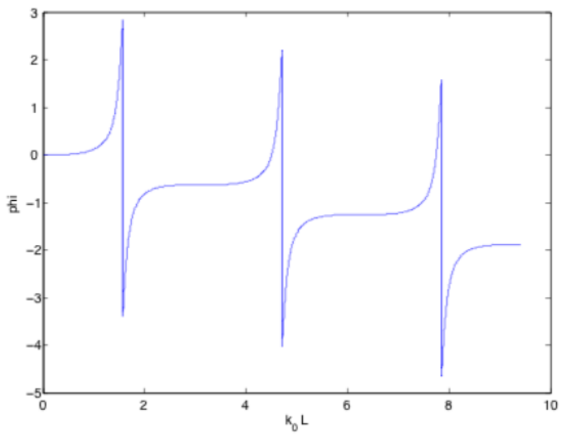
$\psi(x) = C_1\sin(kx) + C_2\cos(kx)$.

The preceding wave function is usually written:

$\psi(x) = D\sin(kx + \gamma)$

At $x = L$ the wave function and its derivative to be continuous:

$C\sin(qL) = D\sin(kL+\gamma)$,
$Cq\cos(qL) = Dk\cos(kL+\gamma)$.
Dividing both equations:
$\tan(qL) = \frac{q}{k}\tan(kL+\gamma)$.
Hence
$\phi = 2\gamma = 2\tan^{-1}\left[\frac{k}{q}\tan(qL)\right] - 2kL$ .
**b)** Plot the function of $\phi$ as a function of $k_0L \equiv \theta$ for fixed energy.
We introduce a number for the fixed energy
$\bar{k} = \frac{k}{k_0} = \sqrt{\frac{E}{V_0}}$, the fixed energy, dimensionless binding energy,
$\frac{k}{q} = \frac{k/k_0}{q/k_0} = \frac{\bar{k}}{\sqrt{\bar{k}^2+1}}$,
$qL = \frac{q}{k_0}k_0L = \sqrt{\bar{k}^2+1}\cdot\theta$,and
$kL = \frac{k}{k_0}k_0L = \bar{k}\theta$.
Hence,
$\phi = 2\tan^{-1}\left[\frac{\bar{k}}{\sqrt{\bar{k}^2+1}}\tan\left(\sqrt{\bar{k}^2+1}\cdot\theta\right)\right] - 2\,\bar{k}\theta$.
A plot is shown for $\bar{k} = 0.1$.
So,
$\phi \approx 2\tan^{-1}[0.1\tan(\theta)] - 0.2\,\theta$ .
The plot, Boccio,




We see sharp spikes near
$\theta = \frac{n\pi}{2} = k_0L$.
At these points $\phi$(phi) jumps $2\pi$. For each new bound states the phase jumps $2\pi$.
**c)** The phase shifted reflected wave is equivalent to that which would arise from a hard wall, but moved a distance $L'$ from the origin
$\frac{\phi}{k} = \frac{2}{k}\tan^{-1}\left[\frac{\bar{k}}{\sqrt{\bar{k}^2+1}}\tan\left(\sqrt{\bar{k}^2+1}\cdot\theta\right)\right] - 2L$ .
What is the effective $L'$ as a function of the phase shift $\phi$ induced by the semi-finite well?
With $\psi(x) = D\sin(kx+\gamma)$, see a), and the virtual potential wall at $x = L'$:
$D\sin(kL'+\gamma) = 0 \rightarrow L' = -\frac{\gamma}{k}$ or $L' = -\frac{\phi}{2k}$.

### 8.15.36 Nuclear $\alpha$ Decay

Nuclear alpha-decays $(A, Z) \to (A-2, Z-2) + \alpha$ have lifetimes ranging from nanoseconds (or shorter) to millions of years (or longer). This enormous range was understood by George Gamov by the exponential sensitivity to underlying parameters in tunneling phenomena. Consider $\alpha = \ {}^4He$ as a point particle in the potential given schematically in the figure below(Boccio)

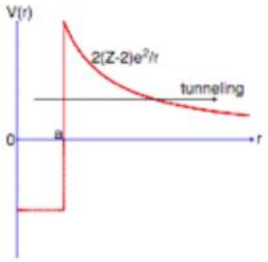



Figure 8.14: Nuclear Potential Model

The potential barrier is due to the Coulomb potential $2(Z-2)e^2/r$ . The probability of tunneling to the so-called Gamov's transmission coefficients in Problem 8.15.31(page 215)

$$T \approx \exp[-2 \int \sqrt{\frac{2m}{\hbar^2}} \cdot \sqrt{V(x) - E}\,dx] \to \exp\,[-\frac{2}{\hbar}\int_a^b \sqrt{2m(V(x)-E)}\,dx],$$

where $a$ and $b$ are the classical turning points: $E = V(x)$. Work out numerically $T$ for the following parameters: $Z = 92$ (Uranium), size of nucleus $a = 5$ fm and the kinetic energy of the $\alpha$ particle 1 MeV, 3 MeV, 10 MeV and 30 MeV.

Below I copy the Matematica code of Bocci

We compute the integral

```
V = 2 (Z - 2) q^2 / r; tp = 2 (Z - 2) q^2 / E0 ;
Tint[r_] = Integrate[Sqrt[2 m (V - E0)], r]
```

$$\sqrt{2}\left(r\sqrt{m\left(-E0+\frac{2q^2(-2+Z)}{r}\right)} - \frac{2q^2\sqrt{r}\sqrt{m\left(-E0+\frac{2q^2(-2+Z)}{r}\right)}(-2+Z)\,\mathrm{Log}\left[2\sqrt{E0}\sqrt{r}+2\sqrt{4q^2+E0\,r-2q^2 Z}\right]}{\sqrt{E0}\sqrt{4q^2+E0\,r-2q^2 Z}}\right)$$

to give the turning points and probabilities

```
ergtomev = 624150.97;
constants = {m -> 3727.37917 / (2.99792458 * 10^10)^2,
   ħ -> 6.58211915 * 10^-22, Z -> 92, a -> 5 * 10^-13, q -> 4.802 * 10^-10 * Sqrt[ergtomev]};
energies = {1, 3, 10, 30};
T = Exp[- 2/ħ (Tint[b] - Tint[a])];
(tp /. E0 -> energies /. constants) * .01
(T /. b -> tp - $MachineEpsilon) /. E0 -> energies /. constants // Re
```

```
{2.59064×10^-13, 8.63545×10^-14, 2.59064×10^-14, 8.63545×10^-15}
```

```
{4.08218×10^-128, 6.29166×10^-63, 3.4855×10^-23, 0.000152428}
```

Mathematica note: The integral blows up at the classical turning point $b$, so this must be handled numerically. In the above computation we take $b \to b - \epsilon$, where *epsilon* is the *MachineEpsilon*, or the upper bound of positive numbers $\delta$ for which $1.0 + \delta = 1.0$ on one's computer.

So, to solve the above problem numerical methods have been used.
Still, approximate methods are useful(Mahan). With iterative numerical methods an approximate solution is useful for making the numerical method efficient.
Then, in this case we have a 3-D problem with a Coulomb potential.
Hence, with a central potential in 3-D, the effective potential is:
$V_l(r) = \frac{2(Z-2)e^2}{r} + \frac{\hbar^2}{2mr^2} l(l+1)$, see also page 655 Eq.(8.700),
the second term in the above expression for the potential is the centrifugal barrier.
The differential equation for the radial part of the wave function is:
$\left\{\frac{d^2}{dr^2} - \frac{2m}{\hbar^2}[V_l(r) - E]\right\}\chi(r)$ .
$\chi(r) = rR(r)$,
where $R(r)$ is the radial part of the wave function. The angular parts are the spherical harmonic parts, translated into the centrifugal barrier. The expression $\frac{2m}{\hbar^2}[V_l(r) - E]$ plays a key role in approximate methods.
The above differential equation can be solved with approximate methods, very similar to the approximation for the Hydrogen Atom, page 655 Undergraduate Course.

### 8.15.37 One Particle, Two Boxes

Consider two boxes in 1-dimension of width $a$, with infinite high walls, separated by a distance $L = 2a$.

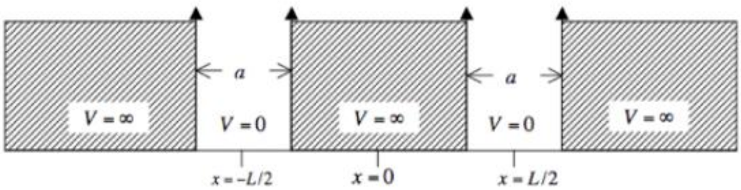



Figure 8.15: Two Boxes

A particle experiences the above potential and its state is described by a wave function.
The energy eigenfunctions are doubly degenerate, $\left\{\phi_n^{(+)}, \phi_n^{(-)} \middle| n = 1,2,3,4,..\right\} \to$
$\to \phi_n^{(\pm)} = u_n\left(x \pm \frac{L}{2}\right)$.
The eigen functions of a particle in a box:

$$u_n(x) = \begin{cases} \left\{\sqrt{\frac{2}{a}}\cos(\frac{n\pi x}{a}), n = 1,3,5, \ldots - a/2 < x < a/2 \right. \\ \left\{\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right), n = 2,4,6, \ldots - a/2 < x < a/2 \right. \\ 0 \qquad\qquad\qquad\qquad |x| > a/2 \end{cases}$$

The eigenvalues
$E_n^{(+)} = E_n^{(-)} = n^2 \frac{\pi^2\hbar^2}{2ma^2}$ .

Suppose at time $t = 0$, the wave function is

$\psi(x) = \frac{1}{2}\phi_1^{(-)} + \frac{1}{2}\phi_2^{(-)} + \frac{1}{\sqrt{2}}\phi_1^{(+)}$ ,

the wave function $\psi(x)$ is normalized.

**a)** What is the probability of finding the particle in the state $\phi_1^{(+)}$?

The probability of finding the particle in the state $\phi_1^{(+)}$?

$P_{1+} = |\left\langle\phi_1^{(+)}\middle|\psi(x)\right\rangle|^2 = \frac{1}{2}$.

**b)** What is the probability of finding the particle with energy $\frac{\pi^2\hbar^2}{2ma^2}$ ?

The probability to find energy $\frac{\pi^2\hbar^2}{2ma^2}$ is the probability to find the eigenvalues $E_1^{(+)} = E_1^{(-)}$.

So,

$P_{1+} = |\left\langle\phi_1^{(+)}\middle|\psi(x)\right\rangle|^2 = \frac{1}{2}$,

and

$P_{1-} = |\left\langle\phi_1^{(-)}\middle|\psi(x)\right\rangle|^2 = \frac{1}{4}$.

The probability of finding $\frac{\pi^2\hbar^2}{2ma^2}$ :

$P_{1+} + P_{1-} = \frac{3}{4}$.

We added the probabilities: The two boxes are “independent”.

**c)** CLAIM: At time $t = 0$, there is a 50-50 chance for finding the particle in either box. Is the claim justified?

We can expand $\psi(x)$ into the eigenfunctions:

$\psi(x) = \sum_n c_n^+ \phi_n^{(+)} + \sum_n c_n^- \phi_n^{(-)}$.

The probability to be in the left well $(+)$:

$P_{left} = \sum_n |c_n^+|^2 = (\frac{1}{\sqrt{2}})^2 = \frac{1}{2}$.

The probability to be in the right well $(-)$:

$P_{right} = \sum_n |c_n^-|^2 = (\frac{1}{2})^2 + (\frac{1}{2})^2 = \frac{1}{2}$.

Hence there is a 50% chance to be in the left well or in the right well.

**d)** What is the state at a later time assuming no measurements are done?

With time development operator

$\psi(x,t) = \left[\frac{1}{2}\phi_1^{(-)} + \frac{1}{\sqrt{2}}\phi_1^{(+)}\right] e^{-\frac{iE_1 t}{\hbar}} + \frac{1}{2}\phi_2^{(-)} e^{-\frac{iE_2 t}{\hbar}}$ .

**e)** Now let us generalize. Suppose we have an arbitrary wave function at $t = 0, \psi(x,0)$, that satisfies all the boundary conditions.

Show that, in general, the probability to find the particle in the left box does not change with time.

The explanation: we have to boxes. When a particle is in the left box at time $t = 0$, it will stay in that box.

The probability for being in the left box

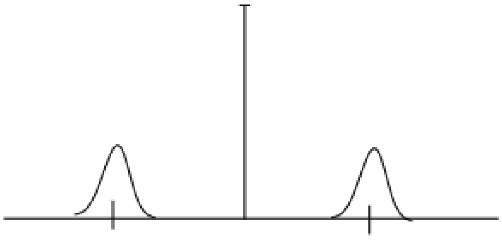
$P_{left} = \sum_n |\left\langle\phi_n^{(+)}\middle|\psi(x,t)\right\rangle|^2 \rightarrow$

$\rightarrow \sum_n | \left\langle\phi_n^{(+)}\middle| \sum_k c_k^+ e^{-\frac{iE_k t}{\hbar}} | \phi_k^{(+)}\right\rangle |^2 \sum_n | \left\langle\phi_n^{(+)}\middle| \sum_k c_k^- e^{-\frac{iE_k t}{\hbar}} | \phi_k^{(-)}\right\rangle |^2 = \sum_n |c_n^+|^2.$

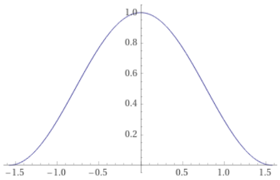
No time dependency.

**f)** Show that the state $\Phi_n(x) = c_1\phi_n^{(+)} + c_2\phi_n^{(-)}$ is a stationary state.
$c_1$ and $c_2$ are complex numbers.
The question to be answered is: is $\Phi_n(x)$ an eigenstate of the Hamiltonian $\widehat{H}$?
$\widehat{H}\Phi_n(x) = c_1\widehat{H}\phi_n^{(+)} + c_2\widehat{H}\phi_n^{(-)} = c_1E_n^{(+)}\phi_n^{(+)} + c_2E_n^{(-)}\phi_n^{(-)}$.
With $E_n^{(+)} = E_n^{(-)} = E_n$
$\widehat{H}\Phi_n(x) = E_n\left(c_1\phi_n^{(+)} + c_2\phi_n^{(-)}\right) = E_n\Phi_n(x)$.

**g)** Next, consider the state described by the wave function
$\psi(x) = (\phi_1^{(+)} + \phi_1^{(-)})/\sqrt{2}$ , normalized.
The probability density in $x$:
The probability density, $|\psi(x)|^2$ is symmetrical distributed. So, we have something like(Boccio):




Note: below a plot of $\cos^2 x$, with WolframAlpha,




The expectation value or mean value $\langle x \rangle$:
for the two independent boxes we expect $\langle x \rangle = 0$ .
To calculate $\langle x \rangle$, we have to evaluate the sum of the following two integrals:

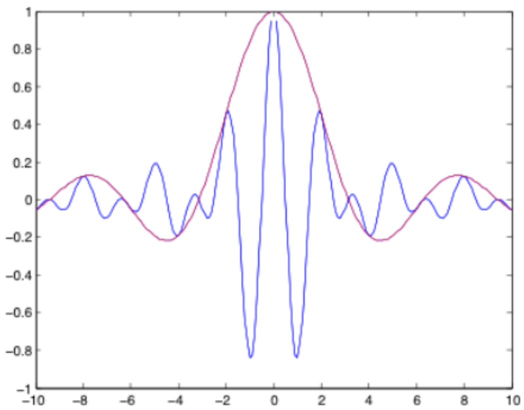
$$\int_{-\frac{L}{2}-\frac{a}{2}}^{-\frac{L}{2}+\frac{a}{2}} x\cos^2\left[\frac{\pi\left(x+\frac{L}{2}\right)}{a}\right]dx + \int_{\frac{L}{2}-\frac{a}{2}}^{\frac{L}{2}+\frac{a}{2}} x\cos^2\left[\frac{\pi\left(x-\frac{L}{2}\right)}{a}\right]dx =$$

$$\int_{-\frac{a}{2}}^{\frac{a}{2}}(y-\tfrac{L}{2})\cos^2\left[\frac{\pi y}{a}\right]dy + \int_{-\frac{a}{2}}^{\frac{a}{2}}(y+\tfrac{L}{2})\cos^2\left[\frac{\pi y}{a}\right]dy = 2\int_{-\frac{a}{2}}^{\frac{a}{2}} y\cos^2\left[\frac{\pi y}{a}\right]dy = 0.$$

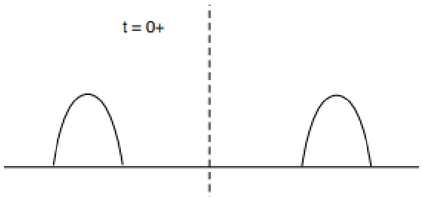
**h)** Show that the momentum space wave function is
$\tilde{\psi}(p) = \sqrt{2}\cos\left(\frac{pL}{2\hbar}\right)\tilde{u}_1(p)$,
where
$\tilde{u}_1(p) = \int_{-\infty}^{\infty} u_1(x)e^{-ipx/\hbar}dx$ ,
is the momentum-space function of $u_1(x)$ .
With $\psi(x) = [\phi_1^{(+)}(x) + \phi_1^{(-)}(x)]/\sqrt{2} \rightarrow$
$\rightarrow \tilde{\psi}(p) = \frac{1}{\sqrt{2}}[\phi_1^{(+)}(p) + \phi_1^{(-)}(p)]$.
We have
$\phi_n^{(\pm)} = u_n\left(x \pm \frac{L}{2}\right)$.

So,
$\tilde{u}_1(p) = e^{\pm ipL/(2\hbar)} \int_{-\infty}^{\infty} u_1\,(x \pm \frac{L}{2}) e^{-ipx/\hbar} dx$ .
Since there is always phase ambiguity, we can write
$\phi_n^{(\pm)}(p) = e^{\pm ipL/(2\hbar)}\, \tilde{u}_n(p)$.
With $\tilde{\psi}(p) = \frac{1}{\sqrt{2}}[\phi_1^{(+)}(p) + \phi_1^{(-)}(p)]$
$\tilde{\psi}(p) = \frac{1}{\sqrt{2}}\left[e^{\frac{ipL}{2\hbar}}\, \tilde{u}_1(p) + e^{-\frac{ipL}{2\hbar}}\, \tilde{u}_1(p)\right] = \sqrt{2}\cos\left(\frac{pL}{2\hbar}\right) \tilde{u}_1(p)$.
**i)** Without calculation, what is $\langle p \rangle$ ?
We have $u(x) \propto \cos x$ .
Then $\tilde{u}(p)$ is the Fourier transform of (Boccio)

Boccio presented a picture of the curves for $\tilde{u}_1(p)$, the red curve, and for $\tilde{\psi}(p)$, the blue curve:




We have $\langle p \rangle$, since $\tilde{\psi}(p)$ is symmetric around the origin.
**j)** Suppose the potential energy was somehow turned off, so the particle is free.
Without doing any calculation, sketch how you expect the position-space wave function to evolve at later times.
Suppose $V(x) \to 0$ instantaneously. Right after the potential is turned off, $\psi(x)$ is in the same state as just before turning of the potential energy:




Then, at $t = 0+$, the two wave packets shown above will spread. Eventually, the wave packets will overlap and interference will occur. Illustrated in the Figure under **i)**.
This picture resembles Figure 8.23 page 636, Undergraduate Course: the two-slit problem.

8.15.38 A half-infinite/half-leaky box

Consider a one dimensional potential

$$V(x) = \begin{cases} \infty & x < 0 \\ U_0\delta(x-a) & x > 0 \end{cases}$$

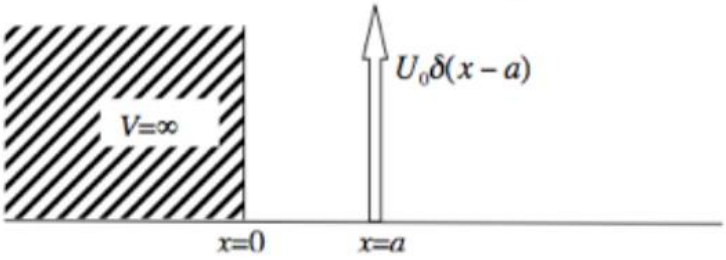



Figure 8.16: Infinite Wall + Delta Function

**a)** Show that the stationary states with energy E can be written as

$$u(x)\begin{cases} 0 & x < 0 \\ A\frac{\sin[ka+\phi(k)]}{\sin\,(ka)}\sin kx & 0 < x < a \\ A\sin[kx+\phi(k)] & x > a \end{cases}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}\ ,\quad \phi(k) = \tan^{-1}[\frac{k\tan(ka)}{k-\gamma_0\tan(ka)}]\quad ,\quad \gamma_0 = \frac{2mU_0}{\hbar^2}\ .$$

Solutions to the time independent Schrödinger equation $\hat{H}u = Eu$,

$\frac{d^2u}{dx^2} = -\frac{2m}{\hbar^2}[E - V(x)]u(x)$,

- $x < 0 \rightarrow u(x) = 0$ , since $V = \infty$ .
- $x > a \rightarrow u(x) = A\sin(kx+\phi)$, the general solution for a free particle.
- $0 < x < a \rightarrow u(x) = B\sin(kx)$ , odd parity .

Three unknowns: $A, B$ and $\phi$. The boundary conditions at $x = a$:

- $u$ is continuous$\rightarrow B\sin(ka) = A\sin(ka+\phi) \rightarrow B = A\frac{\sin(ka+\phi)}{\sin(ka)}$,
- $\frac{du}{dx}$ is discontinuous. Integration of the time independent Schrödinger equation over a small interval $2\varepsilon \rightarrow \int_{a-\varepsilon}^{a+\varepsilon}\frac{d^2u}{dx^2}dx = (\frac{du}{dx})_{a+\varepsilon} - \left(\frac{du}{dx}\right)_{a-\varepsilon} = -\frac{2m}{\hbar^2}\int_{a-\varepsilon}^{a+\varepsilon}[E - V(x)]u(x)dx \rightarrow$

$\rightarrow -\frac{2m}{\hbar^2}Eu(x)|_{a-\varepsilon}^{a+\varepsilon} + \frac{2m}{\hbar^2}\int_{a-\varepsilon}^{a+\varepsilon}U_0\delta(x-a)u(x)dx = 0 + \frac{2mU_0}{\hbar^2}u(a) = \gamma_0 u(a).$

So,

$$\left(\frac{du}{dx}\right)_{a+\varepsilon} - \left(\frac{du}{dx}\right)_{a-\varepsilon} = \gamma_0 u(a).$$

With $\varepsilon \rightarrow 0$:

$(\frac{du}{dx})_{a+\varepsilon} \rightarrow Ak\cos(ka+\phi)$,

$\left(\frac{du}{dx}\right)_{a-\varepsilon} = Bk\cos(ka) = Ak\frac{\sin(ka+\phi)}{\tan(ka)}$ .

Hence,

$$Ak\cos(ka+\phi) - Ak\frac{\sin(ka+\phi)}{\tan(ka)} = \gamma_0 A\sin(ka+\phi) \rightarrow k - k\frac{\tan(ka+\phi)}{\tan(ka)} = \gamma_0\tan(ka+\phi).$$

Then,

$$\tan(ka+\phi)\left[\gamma_0 + \frac{k}{\tan(ka)}\right] = k \rightarrow \tan(ka+\phi) = \frac{k}{\gamma_0+\frac{k}{\tan(ka)}} = \frac{k\tan(ka)}{k+\gamma_0\tan(ka)} \rightarrow$$

$\rightarrow \phi = \tan^{-1}\left[\frac{k\tan(ka)}{k+\gamma_0\tan(ka)}\right] - ka.$

Since we have $u(x) = A\sin(kx+\phi)$ for $x > a$ there are just unbound states.

The question is

$\phi(k) = \tan^{-1}\left[\frac{k\tan(ka)}{k-\gamma_0\tan(ka)}\right] - ka?$

Well, the answer I found is related with a delta function potential barrier, where $\phi(k)$ is related with a delta function potential well.

For a potential well we have:

$\left(\frac{du}{dx}\right)_{a+\varepsilon} - \left(\frac{du}{dx}\right)_{a-\varepsilon} = -\gamma_0 u(a).$

**b)** Show that the limits $\gamma_0 \rightarrow 0$, and $\gamma_0 \rightarrow 0$ give reasonable solutions.

- $\gamma_0 \rightarrow 0 \rightarrow \ \phi = \tan^{-1}\left[\frac{k\tan(ka)}{k}\right] - ka = ka - ka = 0 \rightarrow B = A$, and

$u(x) = A\sin(kx)$, a free particle and odd parity.

- $\gamma_0 \rightarrow \infty \rightarrow \ \phi = \tan^{-1}\left[\frac{k\tan(ka)}{\gamma_0}\right] - ka = 0 - ka = -ka.$

$B = A\frac{\sin(ka+\phi)}{\sin(ka)} \rightarrow B = 0 \rightarrow u(x) = 0$ for $0 < x < a$.

$x > a \rightarrow u(x) = A\sin[k(x-a)].$

**c)** Sketch the energy eigenfunction when $ka = \pi$ . Explain this solution.

When $ka = \pi$ , $\tan(ka) = 0 \rightarrow \ \phi = -ka = -\pi$

$u(x) = A\frac{\sin[ka+\phi]}{\sin(ka)}\sin kx$ , $0 < x < a$ ,

and

$u(x) = A\sin[kx+\phi]$ , $x > a.$

So, at $x = a$, $u(x) = 0$.

Then, we could conclude for $0 < x < a$, $u(x)$ appears to be a bound state.

Note:

$u(x) = A\frac{\sin[ka+\phi]}{\sin(ka)}\sin kx \rightarrow u(x) = A\frac{\sin 0}{\sin\pi}\sin kx$, with l'Hopital Rule, $u(x) = A\sin kx$.

**d)** Sketch the energy eigenfunction when $ka = \frac{\pi}{2}$ . How does the probability to find the particle in the region $0 < x < a$, compare with that found in part c)?

$ka = \frac{\pi}{2}$

$\phi = \tan^{-1}\left[\frac{k\tan(ka)}{k+\gamma_0\tan(ka)}\right] - ka \rightarrow \phi = \tan^{-1}\left[\frac{k\tan\pi/2}{k+\gamma_0\tan\pi/2}\right] - \frac{\pi}{2} = \tan^{-1}\left[\frac{k}{\frac{k}{\tan\pi/2}+\gamma_0}\right] - \frac{\pi}{2} =$

$= \tan^{-1}\left[\frac{k}{\gamma_0}\right] - \frac{\pi}{2}.$

Then, with $\frac{\pi}{2} = ka$

$\frac{\sin[ka+\phi(k)]}{\sin(ka)} = \sin\{\tan^{-1}(\frac{k}{\gamma_0})\} < 1.$

Under c) we found the wave function to be $u(x) = A\sin kx$ .

Here we have $u(x) = A\frac{\sin[ka+\phi]}{\sin(ka)}\sin kx.$

So, the amplitude of the preceding wave function is smaller than the amplitude obtained under c).

**e)** In a scattering scenario, we imagine sending an incident plane wave which is reflected with unit probability, but phase shifted according to the conventions shown in the figure below:

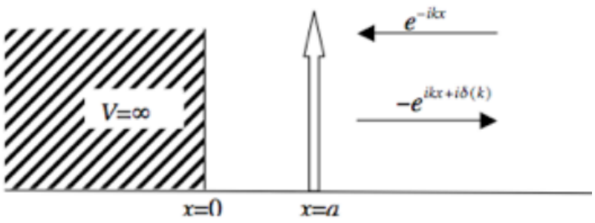



Figure 8.17: Scattering Scenario

Show that the phase shift of the scattered wave is $\beta(k) = 2\,\phi$.
There exist mathematical conditions such that the so-called S[13]-matrix element $e^{i\beta}$ blows up. For these solutions is $k$ real, imaginary, or complex?
The wave function for $x > a$ :

$$u(x) = A\sin[kx + \phi] = A\frac{e^{(kx+\phi)} - e^{-i(kx+\phi)}}{2i} = -A\frac{e^{-i\phi}}{2i}(e^{-ikx} - e^{ikx+2i\phi}).$$

So, $\beta = 2\phi$ is the scattering phase shift. The S-matrix $\rightarrow \infty$ for the quasi bound state, $\phi = -ka = -\pi(?)$. When, for this case $k$ is complex$\rightarrow \phi \neq \pi$.

### 8.15.39 Neutrino Oscillations Redux

Read the article T. Araki, et al, "*Measurement of Neutrino Oscillations with Kam LAND: Evidence of Spectral Distortion,"* Phys. Rev. Lett. 94, 081801 (2005), which shows the neutrino oscillation, a quantum phenomenon demonstrated at the large distance scale yet (about 180 km).

**a)** The Hamiltonian for an ultra-relativistic particle is approximated by

$$H = \sqrt{p^2c^2 + m^2c^4} \approx pc + \frac{m^2c^3}{2p},$$

for $p = |\vec{p}|$.
Suppose in a basis of two states, $m^2$ is given as a $2 \times 2$ matrix

$$m^2 = m_0^2 I + \frac{\Delta m^2}{2}\begin{pmatrix} -\cos 2\theta & \sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{pmatrix}.$$

Write down the eigenstates of $m^2$.
The normalized eigenvalue/eigenvector pairs. We analyse:

$$\begin{pmatrix} -\cos 2\theta & \sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \lambda\begin{pmatrix} a \\ b \end{pmatrix}.$$

Resulting into two expressions:

$$\frac{b}{a} = \frac{\lambda\sin 2\theta}{1 - \lambda\cos 2\theta},$$

and

$$\frac{b}{a} = \frac{1 + \lambda\cos 2\theta}{\lambda\sin 2\theta}.$$

From the two preceding equations follows

$$\lambda = \pm 1.$$

For these values of $\lambda$:

[13] The Scatter Matrix. Dealt with in the Graduate Course?

$\lambda = 1 \rightarrow \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix}$,

$\lambda = -1 \rightarrow \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} -\cos\theta \\ \sin\theta \end{pmatrix}$.

Resulting into the eigenvalues/eigenvectors

$\lambda_+ = m_0^2 + \frac{\Delta m^2}{2}, |\nu_+\rangle = \begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix}$,

$\lambda_- = m_0^2 - \frac{\Delta m^2}{2}, |\nu_-\rangle = \begin{pmatrix} -\cos\theta \\ \sin\theta \end{pmatrix}$.

Note:

$$\begin{vmatrix} m_0^2 - \frac{\Delta m^2}{2}\cos 2\theta - \lambda & \frac{\Delta m^2}{2}\sin 2\theta \\ \frac{\Delta m^2}{2}\sin 2\theta & m_0^2 + \frac{\Delta m^2}{2}\cos 2\theta - \lambda \end{vmatrix} = 0 \rightarrow$$

$$\rightarrow \left(m_0^2 - \lambda - \frac{\Delta m^2}{2}\cos 2\theta\right)\left(m_0^2 - \lambda + \frac{\Delta m^2}{2}\cos 2\theta\right) - \frac{\Delta m^4}{4}\sin^2 2\theta = 0 \rightarrow$$

$$\rightarrow (m_0^2 - \lambda)^2 - \frac{\Delta m^4}{4}(\cos^2 2\theta + \sin^2 2\theta) = 0 \rightarrow$$

$$\lambda_\pm = m_0^2 \pm \frac{\Delta m^2}{2}.$$

**b)** Calculate the probability for the state

$|\psi\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

to be still found in the same state after time interval $t$ for definite momentum $p$.

The probability to measure

$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$,

at time $t$ is $|\langle\psi(0)|\psi(t)\rangle|^2$,

where

$|\psi(t)\rangle = e^{-iEt/\hbar}|\psi(0)\rangle$.

Next, express $|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ into the eigenvectors:

$$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = c_1|\nu_+\rangle + c_2|\nu_-\rangle = c_1\begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix} + c_2\begin{pmatrix} -\cos\theta \\ \sin\theta \end{pmatrix}.$$

Equating the components of the column vectors results into:

$c_1 = \sin\theta$, and $c_2 = -\cos\theta$.

Using the eigenvalues

$$|\psi(t)\rangle = \sin\theta\,|\nu_+\rangle e^{-iE_+t/\hbar} - \cos\theta\,|\nu_-\rangle e^{-iE_-t/\hbar},$$

where

$$E_\pm = pc + \frac{c^3}{2p}\lambda_\pm = pc + \frac{c^3}{2p}\left(m_0^2 \pm \frac{\Delta m^2}{2}\right).$$

The probability

$$|\langle\psi(0)|\psi(t)\rangle|^2 = |(\langle\nu_+|\sin\theta - \langle\nu_-|\cos\theta)|(\sin\theta\,|\nu_+\rangle e^{-iE_+t/\hbar} - \cos\theta\,|\nu_-\rangle e^{-iE_-t/\hbar})|^2.$$

Using orthogonality of the eigenvectors:

$$|\langle\psi(0)|\psi(t)\rangle|^2 = |e^{-\frac{iE_+t}{\hbar}}\sin^2\theta + e^{-\frac{iE_-t}{\hbar}}\cos^2\theta\,|^2 =$$

$$= \sin^4\theta + \cos^4\theta + e^{\frac{i(E_+-E_-)t}{\hbar}}\sin^2\theta\cos^2\theta + e^{-\frac{i(E_+-E_-)t}{\hbar}}\sin^2\theta\cos^2\theta =$$

$$= \sin^4\theta + \cos^4\theta + \frac{1}{2}\sin^2 2\theta\cos\frac{(E_+-E_-)t}{\hbar} = 1 - \frac{1}{2}\sin^2 2\theta + \frac{1}{2}\sin^2 2\theta\cos\frac{(E_+-E_-)t}{\hbar} =$$

$$= 1 - \frac{1}{2}\sin^2 2\theta + \frac{1}{2}\sin^2 2\theta\cos 2\frac{(E_+-E_-)t}{2\hbar} = 1 - \frac{1}{2}\sin^2 2\theta + \frac{1}{2}\sin^2 2\theta\left(1 - 2\sin^2\frac{(E_+-E_-)t}{2\hbar}\right),$$

use has been made of

$$\sin^4\theta + \cos^4\theta = (\sin^2\theta + \cos^2\theta)^2 - 2\sin^2\theta\cos^2\theta = 1 - \frac{1}{2}\sin^2 2\theta \ .$$

Hence,

$$|\langle\psi(0)|\psi(t)\rangle|^2 = 1 - \sin^2 2\theta \sin^2\frac{(E_+ - E_-)t}{2\hbar} = 1 - \sin^2 2\theta \sin^2\left(\frac{\Delta m^2 c^4}{4\hbar c}\frac{t}{p}\right).$$

**c)** Using data shown in Figure 3 of the article, estimate approximately values of $\Delta m^2$ and $\sin^2 2\theta$. Furthermore, $p \cong E/c$ .

$1 - \sin^2 2\theta \sin^2\left(\frac{\Delta m^2 c^4}{4\hbar c}\frac{t}{p}\right)$ is plotted below (Boccio)

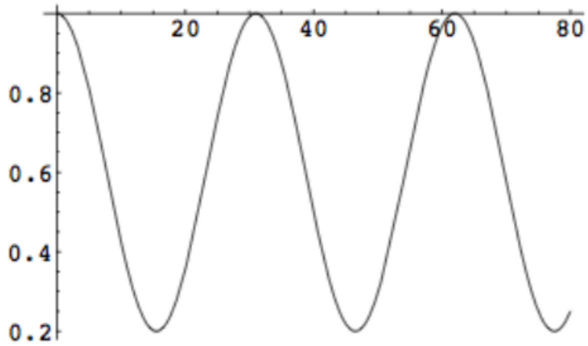



Figure 3 in the paper shows a peak-to-peak wavelength of a bit over $30\,km/MeV$, which is reproduced nicely here with the value of $\Delta m^2 = 8\times 10^{-5}\,eV^2$ quoted in the paper. This is not surprising, as their quoted error is only $\pm 0.5\times 10^{-5}\,eV^2$.

The amplitude and center of oscillation are more problematic, as this is entirely dependent on $\theta$. the authors quote a range of $0.33 < \tan^2\theta < 0.5$, which corresponds to $0.75 < \sin^2\theta < 0.9$; however, this is after including data from solar neutrinos, which puts stong constraints on $\theta$ as shown in Figure 4(a). Looking at the 95% confidence range for just KamLAND, $0.1 < \tan^2\theta < 5$, or $0.33 < \sin^2\theta < 0.56$ passing through $\sin^2 = 1$. Examining Figure 3, the peak and through are at roughly 1.0 and 0.2 respectively, and this is reproduced above with the quoted value of $\sin^2\theta 0.8$ ($\tan^2\theta = 0.4$).

## 8.15.40 Is it the ground state

An infinitely one-dimensional potential well $0 < x < a$ .

The normalized energy eigenstates are:

$$u_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} \ , n = 1,2,3, \ldots$$

A particle is placed in the left-hand half of the well so that its wave function $\psi$ is constant for $x < \frac{a}{2}$ . Meaning: the particle can be anywhere in the interval $0 < \mathrm{x} < \frac{\mathrm{a}}{2}$ . Consequently, the probability density distribution is homogeneous in the interval $0 < \mathrm{x} < \frac{\mathrm{a}}{2}$ .

So,

$$P = \int_0^{a/2}|\psi|^2 dx = 1 \to \psi = \sqrt{\frac{2}{a}} .$$

If the energy of the particle is now measured, what is the probability of finding it in the ground state?

The wavefunction

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{a}} & 0 < \mathrm{x} < \frac{\mathrm{a}}{2} \\ 0 & otherwise \end{cases}.$$

Note: $\psi(x)$ is a constant. What about the boundary condition at $x = 0$? Do we have a hat function here? I assume $\psi(x)$ can be expressed in the eigenstates. So it looks like the Fourier transform of the hat function.

The probability of finding the particle in the ground state, $n = 1$, in the interval $0 < \mathrm{x} < \frac{\mathrm{a}}{2}$.
Expand $\psi(x)$ in terms of the eigenstates:

$$\psi(x) = \sqrt{\frac{2}{a}} \sum_n c_n \sin\frac{n\pi x}{a}.$$

The probability to find the particle in the state $n$ is:

$$P_n = |c_n|^2 = |\langle\psi(x)|u_n\rangle|^2 = |\int_0^{a/2} \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} dx\,|^2.$$

With $n = 1$

$$P_1 = |\frac{2}{a}\frac{a}{\pi}\int_0^{\pi/2} \sin\alpha\, d\alpha|^2 = \frac{4}{\pi^2}.$$

### 8.15.41 Some Thoughts of T- Violation

Any Hamiltonian can be recast to the form

$$H = U\begin{pmatrix} E_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & E_n \end{pmatrix} U^\dagger,$$

where $U$ is a general $n \times n$ unitary matrix.

$$H = UHU^\dagger \longrightarrow H^\dagger = (UHU^\dagger)^\dagger \longrightarrow H = U^{\dagger\dagger}(UH)^\dagger = UHU^\dagger.$$

**a)** Show that the time evolution operator is given by

$$e^{-iHt/\hbar} = U\begin{pmatrix} e^{-iE_1t/\hbar} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{-iE_nt/\hbar} \end{pmatrix} U^\dagger.$$

The time evolution operator can be expanded into

$$e^{-iHt/\hbar} = \sum_k \frac{(-it/\hbar)^k}{k!} H^k = \sum_k \frac{(-it/\hbar)^k}{k!} (UEU^\dagger)^k,$$

where $E$ is the diagonal matrix element of the Hamiltonian eigenvalues $E_n$ given in the above matrices.

Using

$$UEU^\dagger UEU^\dagger = UE^2U^\dagger,$$

$$e^{-iHt/\hbar} = U\sum_k \frac{(-it/\hbar)^k}{k!} (E)^k U^\dagger = Ue^{-iEt/\hbar}U^\dagger.$$

Now, using matrix multiplication, we obtain

$$e^{-iHt/\hbar} = U\begin{pmatrix} e^{-iE_1t/\hbar} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{-iE_nt/\hbar} \end{pmatrix} U^\dagger.$$

**b)** For a two-state problem, the most general unitary matrix is

$$U = e^{i\theta}\begin{pmatrix} e^{i\phi}\cos\theta & -e^{i\eta}\sin\theta \\ e^{-i\eta}\sin\theta & e^{-i\phi}\cos\theta \end{pmatrix}.$$

Work out the probabilities $P(1 \to 2)$ and $P(2 \to 1)$ over time interval $t$ and verify that they are the same despite the apparent T-violation due to complex phases.
NOTE: This is the same problem as the neutrino oscillation (problem 8.15.39) if you set $E_i = \sqrt{p^2c^2 + m^2c^4} \approx pc + \frac{m^2c^3}{2p}$, and set all phases to zero.
The probabilities are:

$$P(1 \to 2) = |\langle 2|e^{-iHt/\hbar}|1\rangle|^2 = |\langle 2|Ue^{-iEt/\hbar}U^\dagger|1\rangle|^2 ,$$
$$P(2 \to 1) = |\langle 1|e^{-iHt/\hbar}|2\rangle|^2 = |\langle 1|Ue^{-iEt/\hbar}U^\dagger|2\rangle|^2 .$$

There will be no T-violation when

$$P(1 \to 2) - P(2 \to 1) = 0.$$

With $|1\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, and $|2\rangle = \begin{pmatrix}0\\1\end{pmatrix}$
we need to evaluate

$$(0 \quad 1)\, Ue^{-iEt/\hbar}U^\dagger \begin{pmatrix}1\\0\end{pmatrix},$$

and

$$(1 \quad 0)\, Ue^{-iEt/\hbar}U^\dagger \begin{pmatrix}0\\1\end{pmatrix}.$$

For convenience we write with $n = 2$

$$U\begin{pmatrix} e^{-iE_1t/\hbar} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{-iE_nt/\hbar} \end{pmatrix}U^\dagger = U\begin{pmatrix} m_{11} & 0 \\ 0 & m_{22} \end{pmatrix}U^\dagger.$$

Furthermore

$$U^\dagger = e^{-i\theta}\begin{pmatrix} e^{-i\phi}\cos\theta & e^{i\eta}\sin\theta \\ -e^{-i\eta}\sin\theta & e^{i\phi}\cos\theta \end{pmatrix}.$$

With these ingredients we obtain:

$$(0 \quad 1)Ue^{-\frac{iEt}{\hbar}}U^\dagger\begin{pmatrix}1\\0\end{pmatrix} = e^{-i(\eta+\phi)}(m_{11} - m_{22}),$$

and

$$(1 \quad 0)Ue^{-\frac{iEt}{\hbar}}U^\dagger\begin{pmatrix}0\\1\end{pmatrix} = e^{i(\eta+\phi)}(m_{11} - m_{22}).$$

Hence

$$P(1 \to 2) = |e^{-i(\eta+\phi)}(m_{11} - m_{22})|^2$$

and

$$P(2 \to 1) = |e^{i(\eta+\phi)}(m_{11} - m_{22})|^2.$$

Consequently

$$P(1 \to 2) - P(2 \to 1) = 0.$$

**c)** For a three state problem, however, the time(T)-reversal variance can be broken.
Calculate the difference $P(1 \to 2) - P(2 \to 1)$ for the following form of the unitary matrix

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix}\begin{pmatrix} c_{13} & 0 & s_{13}e^{-i\delta} \\ 0 & 1 & 0 \\ -s_{13}e^{i\delta} & 0 & c_{13} \end{pmatrix}\begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix} =$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix}\begin{pmatrix} c_{12}c_{13} & c_{13}s_{12} & s_{13}e^{-i\delta} \\ -s_{12} & c_{12} & 0 \\ -c_{12}s_{13}e^{i\delta} & -s_{12}s_{13}e^{i\delta} & c_{13} \end{pmatrix} =$$

$$= \begin{pmatrix} c_{12}c_{13} & c_{13}s_{12} & s_{13}e^{-i\delta} \\ -c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta} & c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta} & c_{13}s_{23} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta} & -c_{12}s_{23} - c_{23}s_{12}s_{13}e^{i\delta} & c_{13}c_{23} \end{pmatrix}.$$

The notation is: $s_{12} = \sin\theta_{12} \neq 0$ , $c_{23} = \cos\theta_{23} \neq 0$, etc. Furthermore, $\delta \neq 0$.
Again, for convenience, we use for the eigenvalue matrix,

$$\begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix}.$$

Furthermore

$$U^\dagger = \begin{pmatrix} c_{12}c_{13} & -c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta} & s_{12}s_{23} - c_{12}c_{23}s_{13}e^{-i\delta} \\ c_{13}s_{12} & c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta} & -c_{12}s_{23} - c_{23}s_{12}s_{13}e^{-i\delta} \\ s_{13}e^{i\delta} & c_{13}s_{23} & c_{13}c_{23} \end{pmatrix}.$$

Next, we evaluate

$$(0 \quad 1 \quad 0)U\begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix}U^\dagger\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},$$

and

$$(1 \quad 0 \quad 0)U\begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix}U^\dagger\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

First

$$(0 \quad 1 \quad 0)U\begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix}U^\dagger\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = (0 \quad 1 \quad 0)U\begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix}\begin{pmatrix} c_{12}c_{13} \\ c_{13}s_{12} \\ s_{13}e^{i\delta} \end{pmatrix} =$$

$$= (0 \quad 1 \quad 0)U\begin{pmatrix} c_{12}c_{13}m_{11} \\ c_{13}s_{12}m_{22} \\ s_{13}e^{i\delta}m_{33} \end{pmatrix}.$$

From $(0 \quad 1 \quad 0)U$ we obtain

$$\begin{pmatrix} -c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta} & c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta} & c_{13}s_{23} \end{pmatrix}.$$

With the preceding expressions

$$\begin{pmatrix} -c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta} & c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta} & c_{13}s_{23} \end{pmatrix} \cdot \begin{pmatrix} c_{12}c_{13}m_{11} \\ c_{13}s_{12}m_{22} \\ s_{13}e^{i\delta}m_{33} \end{pmatrix} =$$

$$= \left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta}\right)c_{12}c_{13}m_{11} + \left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta}\right)c_{13}s_{12}m_{22} + \\ + c_{13}s_{23}s_{13}e^{i\delta}m_{33}.$$

Then

$$\boldsymbol{P}(\mathbf{1} \to \mathbf{2}) = \left[\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta}\right)c_{12}c_{13}m_{11}^* + \left(c_{12}c_{23} + \\ -s_{12}s_{13}s_{23}e^{-i\delta}\right)c_{13}s_{12}m_{22}^* + c_{13}s_{23}s_{13}e^{-i\delta}m_{33}^*\right]\left[\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta}\right)c_{12}c_{13}m_{11} + \\ + \left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta}\right)c_{13}s_{12}m_{22} + c_{13}s_{23}s_{13}e^{i\delta}m_{33}\right].$$

The other expression

$$(1 \quad 0 \quad 0)U\begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix}U^\dagger\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} =$$

$$= (1 \quad 0 \quad 0)U \begin{pmatrix} (-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta})m_{11} \\ (c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta})m_{22} \\ c_{13}s_{23}m_{33} \end{pmatrix}.$$

From $(1 \quad 0 \quad 0)U$ we obtain

$$(1 \quad 0 \quad 0)U = \begin{pmatrix} c_{12}c_{13} & c_{13}s_{12} & s_{13}e^{-i\delta} \end{pmatrix}.$$

With the preceding expressions

$$\begin{pmatrix} c_{12}c_{13} & c_{13}s_{12} & s_{13}e^{-i\delta} \end{pmatrix} \cdot \begin{pmatrix} (-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta})m_{11} \\ (c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta})m_{22} \\ c_{13}s_{23}m_{33} \end{pmatrix} =$$

$$= (-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta})c_{12}c_{13}m_{11} + (c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta})c_{13}s_{12}m_{22} +$$
$$+c_{13}s_{23}s_{13}e^{-i\delta}m_{33}.$$

$$\boldsymbol{P(2 \to 1)} = [(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta})c_{12}c_{13}m_{11}^* + ((c_{12}c_{23} +$$
$$-s_{12}s_{13}s_{23}e^{i\delta})c_{13}s_{12}m_{22}^* + c_{13}s_{23}s_{13}e^{i\delta}m_{33}^*][(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta})c_{12}c_{13}m_{11} +$$
$$+(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta})c_{13}s_{12}m_{22} + c_{13}s_{23}s_{13}e^{-i\delta}m_{33}].$$

Next we evaluate

$P(1 \to 2) - P(2 \to 1)$.

After inspection with $\delta = 0$ in both expressions for $P(1 \to 2)$ and $P(2 \to 1)$ respectively we have:

$P(1 \to 2) - P(2 \to 1) = 0$.

After inspection with $\theta_{13} = 0$ in both expressions for $P(1 \to 2)$ and $P(2 \to 1)$ respectively we have:

$P(1 \to 2) - P(2 \to 1) = 0$.

Hence, with $\delta \neq 0$, and/or $\sin\theta_{13} \equiv s_{13} \neq 0$, the time-reversal can be broken.

Let us evaluate

$P(1 \to 2) - P(2 \to 1)$ step by step

First

$$(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta})(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta})c_{12}c_{13}^2s_{12}m_{11}m_{22}^* +$$
$$+(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta})(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta})c_{12}c_{13}^2s_{12}m_{22}m_{11}^* +$$
$$-(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta})(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta})c_{12}c_{13}^2s_{12}m_{22}m_{11}^* +$$
$$-(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta})(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta})c_{12}c_{13}^2s_{12}m_{11}m_{22}^* =$$
$$= c_{12}c_{13}^2s_{12}(m_{11}m_{22}^* - m_{22}m_{11}^*)[(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta})(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta}) +$$
$$-(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta})(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta})] = -c_{12}c_{13}^2s_{12}(m_{11}m_{22}^* - m_{22}m_{11}^*) \cdot$$
$$\cdot c_{23}s_{13}s_{23}2i\sin\delta = c_{12}c_{13}^2s_{12}c_{23}s_{13}s_{23}2i\sin[\tfrac{(E_1-E_2)}{\hbar}t]2i\sin\delta =$$
$$= -4c_{12}c_{13}^2s_{12}c_{23}s_{13}s_{23}\sin[\tfrac{(E_1-E_2)}{\hbar}t]\sin\delta,$$

next

$$(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta})c_{13}s_{23}s_{13}e^{-i\delta}c_{12}c_{13}m_{11}m_{33}^* +$$
$$+c_{13}s_{23}s_{13}e^{i\delta}(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta})c_{12}c_{13}m_{33}m_{11}^* +$$
$$-(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta})c_{13}s_{23}s_{13}e^{-i\delta}c_{12}c_{13}m_{33}m_{11}^* +$$
$$-c_{13}s_{23}s_{13}e^{i\delta}(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta})c_{12}c_{13}m_{11}m_{33}^* =$$
$$= c_{12}c_{13}^2s_{13}s_{23}(m_{11}m_{33}^* - m_{33}m_{11}^*)[(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta})e^{-i\delta} +$$
$$-e^{i\delta}(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta})] = 4c_{12}c_{13}^2c_{23}s_{12}s_{13}s_{23}\sin(\tfrac{E_1-E_3}{\hbar}t)\sin\delta,$$

and

$$(c_{12}c_{23}-s_{12}s_{13}s_{23}e^{i\delta})c_{13}s_{23}s_{13}e^{-i\delta}c_{13}s_{12}m_{22}m_{33}^{*}+$$
$$+c_{13}s_{23}s_{13}e^{i\delta}(c_{12}c_{23}-s_{12}s_{13}s_{23}e^{-i\delta})c_{13}s_{12}m_{33}m_{22}^{*}+$$
$$-(c_{12}c_{23}-s_{12}s_{13}s_{23}e^{i\delta})c_{13}s_{23}s_{13}e^{-i\delta}c_{13}s_{12}m_{33}m_{22}^{*}+$$
$$-c_{13}s_{23}s_{13}e^{i\delta}(c_{12}c_{23}-s_{12}s_{13}s_{23}e^{-i\delta})c_{13}s_{12}m_{22}m_{33}^{*}=$$
$$=c_{13}^{2}s_{12}s_{23}(m_{22}m_{33}^{*}-m_{33}m_{22}^{*})[(c_{12}c_{23}-s_{12}s_{13}s_{23}e^{i\delta})e^{-i\delta}+$$
$$-e^{i\delta}(c_{12}c_{23}-s_{12}s_{13}s_{23}e^{-i\delta})]=-4c_{12}c_{13}^{2}c_{23}s_{12}s_{13}s_{23}\sin(\tfrac{E_2-E_3}{\hbar}t)\sin\delta.$$

Then

$$P(1\rightarrow 2)-P(2\rightarrow 1)=$$
$$=-4c_{12}c_{13}^{2}c_{23}s_{12}s_{13}s_{23}\sin\delta\left[\sin\left(\tfrac{E_1-E_2}{\hbar}t\right)-\sin\left(\tfrac{E_1-E_3}{\hbar}t\right)+\sin\left(\tfrac{E_2-E_3}{\hbar}t\right)\right]=$$
$$=-\cos^2\theta_{13}\sin 2\theta_{12}\sin 2\theta_{23}\sin\theta_{13}\sin\delta\left[\sin\left(\tfrac{E_1-E_2}{\hbar}t\right)-\sin\left(\tfrac{E_1-E_3}{\hbar}t\right)+\sin\left(\tfrac{E_2-E_3}{\hbar}t\right)\right].$$

This expression proves, given $0<\theta<\pi/2$ , with $\delta\neq 0$ the time-reversal can be broken.

**d)** Wikipedia:

In particle physics, **CP violation** is a violation of **CP-symmetry** (or **charge conjugation parity symmetry**): the combination of C-symmetry (charge symmetry) and P-symmetry (parity symmetry). CP-symmetry states that the laws of physics should be the same if a particle is interchanged with its antiparticle (C-symmetry) while its spatial coordinates are inverted ("mirror" or P-symmetry). The discovery of CP violation in 1964 in the decays of neutral kaons resulted in the Nobel Prize in Physics in 1980 for its discoverers James Cronin and Val Fitch.

**Charge, parity, and time reversal symmetry** is a fundamental symmetry of physical laws under the simultaneous transformations of charge conjugation (C), parity transformation (P), and time reversal (T). CPT is the only combination of C, P, and T that is observed to be an exact symmetry of nature at the fundamental level.[1][2] The **CPT theorem** says that CPT symmetry holds for all physical phenomena, or more precisely, that any Lorentz invariant local quantum field theory with a Hermitian Hamiltonian must have CPT symmetry.

For CP-conjugate states, e.g. anti-neutrinos ($\bar{\nu}$) versus neutrinos($\nu$), the Hamiltonian is given by substituting $U^*$ in place of $U$ in case of evaluating $P(\bar{1}\rightarrow\bar{2})$. I suppose $U^\dagger$ is replaced by $U^{*\dagger}$.

Show that the probabilities $P(1\rightarrow 2)$ and $P(\bar{1}\rightarrow\bar{2})$ can differ (CP violation) yet CPT is respected, i.e., $P(1\rightarrow 2)=P(\bar{1}\rightarrow\bar{2})$. I suppose the probabilities have to be worked out again over a time interval $t$. We need the time evolution operator as given under **a)** with $U$ replaced by $U^*$:

$$U=\begin{pmatrix} c_{12}c_{13} & c_{13}s_{12} & s_{13}e^{-i\delta} \\ -c_{23}s_{12}-c_{12}s_{13}s_{23}e^{i\delta} & c_{12}c_{23}-s_{12}s_{13}s_{23}e^{i\delta} & c_{13}s_{23} \\ s_{12}s_{23}-c_{12}c_{23}s_{13}e^{i\delta} & -c_{12}s_{23}-c_{23}s_{12}s_{13}e^{i\delta} & c_{13}c_{23} \end{pmatrix},$$

$$U^*=\begin{pmatrix} c_{12}c_{13} & c_{13}s_{12} & s_{13}e^{i\delta} \\ -c_{23}s_{12}-c_{12}s_{13}s_{23}e^{-i\delta} & c_{12}c_{23}-s_{12}s_{13}s_{23}e^{-i\delta} & c_{13}s_{23} \\ s_{12}s_{23}-c_{12}c_{23}s_{13}e^{-i\delta} & -c_{12}s_{23}-c_{23}s_{12}s_{13}e^{-i\delta} & c_{13}c_{23} \end{pmatrix},$$

and

$$U^{*\dagger}=\begin{pmatrix} c_{12}c_{13} & -c_{23}s_{12}-c_{12}s_{13}s_{23}e^{i\delta} & s_{12}s_{23}-c_{12}c_{23}s_{13}e^{i\delta} \\ c_{13}s_{12} & c_{12}c_{23}-s_{12}s_{13}s_{23}e^{i\delta} & -c_{12}s_{23}-c_{23}s_{12}s_{13}e^{i\delta} \\ s_{13}e^{-i\delta} & c_{13}s_{23} & c_{13}c_{23} \end{pmatrix}.$$

$$H = U^* \begin{pmatrix} E_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & E_n \end{pmatrix} U^{*\dagger}.$$

We already derived $P(1 \to 2)$ :

$\boldsymbol{P(1 \to 2)} = \left[\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta}\right)c_{12}c_{13}m_{11}^* + \left(c_{12}c_{23} + \right.\right.$
$\left.-s_{12}s_{13}s_{23}e^{-i\delta}\right)c_{13}s_{12}m_{22}^* + c_{13}s_{23}s_{13}e^{-i\delta}m_{33}^*\big]\big[\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta}\right)c_{12}c_{13}m_{11} +$
$+\left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta}\right)c_{13}s_{12}m_{22} + c_{13}s_{23}s_{13}e^{i\delta}m_{33}].$

Now,

$$\boldsymbol{P(\overline{1} \to \overline{2})} = |(0 \quad 1 \quad 0)U^* \begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix} U^{*\dagger} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} |^2,$$

where $m_{jj} = e^{-iE_j t/\hbar}$.

$$\begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix} U^{*\dagger} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} c_{12}c_{13}m_{11} \\ c_{13}s_{12}m_{22} \\ s_{13}e^{-i\delta}m_{33} \end{pmatrix}.$$

Next

$$(0 \quad 1 \quad 0)U^* = (0 \quad 1 \quad 0) \begin{pmatrix} c_{12}c_{13} & c_{13}s_{12} & s_{13}e^{i\delta} \\ -c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta} & c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta} & c_{13}s_{23} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{-i\delta} & -c_{12}s_{23} - c_{23}s_{12}s_{13}e^{-i\delta} & c_{13}c_{23} \end{pmatrix}.$$

So,

$$(0 \quad 1 \quad 0)U^* = \left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta} \quad c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta} \quad c_{13}s_{23}\right) \ .$$

Then,

$$(0 \quad 1 \quad 0)U^* \begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix} U^{*\dagger} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} =$$

$$= \left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta} \quad c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta} \quad c_{13}s_{23}\right) \begin{pmatrix} c_{12}c_{13}m_{11} \\ c_{13}s_{12}m_{22} \\ s_{13}e^{-i\delta}m_{33} \end{pmatrix} =$$

$= \left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta}\right)c_{12}c_{13}m_{11} + \left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta}\right)c_{13}s_{12}m_{22} +$
$+c_{13}s_{23}s_{13}e^{-i\delta}m_{33}.$

$\boldsymbol{P(\overline{1} \to \overline{2})} = \left[\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta}\right)c_{12}c_{13}m_{11}^* + \left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta}\right)c_{13}s_{12}m_{22}^* +\right.$
$\left.c_{13}s_{23}s_{13}e^{i\delta}m_{33}^*\right]\left[\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta}\right)c_{12}c_{13}m_{11} +\right.$
$\left.+\left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta}\right)c_{13}s_{12}m_{22} + c_{13}s_{23}s_{13}e^{-i\delta}m_{33}\right]$ .

$\boldsymbol{P(2 \to 1)} = [\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta}\right)c_{12}c_{13}m_{11}^* + ((c_{12}c_{23} +$
$-s_{12}s_{13}s_{23}e^{i\delta})c_{13}s_{12}m_{22}^* + c_{13}s_{23}s_{13}e^{i\delta}m_{33}^*][\ \left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta}\right)c_{12}c_{13}m_{11} +$
$+(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta})c_{13}s_{12}m_{22} + c_{13}s_{23}s_{13}e^{-i\delta}m_{33}]$ .

Comparing $\boldsymbol{P(\overline{1} \to \overline{2})}$ and $\boldsymbol{P(2 \to 1)}$

$\boldsymbol{P(\overline{1} \to \overline{2}) = P(2 \to 1).}$

Consequently

$P(1 \to 2) - P(\overline{1} \to \overline{2}) =$

$= -4c_{12}c_{13}^2c_{23}s_{12}s_{13}s_{23}\sin\delta\left[\sin\left(\frac{E_1-E_2}{\hbar}t\right) - \sin\left(\frac{E_1-E_3}{\hbar}t\right) + \sin\left(\frac{E_2-E_3}{\hbar}t\right)\right] =$

$= -\cos^2\theta_{13}\sin 2\theta_{12}\sin 2\theta_{23}\sin\theta_{13}\sin\delta\left[\sin\left(\frac{E_1-E_2}{\hbar}t\right) - \sin\left(\frac{E_1-E_3}{\hbar}t\right) + \sin\left(\frac{E_2-E_3}{\hbar}t\right)\right].$

Next,

$P(1 \to 2) - P(\bar{2} \to \bar{1})$.

$\boldsymbol{P(1 \to 2)} = \left[\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta}\right)c_{12}c_{13}m_{11}^* + \left(c_{12}c_{23} + \right.\right.$
$\left.-s_{12}s_{13}s_{23}e^{-i\delta}\right)c_{13}s_{12}m_{22}^* + c_{13}s_{23}s_{13}e^{-i\delta}m_{33}^*\big]\big[\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta}\right)c_{12}c_{13}m_{11} +$
$+\left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta}\right)c_{13}s_{12}m_{22} + c_{13}s_{23}s_{13}e^{i\delta}m_{33}\big]$.

$\boldsymbol{P(\bar{2} \to \bar{1})}$:

we need to evaluate $(1 \quad 0 \quad 0)U^* \begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix} U^\dagger \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$.

$$\begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix} U^{*\dagger} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta}\right)m_{11} \\ \left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta}\right)m_{22} \\ c_{13}s_{23}m_{33} \end{pmatrix},$$

and

$(1 \quad 0 \quad 0)U^* = (c_{12}c_{13} \quad c_{13}s_{12} \quad s_{13}e^{i\delta})$.

Then

$$(1 \quad 0 \quad 0)U^* \begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & 0 \\ 0 & 0 & m_{33} \end{pmatrix} U^\dagger \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} =$$

$$= (c_{12}c_{13} \quad c_{13}s_{12} \quad s_{13}e^{i\delta}) \begin{pmatrix} \left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta}\right)m_{11} \\ \left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta}\right)m_{22} \\ c_{13}s_{23}m_{33} \end{pmatrix} =$$

$= c_{12}c_{13}\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta}\right)m_{11} + c_{13}s_{12}\left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta}\right)m_{22} +$
$+s_{13}e^{i\delta}c_{13}s_{23}m_{33}$.

Hence,

$\boldsymbol{P(\bar{2} \to \bar{1})}$=$\left[c_{12}c_{13}\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{-i\delta}\right)m_{11}^* + \right.$
$+c_{13}s_{12}\left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{-i\delta}\right)m_{22}^* + s_{13}e^{-i\delta}c_{13}s_{23}m_{33}^*\big]\big[s_{13}e^{i\delta}c_{13}s_{23}m_{33} +$
$\left.+c_{12}c_{13}\left(-c_{23}s_{12} - c_{12}s_{13}s_{23}e^{i\delta}\right)m_{11} + c_{13}s_{12}\left(c_{12}c_{23} - s_{12}s_{13}s_{23}e^{i\delta}\right)m_{22}\right]$ .

Comparing the expressions for $\boldsymbol{P(1 \to 2)}$ and $\boldsymbol{P(\bar{2} \to \bar{1})}$ results into

$\boldsymbol{P(1 \to 2)} = \boldsymbol{P(\bar{2} \to \bar{1})} \to \boldsymbol{P(1 \to 2)} - \boldsymbol{P(\bar{2} \to \bar{1})} = 0$.

### 8.15.42 Kronig-Penney Model

Consider a periodic repulsive potential of the form

$V = \sum_{n=-\infty}^{\infty} \lambda\delta(x - na)$,

with $\lambda > 0$. The general solution for $-a < x < 0$ is given by

$\psi(x) = Ae^{i\kappa x} + Be^{-i\kappa x}$,

with $\kappa = \frac{\sqrt{2mE}}{\hbar}$.

Using Bloch's theorem[14] , the wave function for the next period $0 < x < a$ is given by

$\psi(x) = e^{ika}\left(Ae^{i\kappa(x-a)} + Be^{-i\kappa(x-a)}\right)$

for $|k| \leq \frac{\pi}{a}$.

Questions:

**a)** Write down the continuity condition for the wave function and the required discontinuity for its derivative at $x = 0$. Show that the phase $e^{i\kappa a}$ under the discrete translation

[14] Bloch's theorem: solutions to the Schrödinger equation in a periodic potential take the form of a plane wave modulated by a periodic function, www.en.wikipedia.org .

$x \to x + a$ is given by

$$e^{ika} = \cos\kappa a + \frac{1}{\kappa d}\sin\kappa a \pm i\sqrt{1 - \left(\cos\kappa a + \frac{1}{\kappa d}\sin\kappa a\right)^2},$$

where $d = \frac{\hbar^2}{m\lambda}$.

**Note** : the above expression for $e^{ika}$ represents the roots of a quadratic equation.

$$[e^{ika} - (\cos\kappa a \ + \frac{1}{\kappa d}\sin\kappa a)]^2 = \left(\cos\kappa a + \frac{1}{\kappa d}\sin\kappa a\right)^2 - 1 \to$$

$$\to e^{2ika} - 2\,e^{ika}(\cos\kappa a \ + \frac{1}{\kappa d}\sin\kappa a) = -1 \to e^{2ika} = 2e^{ika}\,(\cos\kappa a \ + \frac{1}{\kappa d}\sin\kappa a) - 1$$

The latter expression can be of some help by evaluating $e^{ika}$.

At $x = 0$, we have a discontinuity of the derivatives.

We evaluate $\psi(x)$ and $\frac{d\psi(x)}{dx}$ for $-\epsilon < x < \epsilon$ and $\epsilon \to 0$ :

$\psi(-\epsilon) = A + B$ ,

$\psi(+\epsilon) = e^{ika}\left(Ae^{-i\kappa a} + Be^{i\kappa a}\right)$,

$\frac{d\psi(x)}{dx}|_{x=-\epsilon} = i\kappa(A - B)$,

$\frac{d\psi(x)}{dx}|_{x=+\epsilon} = \ i\kappa e^{ika}\left(Ae^{-i\kappa a} - Be^{i\kappa a}\right)$.

Furthermore, integrating the Schrödinger equation, we have with the delta function potential and $n = 0$

$$\frac{d\psi(x)}{dx}|_{x=+\epsilon} - \ \frac{d\psi(x)}{dx}|_{x=-\epsilon} = \frac{2}{d}\psi(0) = \frac{2}{d}(A + B) .$$

At $x = 0$

$$A + B = e^{ika}\left(Ae^{-i\kappa a} + Be^{i\kappa a}\right) \to A\left(1 - e^{ika}e^{-i\kappa a}\right) = B(e^{ika}e^{i\kappa a} - 1) \to$$

$$\to A = B\,\frac{e^{ika}e^{i\kappa a} - 1}{1 - e^{ika}e^{-i\kappa a}},$$

and with the derivatives

$$i\kappa e^{ika}\left(Ae^{-i\kappa a} - Be^{i\kappa a}\right) - i\kappa(A - B) = \frac{2}{d}(A + B) \to$$

$$\to e^{ika}\left(Ae^{-i\kappa a} - Be^{i\kappa a}\right) - A + B = -\frac{2i}{\kappa d}(A + B) \to$$

$$A\left(e^{ika}e^{-i\kappa a} - 1 + \frac{2i}{\kappa d}\right) = B\left(e^{ika}e^{i\kappa a} - 1 - \frac{2i}{\kappa d}\right).$$

Take the quotient of

$$A\left(1 - e^{ika}e^{-i\kappa a}\right) = B(e^{ika}e^{i\kappa a} - 1),$$

and

$$A\left(e^{ika}e^{-i\kappa a} - 1 + \frac{2i}{\kappa d}\right) = B\left(e^{ika}e^{i\kappa a} - 1 - \frac{2i}{\kappa d}\right):$$

$$\frac{1 - e^{ika}e^{-i\kappa a}}{e^{ika}e^{-i\kappa a} - 1 + \frac{2i}{\kappa d}} = \frac{e^{ika}e^{i\kappa a} - 1}{e^{ika}e^{i\kappa a} - 1 - \frac{2i}{\kappa d}}.$$

Next we need to eliminate $e^{ika}$ from the above expression:

$$\left(1 - e^{ika}e^{-i\kappa a}\right)\left(e^{ika}e^{i\kappa a} - 1 - \frac{2i}{\kappa d}\right) = (e^{ika}e^{i\kappa a} - 1)(e^{ika}e^{-i\kappa a} - 1 + \frac{2i}{\kappa d}) \to$$

$$\to -e^{2ika} + e^{ika}\left(e^{i\kappa a} + e^{-i\kappa a}\right) - \frac{i}{\kappa d}e^{ika}\left(e^{i\kappa a} - e^{-i\kappa a}\right) - 1 = 0 \to$$

$$\to e^{2ika} = 2e^{ika}\,(\cos\kappa a + \frac{1}{\kappa d}\sin\kappa a) - 1,$$

as we obtained above.

**b)** Take the limit od zero potential, i.e. $d \to \infty$, and show that there are no gaps between the bands as expected for a free particle.
With

$e^{ika} = \cos \kappa a + \frac{1}{\kappa d} \sin \kappa a \pm i\sqrt{1 - \left(\cos \kappa a + \frac{1}{\kappa d} \sin \kappa a\right)^2}$, and $d \to \infty$ , we have

$e^{ika} = \cos \kappa a \pm i \sin \kappa a = e^{\pm i\kappa a}$.

This is the result for a free particle and a continuous energy spectrum.

**c)** When the potential is weak but finite (large $d$) show analytically that there appear gaps between the bands at $k = \pm\pi/a$ .

$e^{ika} = \cos ka \pm i \sin ka,$

then $1 - \left(\cos \kappa a + \frac{1}{\kappa d} \sin \kappa a\right)^2 > 0$ .

When $1 - \left(\cos \kappa a + \frac{1}{\kappa d} \sin \kappa a\right)^2 < 0,$

there are no solutions.

For $k \approx \kappa$ , we rewrite the expression

$e^{ika} = \cos ka + \frac{1}{kd} \sin ka \pm i\sqrt{1 - \left(\cos ka + \frac{1}{kd} \sin ka\right)^2}$,

and

$|\cos ka + \frac{1}{kd} \sin ka\,| > 1.$

For large $d$ the preceding expression can be larger than 1. There are no solutions. There is a band with gaps.

Assume the gaps to be small and equal to $\epsilon$

$ka = n\pi + \epsilon$ .

To investigate the width of the gap, we expand

$\cos ka = \cos(n\pi + \epsilon) = \cos n\pi \cos \epsilon = (-1)^n\,(1 - \frac{\epsilon^2}{2} + O(\epsilon^4))$

$\sin ka = \sin(n\pi + \epsilon) = \cos n\pi \sin \epsilon = (-1)^n(\epsilon + O(\epsilon^3))$ .

Then

$\cos ka + \frac{1}{\kappa d} \sin ka = (-1)^n(1 + \frac{1}{kd}\epsilon - \frac{\epsilon^2}{2} + \, O(\epsilon^3)).$

For $\frac{1}{kd}\epsilon - \frac{\epsilon^2}{2} > 0 \to 0 < \epsilon < \frac{2}{kd} (= \frac{2a}{n\pi d}).$

Hence, there exists a gap at $k \approx \kappa = \pm\frac{\pi}{a}$.

**d)** The relation between $\kappa$ and $k$ can be illustrated, including the gap by plotting the relationship

$e^{ika} = \cos \kappa a + \frac{1}{\kappa d} \sin \kappa a \pm i\sqrt{1 - \left(\cos \kappa a + \frac{1}{\kappa d} \sin \kappa a\right)^2}$,

for a weak potential, $d = 3a$, and a strong potential, $d = a/3$ .

**e)** You always find two values of $k$ at the same energy $\kappa = \frac{\sqrt{2mE}}{\hbar}$ .

What discrete symmetry guarantees this degeneracy?

Let us investigate parity.

We have

$\psi(x) = Ae^{i\kappa x} + Be^{-i\kappa x}$ , for $-a < x < 0$

and
$\psi(x) = e^{ika}\left(Ae^{i\kappa(x-a)} + Be^{-i\kappa(x-a)}\right)$, for $0 < x < a$.
Apply parity transformation for the latter expression $x \to -x$ :
$\psi(x) = e^{ika}\left(Ae^{i\kappa(-x-a)} + Be^{-i\kappa(-x-a)}\right) = Be^{i(k+\kappa)a}e^{i\kappa x} + Ae^{i(k-\kappa)a}e^{-i\kappa x} =$
$= A'e^{i\kappa x} + B'e^{-i\kappa x}$.
Next we investigate the former expression, $\psi(x) = Ae^{i\kappa x} + Be^{-i\kappa x}$ , $x \to a - x$
$\psi(x) = Ae^{i\kappa x} + Be^{-i\kappa x} = Ae^{-i\kappa(x-a)} + Be^{i\kappa(x-a)} \to$
$\to e^{ika}(Be^{ika}e^{i\kappa(x-a)} + \ Ae^{-ika}e^{-i\kappa(x-a)} = e^{ika}\left(A'e^{i\kappa(x-a)} + B'e^{-i\kappa(x-a)}\right)$.

### 8.15.43 Operator Moments and Uncertainty.

Consider an observable $O_A$ for a finite-dimensional quantum system with spectral decomposition
$O_A = \sum_i \lambda_i P_i$ ,
with the projection operator
$P_i = |\lambda_i\rangle\langle\lambda_i|$.
**a)** Show that the exponential operator $E_A = e^{O_A}$ has spectral decomposition
$E_A = \sum_i e^{\lambda_i P_i}$.
Do this by inserting the spectral decomposition of $O_A$ into the power series expansion of the exponential.
We know
$e^{O_A} = I + O_A + \frac{1}{2!}O_A^2 + \frac{1}{3!}O_A^3 + \cdots$.
Hence,
$e^{O_A} = I + \sum_i \lambda_i P_i + \frac{1}{2!}(\sum_i \lambda_i P_i)^2 + \frac{1}{3!}(\sum_i \lambda_i P_i)^3 + \cdots$.
With
$\sum_i P_i = \sum_i |\lambda_i\rangle\langle\lambda_i| = I$ ,
$P_i^2 = |\lambda_i\rangle\langle\lambda_i||\lambda_i\rangle\langle\lambda_i| = |\lambda_i\rangle\langle\lambda_i| = P_i$, etc…,
and $P_i P_j = \delta_{ij}$
$\to e^{O_A} = \sum_i P_i + \sum_i \lambda_i P_i + \frac{1}{2!}\sum_i \lambda_i^2 \ P_i + \frac{1}{3!}\sum_i \lambda_i^3 \ P_i + \cdots = \sum_i(\sum_{n=0}^{\infty}\frac{\lambda_i^n}{n!})P_i =$
$= \sum_i(\sum_{n=0}^{\infty}\frac{\lambda_i^n}{n!}P_i^n) = \sum_i e^{\lambda_i P_i} = \sum_i e^{\lambda_i} P_i$.
**b)** Prove that for any state $|\Psi_A\rangle$ such that $\Delta O_A = 0$, we automatically have $\Delta E_A = 0$.
In order to have $\Delta O_A = 0$ , it must be the case that $P_i|\Psi_A\rangle = |\Psi_A\rangle$ for some eigenspace projector.
$\Delta O_A = \sqrt{\langle O_A^2\rangle - \langle O_A\rangle^2}$ .
Now
$\sqrt{\langle O_A^2\rangle - \langle O_A\rangle^2} = 0 \to \langle O_A^2\rangle = \langle O_A\rangle^2 \to \langle\Psi_A|O_A^2|\Psi_A\rangle = \langle\Psi_A|O_A|\Psi_A\rangle^2$.
We expand $|\Psi_A\rangle$
$|\Psi_A\rangle = \sum_i c_i\,|\lambda_i\rangle$.
Then,
$\langle\Psi_A|O_A^2|\Psi_A\rangle = \sum_i |c_i|^2\,\lambda_i^2$ , and $\langle\Psi_A|O_A|\Psi_A\rangle^2 = (\sum_i |c_i|^2\,\lambda_i)^2 \to$
$\to \sum_i |c_i|^2\,\lambda_i^2 - (\sum_i |c_i|^2\,\lambda_i)^2 = 0$.
Plug into the preceding equation $|c_i|^2 = 1 - \sum_{i\neq j}|c_j|^2$:

$\sum_i \lambda_i^2 \,(1 - \sum_{i\neq j}|c_j|^2) - \left(\sum_i \lambda_i (1 - \sum_{i\neq j}|c_j|^2)\right)^2 = 0\,.$

The summation in the preceding expression is over all $i$. Consequently

$\sum_{i\neq j} |c_j|^2 = 0 \rightarrow |c_i|^2 = 1.$

We use this result to investigate $P_i|\Psi_A\rangle$ :

$|\lambda_i\rangle\langle\lambda_i| \sum_j c_j \,|\lambda_j\rangle = c_i|\lambda_i\rangle.$

Since we have $\Delta O_A = 0 \rightarrow |c_i|^2 = 1 \rightarrow c_i = e^{i\theta}$ and choose to set $\theta = 0$ .

Then,

$|\lambda_i\rangle\langle\lambda_i| \sum_j c_j \,|\lambda_j\rangle = c_i|\lambda_i\rangle \rightarrow |\lambda_i\rangle\langle\lambda_i|\,|\lambda_i\rangle = |\lambda_i\rangle \rightarrow P_i|\Psi_A\rangle = |\Psi_A\rangle$ .

Next

$\Delta E_A = ?$

$E_A|\Psi_A\rangle = \sum_i e^{\lambda_i} P_i|\Psi_A\rangle = e^{\lambda_i}|\Psi_A\rangle \rightarrow \langle\Psi_A|E_A|\Psi_A\rangle^2 = e^{2\lambda_i}.$

Consequently

$E_A^2|\Psi_A\rangle = e^{2\lambda_i}|\Psi_A\rangle \rightarrow \langle\Psi_A|E_A^2|\Psi_A\rangle = e^{2\lambda_i}.$

Hence

$\Delta E_A = 0$ .

**Note:**

An exercise with projection operators.

$\sqrt{\langle O_A^2\rangle - \langle O_A\rangle^2} = 0? \rightarrow \langle O_A^2\rangle = \langle O_A\rangle^2 \rightarrow \langle\Psi_A|O_A^2|\Psi_A\rangle - \langle\Psi_A|O_A|\Psi_A\rangle^2 =$

$= \langle\Psi_A|O_A^2|\Psi_A\rangle - \langle\Psi_A|O_A|\Psi_A\rangle\langle\Psi_A|O_A|\Psi_A\rangle.$

We define $P_A = |\Psi_A\rangle\langle\Psi_A|$ and $|\Psi_A\rangle$ is an eigenvector of $O_A$ and of $P_A$.

$P_A|\Psi_A\rangle = |\Psi_A\rangle\langle\Psi_A\,|\Psi_A\rangle = |\Psi_A\rangle.$

When $O_A$ and $P_A$ commute, do both operators have the same eigenvectors?

$(P_A O_A - O_A P_A)|\Psi_A\rangle = (P_A - 1)O_A|\Psi_A\rangle = 0 \rightarrow P_A O_A|\Psi_A\rangle = O_A|\Psi_A\rangle \rightarrow O_A|\Psi_A\rangle$ is an eigenstate of $P_A$ with eigenvalue 1. Consequently, $|\Psi_A\rangle$ is an eigenstate of $O_A$.

Then

$\langle\Psi_A|O_A^2|\Psi_A\rangle - \langle\Psi_A|O_A|\Psi_A\rangle\langle\Psi_A|O_A|\Psi_A\rangle = \langle\Psi_A|O_A(O_A - P_A O_A)|\Psi_A\rangle =$

$= \langle\Psi_A|O_A(O_A - O_A P_A + O_A P_A - P_A O_A)|\Psi_A\rangle = \langle\Psi_A|O_A(O_A - O_A P_A + [O_A, P_A]|\Psi_A\rangle =$

$= \langle\Psi_A|O_A^2(1 - P_A)|\Psi_A\rangle,$

where use has been made of $[O_A, P_A] = 0$ , since both operators have the same eigenvectors.

Furthermore both operators are Hermitian, consequently, the eigenvalues are real.

What about $(1 - P_A)|\Psi_A\rangle$?

$P_A|\Psi_A\rangle = |\Psi_A\rangle.$

Consequently

$(1 - P_A)|\Psi_A\rangle = 0 \rightarrow \sqrt{\langle O_A^2\rangle - \langle O_A\rangle^2} = 0.$

### 8.15.44 Uncertainty and Dynamics

Consider the observable in matrix representation

$O_X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$

and the initial state

$|\Psi_A(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$

**a)** Compute the uncertainty $\Delta O_x$, with respect to the initial state $|\Psi_A(0)\rangle$ .

$\Delta O_X = \sqrt{\langle O_X^2\rangle - \langle O_X\rangle^2}$.

The ingredients to calculate $\Delta O_X$ are available.

$\langle O_X\rangle = \langle \Psi_A(0)|O_X|\Psi_A(0)\rangle = (1 \quad 0)\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = (1 \quad 0)\begin{pmatrix}0\\1\end{pmatrix} = 0$ .

$\langle O_X^2\rangle = \langle \Psi_A(0)|O_X^2|\Psi_A(0)\rangle = (1 \quad 0)\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = (1 \quad 0)\begin{pmatrix}1\\0\end{pmatrix} = 1$.

Hence $\Delta O_x = 1$ , with respect to the initial state $|\Psi_A(0)\rangle$ .

A surprise with respect to the result presented in the note of the preceding problem 8.15.43? Keep in mind:

$|\Psi_A(0)\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ is not an eigenvector of $O_X = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$.

The eigenvectors of $O_X = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$ are $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$, and $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$.

Furthermore $|\Psi_A(0)\rangle\langle\Psi_A(0)|$ and $O_X$ do not commute.

**b)** Now let the state evolve according to the Schrödinger equation, with the Hamiltonian operator

$H = \hbar\begin{pmatrix}0 & i\\-i & 0\end{pmatrix}$ .

Compute the uncertainty $\Delta O_X$ as a function of $t$.

The time dependent Schrödinger equation:

$\frac{d}{dt}|\Psi_A(t)\rangle = -\frac{i}{\hbar}H|\Psi_A(t)\rangle \rightarrow |\Psi_A(t)\rangle = e^{-\frac{iHt}{\hbar}}|\Psi_A(0)\rangle$, the well-known time dependency.

The eigenvalues of $\begin{pmatrix}0 & i\\-i & 0\end{pmatrix}$:

$\begin{vmatrix}-\lambda & i\\-i & -\lambda\end{vmatrix} = 0 \rightarrow \lambda = \pm 1 \rightarrow \lambda = 1 \rightarrow |\lambda_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}$; $\lambda = 1 \rightarrow |\lambda_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}$.

The normalized eigen vectors of $\frac{1}{\hbar}H$ can be used to diagonalize $\frac{1}{\hbar}H$.

We expand $e^{-\frac{iHt}{\hbar}}$ to obtain $|\Psi_A(t)\rangle$

$e^{-\frac{iHt}{\hbar}} = \sum_{n=0}^{\infty}\frac{(-it)^n}{n!}\left(\frac{1}{\hbar}H\right)^n$.

For convenience , we diagonalize $\frac{1}{\hbar}H$:

$\frac{1}{4}\begin{pmatrix}1 & i\\1 & -i\end{pmatrix}\begin{pmatrix}0 & i\\-i & 0\end{pmatrix}\begin{pmatrix}1 & 1\\-i & i\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$.

Then

$$e^{-\frac{iHt}{\hbar}} = \sum_{n=0}^{\infty}\frac{(-it)^n}{n!}\left(\frac{1}{\hbar}H\right)^n = \sum_{n=0}^{\infty}\frac{(-it)^n}{n!}\begin{pmatrix}\frac{1}{2} & 0\\0 & -\frac{1}{2}\end{pmatrix}^n = \begin{pmatrix}e^{-it/2} & 0\\0 & e^{it/2}\end{pmatrix}.$$

With $|\Psi_A(0)\rangle = \begin{pmatrix}1\\0\end{pmatrix}$,

$|\Psi_A(t)\rangle = e^{-\frac{iHt}{\hbar}}|\Psi_A(0)\rangle = \begin{pmatrix}e^{-it/2} & 0\\0 & e^{it/2}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}e^{-it/2}\\0\end{pmatrix}$.

**Note:**

$n = 1 \rightarrow \frac{1}{\hbar}H = \begin{pmatrix}0 & i\\-i & 0\end{pmatrix}$; $n = 2 \rightarrow \frac{1}{\hbar}H = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$; $n = 3 \rightarrow \frac{1}{\hbar}H = \begin{pmatrix}0 & i\\-i & 0\end{pmatrix}$; etc.

With $O_X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$,

$\langle O_X \rangle = \langle \Psi_A(t)|O_X|\Psi_A(t)\rangle = \begin{pmatrix} e^{it/2} & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{-it/2} \\ 0 \end{pmatrix} = 0$ .

$O_X^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \to \langle O_x^2 \rangle = 1.$

Then

$\Delta O_X = \sqrt{\langle O_X^2 \rangle - \langle O_X \rangle^2} = 1.$

**c)** Repeat part b), but replace $O_X$ with the observable

$O_Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

Compute the uncertainty $\Delta O_Z$ as a function of $t$ assuming evolution according to the Schrödinger equation with the Hamiltonian above.

$O_Z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \to \langle O_Z^2 \rangle = 1$ .

$\langle O_Z \rangle = \langle \Psi_A(t)|O_Z|\Psi_A(t)\rangle = \begin{pmatrix} e^{it/2} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} e^{-it/2} \\ 0 \end{pmatrix} = 1.$

$\Delta O_Z = \sqrt{\langle O_Z^2 \rangle - \langle O_Z \rangle^2} = 0.$

**d)** Show that the answers to parts b) an c) always respect the Heisenberg Uncertainty Relation

$\Delta O_X \Delta O_Z \geq \frac{1}{2}|\langle [O_X, O_Z] \rangle|,$

Are there any times $t$ which the Heisenberg Uncertainty Relation satisfies the preceding equality?

$[O_X, O_Z] = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix}.$

At time $t$

$\frac{1}{2}|\langle [O_X, O_Z] \rangle| = \frac{1}{2}\left| \left\langle \Psi_A(t) \right| \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix} \left| \Psi_A(t) \right\rangle \right| = 0$ .

We already obtained

$\Delta O_X \Delta O_Z = 1 \cdot 0 = 0$ .

Hence,

the equality in $\Delta O_X \Delta O_Z \geq \frac{1}{2}|\langle [O_X, O_Z] \rangle|$ is always obtained.

# Chapter 9 Angular Momentum;2- and 3- Dimensions

## 9.1 Angular Momentum Eigenvalues and Eigenvectors

In Chapter 6, the commutation relations that define angular momentum operators, Eqs. (9.1) and (9.2) are derived. It is about Hermitian operators.

For example $\hat{J}_x$:

$\hat{J}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \to \hat{J}_x^\dagger = \hat{p}_z^\dagger \hat{y}^\dagger - \hat{p}_y^\dagger \hat{z}^\dagger.$

$\hat{p}_y, \hat{p}_z, \hat{y}$, and $\hat{z}$ are Hermitian $\to \hat{J}_x^\dagger = \hat{p}_z \hat{y} - \hat{p}_y \hat{z}.$

Furthermore, in classical notation

$[q_i, p_j] = i\hbar\delta_{ij} \to \hat{J}_x^\dagger = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = \hat{J}_x$ .

The eigenvectors and eigenvalues of the angular momentum operators can be derived using

the commutators.
$\hat{J}_x$ , $\hat{J}_y$ , and $\hat{J}_z$ do not commute. For example
$[\hat{J}_x , \hat{J}_y ] = i\hbar \hat{J}_z$ ,
similar to the momentum operator.
With Eq.(9.3), it can be shown:
$[\hat{J}^2 , J_i] = 0$, Eq.(9.4),
using $[A^2, B] = A[A, B] + [[A, B]A$.
The eigenvalues and eigenvector relations are presented by Eqs.(9.5) and (9.6).
In Eqs.(9.7)-(9.14), the relations between the angular momentum operators and the raising and lowering operators are presented.
Remark: Eq.(9.11) can be derived by Eqs.(9.12) and (9.13), representing the elements of the commutator $[\hat{J}_+, \hat{J}_-]$.

### 9.1.1 Derivation of Eigenvalues

With Eqs.(9.3) and (9.5), Eqs.(9.15) and (9.16) are obtained.
See also section 8.5 and 8.6 of Fitzpatrick, *Undergraduate Course* and Mahan, Section 4.1.3.
Eqs.(9.21), (9.6) and (9.10):
$(\hat{J}_+\hat{J}_3 + \hbar\hat{J}_+)|\lambda m\rangle = \hat{J}_+\hat{J}_3 |\lambda m\rangle + \hbar\hat{J}_+|\lambda m\rangle = \hbar m\hat{J}_+|\lambda m\rangle + \hbar\hat{J}_+|\lambda m\rangle = \hbar(m + 1)\hat{J}_+|\lambda m\rangle$.
Eq.(9.28) is found using Eq.(9.25): $\lambda = j(j + 1)$.
At the top of page 691: *"which implies that* $2j$ *= integer…..".*
Assume $2j$ not to be an integer, consequently the symmetrical number array of $m$ does not exist.
Demonstrate by an example: $2j = \frac{9}{4} \to j = \frac{9}{8} \to m = \frac{1}{8}, -\frac{7}{8}$.
Page 689 below Eq(9.21):
$\hat{J}_+|\lambda m\rangle \propto |\lambda, m + 1\rangle \to \hat{J}_+|jm\rangle = C_+|j, m + 1\rangle = |\alpha_+\rangle$, Eq.(9.37).
In this way the relations for raising/lowering operators are found, Eq.(9.45).

## 9.2 Transformations and Generators; Spherical Harmonics.

Boccio introduced some notation conventions.
Generators of momentum operators are discussed in section 6.10: *Generators of the Group Transformations,* Eq.(6.172). The unitary transformation is given in Eq.(9.46).
Eq.(9.51) is the expansion to first order of Eq.(9.46).
As given in Eq.(9.57), the angular momentum operator is Hermitian. This has been proven above, page 273.
Furthermore, the operators are presented in Cartesian Coordinates and Spherical-Polar Coordinates, Eqs.(9.82)-(9.94).

### 9.2.1 Eigenfunctions; Eigenvalues; Position Representation.

Eqs(9.95)-(9.99) summarize the results of the foregoing sections.
I prefer Eq.(9.101) in the following way, with Eq.(9.96)
$\langle\theta\varphi|\vec{L}^2_{op}|lm\rangle = \hbar^2 l(l + 1)\langle\theta\varphi|lm\rangle = \vec{L}^2_{op}\langle\theta\varphi|lm\rangle = \vec{L}^2_{op}Y_{lm}(\theta, \varphi)$.
With Eq.(9.106) use has been made of Eq.(9.90).
To derive Eq.(9.114) use have been made of Eq.(9.45).
The general result for the spherical harmonics is presented by Eq.(9.118). As mentioned by

Boccio, the algebra is complicated.
For the details see, e.g., Fitzpatrick, *Undergraduate Course,* Section 8.7, *Spherical Harmonics.*

## 9.3 Spin

Spin is the second kind of angular momentum.
The relations of orbital angular momentum need to be satisfied.

### 9.3.1 Spin ½

The Pauli spin operators are introduced.
Matrix Representations
Using the matrix elements of $S_z$, the Pauli spin operator $\sigma_z$ in matrix representation is obtained, Eq.(9.137).
For example the matrix element $\langle z\uparrow|\hat{S}_z|z\downarrow\rangle = \left\langle z\uparrow\left|-\frac{\hbar}{2}\right|z\downarrow\right\rangle = -\frac{\hbar}{2}\langle z\uparrow|z\downarrow\rangle = 0.$
The other Pauli matrix representation of the operator $S_x$, using raising and lowering operators, Eqs.(9.138) and (9.139), an example,
$\langle z\uparrow|\hat{S}_x|z\downarrow\rangle = \left\langle z\uparrow\left|\frac{\hat{S}_+\hat{S}_-}{2}\right|z\downarrow\right\rangle = \left\langle z\uparrow\left|\frac{\hbar}{2}\right|z\uparrow+0\right\rangle = \frac{\hbar}{2}\langle z\uparrow|z\uparrow\rangle = \frac{\hbar}{2}.$
In this way $\sigma_x$ is obtained, Eq.(9.140). Similarly $\sigma_y$, Eq.(9.141).
Properties of the $\hat{\boldsymbol{\sigma}}_i$
The commutation relations for the Pauli matrices are presented, Eq.(9.142).
Rotations in Spin Space
Eq.(9.152) presents the spin operator in the elements of the Cartesian basis for the unit vector.
Deriving Eqs.(159) and (9.160), use have been made of
$n_x^2 + n_y^2 + n_z^2 = 1.$
The calculations are presented also in spherical coordinates, Eqs.(9.163)-(9.165).
Plugging $n_z = \cos\theta$ into Eq.(9.160) gives:
$|\hat{n}+\rangle = \begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}\end{pmatrix}$ instead of $\begin{pmatrix}\cos\frac{\theta}{2}\\ e^{i\varphi}\sin\frac{\theta}{2}\end{pmatrix}.$
Let us present the derivation of the above result in more detail.
Substitute $n_z = cos\theta$, $n_x = sin\theta cos\varphi$, and $n_y = sin\theta sin\varphi$ into

$$\hat{S}_{op} = \frac{\hbar}{2}\begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix} \to \frac{\hbar}{2}\begin{pmatrix} cos\theta & sin\theta(cos\varphi - isin\varphi) \\ sin\theta(cos\varphi + isin\varphi) & -cos\theta \end{pmatrix}$$

$$\to \frac{\hbar}{2}\begin{pmatrix} cos\theta & e^{-i\varphi}sin\theta \\ e^{i\varphi}sin\theta & -cos\theta \end{pmatrix}.$$

The determinant to obtain the eigenvalues is:

$$\begin{vmatrix} cos\theta - \lambda & e^{-i\varphi}sin\theta \\ e^{i\varphi}sin\theta & -cos\theta - \lambda \end{vmatrix} = 0.$$

The equation for the eigenvalues is:

$$(cos\theta - \lambda)\cdot(-cos\theta - \lambda) - sin\theta\cdot\ sin\theta = \lambda^2 - 1 = 0 \to \lambda = \pm 1.$$

For the eigenvector $|\hat{n}+\rangle$ and eigenvalue $\lambda = 1$, the components of the eigenvector are $\beta_1$ and $\beta_2$.

$$\begin{pmatrix} cos\theta & e^{-i\varphi}sin\theta \\ e^{i\varphi}sin\theta & -cos\theta \end{pmatrix}\begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \to \frac{\beta_1}{\beta_2} = e^{-i\varphi}\frac{sin\theta}{1-cos\theta} = e^{-i\varphi}\frac{cos\frac{\theta}{2}}{sin\frac{\theta}{2}}.$$

Then, using normalization

$$|\hat{n}+\rangle = \begin{pmatrix} e^{-i\varphi}\cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}.$$

For the eigenvector $|\hat{n}-\rangle$ and eigenvalue $\lambda = -1$, we obtain

$$|\hat{n}-\rangle = \begin{pmatrix} -e^{-i\varphi}\sin\frac{\theta}{2} \\ cos\frac{\theta}{2} \end{pmatrix}.$$

Page 705: Any $2 \times 2$ *Hermitian matrix* $\hat{B}$ *can be written as the sum of four terms,*

$\hat{B} = a\sigma_x + b\sigma_y + c\sigma_z + dI,$

*where* $a, b, c,$ *and* $d$ *are real numbers.*

*Hence* $\hat{B} = a\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + b\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + c\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + d\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} c+d & a-ib \\ a+ib & -c+d \end{pmatrix} \to$ An Hermitian matrix: *the diagonal elements being real and the other two being conjugate complex.*

On pages 707-710 Boccio discussed rotations in spin space.

Fitzpatrick evaluate the subject matter in The Graduate Course pages76-78.

On page 709, Eq (9.190). to prevent confusion it is preferred to write for the product state, a product state is a product of two independent states,

$|\psi\rangle = |\psi_{external}\rangle \otimes |\psi_{internal}\rangle$ .

In Eq.(9.193) the formula for the total angular momentum of a spinning particle is presented: the sum of the orbital and spin angular momenta.

### 9.3.2 Super Selection Rules

Boccio starts with the $2\pi$ rotation transformation operator, Eq.(9.201).

At the bottom of page 710, Boccio mentioned $\hat{A}$ to be any physical observable. $\hat{A}$?

Eq.(9.210) is found by using Eq.(9.209).

Eq.(9.213) is obtained using Eq.(9.208).

### 9.3.3 A Box with 2 Slides

An example of a two-sided box using both the Schrödinger and Heisenberg pictures.

## 9.4 Magnetic Resonance

How to observe the spin of a particle?

The magnetic momentum operator, in non-relativistic quantum mechanics is the sum of the orbital momentum operator and the spin operator.

Eq.(9.247) represents the spin contribution to the Hamiltonian in a magnetic field.

See also Fitzpatrick 10.6 *Spin Precession* Undergraduate Course.

### 9.4.1 Spin Resonance

An oscillating magnetic field perpendicular to the applied field is added.

## 9.5 Addition of Angular Momentum

Boccio presented the special case of two spin ½ systems.
See also: Fitzpatrick chapter 11 and section 11.4, Undergraduate Course.

### 9.5.1 Addition of Two Spin ½ Angular Momenta

Two systems are defined. The operators for the two systems do commute, Eq.(9.132).

### 9.5.2 General Addition of two Angular Momenta

The operators and states are presented, page 732.

### 9.5.3 Actual Construction of States

In the beginning of this section Boccio presented the notation used, page 735.
For the second subsection of 9.5.3 “**Notation**”, I prefer “**Procedure**”.

## 9.6 Two- and Three- Dimensional Systems

The wave function representing such systems is given by Eq.(9.391).

### 9.6.1 2- and 3- Dimensional Infinite Wells

**2- Dimensional Infinite Square Well-Cartesian Coordinates**
The potential energy function is given in Eq.(9.394).
Two major changes with respect to the 1-Dimensional case:
- the energy level structure is more complex, Fig.9.4,
- degeneracy→ different sets of quantum numbers give the same energy eigenvalue.

### 9.6.2 Two-Dimensional Infinite circular well

The potential is given in Eq.(9.418).
In Figure 9.7 Boccio presented the energy levels of the infinite square and circular wells.
Next, Boccio dealt with the 3-dimensional infinite square and spherical wells.

### 9.6.3 3-Dimensional Finite well

The potential function in three dimensions is presented in Eq.(9.450).
A graphical solution is presented by Boccio Figure 9.16, page 751.

### 9.6.4 Two-Dimensional Harmonic Oscillator

The Hamiltonian for the two-dimensional oscillator is presented by Eq.(9.487).
The energy level structure is given in Table 9.1, page 753.
At the bottom of page 753, Boccio introduced the general rule: the existence of degeneracy indicates that there is another operator that commutes with the Hamiltonian operator.

### 9.6.5 What happens in 3 dimensions?

For Cartesian coordinates Boccio presented the energy eigenvalues in Eq.(9.557). An extension of the 2-dimensional case.
The energy levels and degeneracy are given in Table 9.6, page 760.

### 9.6.6 Two dimensional Finite Circular Well

The 2-dimensional finite well is considered to be a very difficult case.

### 9.6.7 The 3-Dimensional Delta Function

The delta function potential is given by Eq.(9.582).
The delta function is dealt with similarly to the 1-dimensional case.

### 9.6.8 The Hydrogen Atom

The potential is given by Eq.(9.604).
See also Mahan Section 5.4, Coulomb Potentials. There the nucleus is assumed to be fixed at the origin.
Boccio started with the equations of a two particle system. Then the two particle system is reduced to a particle with reduced mass in an external potential. Finally , the reduced mass is approximated by the mass of the electron, Eq.(9.162).

### 9.6.9 Algebraic Solution of the Hydrogen atom.

**Review of the Classical Kepler Problem**
The orbit equation of motion has been derived: Eq.(9.656).
**The Quantum Mechanical Problem**
The set of states are presented in Eq. (9.676),
with the ladder operators $\vec{I}_{op}^{\pm}$ defined in Eq.(9.673).
The degeneracy is given in Eq.(9.681).

### 9.6.10 The Deuteron

Boccio: "*A deuteron is a bound state of a neutron and a proton*".
The potential of the proton and neutron is such that the deuteron is weakly bound.
The potential is assumed to be a finite square well.

### 9.6.11 The Deuteron-Another Way.

Boccio mentioned the square well representation of the potential to be realistic.
The actual potential is given in Eq.(9.695).
The bound state energy ($l = 0$) is presented in Eq.(9.712).

### 9.6.12 Linear Potential

The linear central potential is presented in Eq.(9.7.13).
For $l > 0$ numerical methods needs to be applied to solve the differential equation given in Eq.(9.7.18).
Boccio analysed solutions for $l = 0$.
The allowed energies are given in Eq.(9.730).

### 9.6.13 Modified Linear Potential and Quark Bound States.

The quark-quark force is given by an effective potential, Eq.(9.734).
The energy levels are presented in Table 9.8

## 9.7 Problems

### 9.7.1 Position representation of the wave function.

A system is found in the state

$$\psi(\theta,\varphi) = \sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta\cos\varphi$$

(a) What are the possible values of $\hat{L}_z$ that measurement will give and with what probabilities?

(b) Determine the expectation value of $\hat{L}_x$ in this state.

**a)** For the spherical harmonics solution we write

$\psi(\theta,\varphi) = \sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta\cos\varphi = \sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta\,(\frac{e^{i\varphi}+e^{-i\phi}}{2})$.

With the spherical harmonics we know for $m = \pm1$:

$Y_{2,\pm1} = \mp\sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta\, e^{\pm i\varphi}$ or $Y_2^{\pm1} = \mp\sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta\, e^{\pm i\varphi}$ .

Then,

$\psi(\theta,\varphi) = \sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta\cos\varphi = \frac{1}{2}(-Y_{2,1} + Y_{2,1})$.

In the $(l,m)$ notation:

$\psi(\theta,\varphi) = \frac{1}{2}(-|2,1\rangle + |2,-1\rangle),\, l = 2, m = \pm1.$

With normalization

$\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta\, \psi(\theta,\varphi)^*\, \psi(\theta,\varphi) = \delta_{ll'}\delta_{mm'}$,

we obtain for the normalized state.

Obviously, evaluation of the integral gives the desired result. However, using

$\langle\psi|\psi\rangle = \frac{1}{4}(-\langle 2,1| + \langle 2,-1|)(-|2,1\rangle + |2,-1\rangle) = \frac{1}{2}$,

$\psi(\theta,\varphi) = \frac{1}{\sqrt{2}}(-|2,1\rangle + |2,-1\rangle)$.

We know

$L_z Y_{2,\pm1} = m\hbar Y_{2,\pm1} \rightarrow L_z = \pm\hbar \rightarrow$ consequently, the probability is $\frac{1}{2}$.

Hence, the expectation value of $L_z = 0$ .

This result, $L_z = 0$, is obtained also from evaluating the integral

$\langle L_z\rangle = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta\, \psi(\theta,\varphi)^* L_z\, \psi(\theta,\varphi) = m\hbar \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta\, \psi(\theta,\varphi)^*\, \psi(\theta,\varphi)$ .

**b)** $\langle L_x\rangle$?

With the raising and lowering operators:

$L_\pm = L_x \pm iL_y \rightarrow L_x = 1/2(L_+ + L_-)$.

So,

$\langle L_x\rangle = \frac{1}{2}\langle L_+ + L_-\rangle$.

Then, using the Dirac notation for the state and applying the raising and lowering operators:

$\frac{1}{2}\langle L_+ + L_-\rangle = \frac{1}{4}(-\langle 2,1| + \langle 2,-1|)(L_+ + L_-)(-|2,1\rangle + |2,-1\rangle) =$

$= \frac{1}{4}(-\langle 2,1| + \langle 2,-1|)(-|2,2\rangle + |2,-0\rangle - |2,0\rangle + |2,-2\rangle) = 0.$
$\langle L_x \rangle = 0$ .

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