

Quantum Mechanics in Texas. *The Undergraduate Course.*

Updated 2020-09-12 Sections 15.6-15.8

dr.l.noordzij@leennoordzij.nl

www.leennoordzij.me

Remarks, Questions and Exercises.

Based on the *Undergraduate Course* by Fitzpatrick, Professor of Physics

The University of Texas at Austin

<http://farside.ph.utexas.edu>

Quantum Mechanics, Home page for Richard Fitzpatrick.

1.Introduction.....	7
2. Probability Theory.	7
2.1 Introduction.....	7
2.2 What is probability?	7
2.3 Combining Probabilities.	7
2.4 Mean, Variance and Standard Deviation.....	8
2.5 Continuous Probability Distributions.	8
Exercises.	8
Exercise 2.1 About Russian Roulette	8
Exercise 2.2 About the speed of a car	9
Exercise 2.3 About the probability of decay.....	9
3 Wave-Particle Duality	10
3.1 Introduction.....	10
3.2 Wavefunctions.....	10
3.3 Plane Waves	10
3.4 Representation of Waves via Complex Functions	10
3.5 Classical Light Waves	10
3.6 Photoelectric Effect.	10
3.7 Quantum Theory of Light	10
3.8 Classical Interference of Light Waves.....	11
3.9 Quantum Interference of Light	11
3.10 Classical Particles.....	11

3.11 Quantum Particles	11
3.12 Wave Packets	12
3.13 Evolution of Wave Packets	12
3.14 Heisenberg's Uncertainty Principal	13
3.15 Schrödinger's Equation	13
3.16 Collapse of the Wave Function.....	13
Exercises.	13
Exercise 3.1 About a He-Ne laser	13
Exercise 3.2 The Ionization of a Hydrogen atom.....	14
Exercise 3.3 Planck's constant and the Work Function.....	14
Exercise 3.4 de Broglie Wavelength	15
Exercise 3.5 Electron Diffraction from a Crystal.....	16
Exercise 3.6 Group and Phase Velocities.....	17
Exercise 3.7 Application of the Uncertainty Principle	18
Exercise 3.8 Potential Energy	20
4 Fundamentals of Quantum Mechanics	20
4.1 Introduction.....	20
4.2 Schrödinger's Equation.....	20
4.3 Normalization of the Wavefunction.....	20
4.4 Expectation Values and Variances.....	21
4.5 Ehrenfest's Theorem	21
4.6 Operators.....	22
4.7 Momentum Representation.....	23
4.8 Heisenberg's Uncertainty Principle	24
4.9 Eigenstates and Eigenvalues.	25
4.10 Measurement	27
4.11 Continuous Eigenvalues.	29
4.12 Stationary States	32
Exercises.	33
Exercise 4.1 The spreading of wave lengths.....	33
Exercise 4.2 About expectation values and the variances for a given wave function	34
Exercise 4.3 One-dimensional particle in a box	35
Exercise 4.4 A one-dimensional bound particle and its momentum expectation value.....	35

Exercise 4.5 About a complex potential	36
Exercise 4.6 About degeneracy	37
Exercise 4.7 Proof the momentum operator to be a Hermitian operator	39
Exercise 4.8 About the collapse of the wave function	39
Exercise 4.9 About commutation	41
Exercise 4.10 About commutation and time dependency	41
5. One-Dimensional Potentials	45
5.1 Introduction	45
5.2 Infinite Potential Well	45
5.3 Square Potential Barrier	46
5.4 WKB Approximation	46
5.5 Cold Emission	47
5.6 Alpha Decay	48
5.7 Square Potential Well	48
5.8 Simple Harmonic Oscillator	51
Exercises.	52
Exercise 5.1 An infinite one-dimensional well	52
Exercise 5.2 The time evolution of the wave function	53
Exercise 5.3 A particle in an infinite square well expanded suddenly	54
Exercise 5.4 A potential step. Reflection and transmission	55
Exercise 5.5 A delta function potential, reflection and a bound state	56
Exercise 5.6 Two potential wells and tunneling	57
Exercise 5.7 Bound particle in a half-infinite well	60
Exercise 5.8 About the energy eigenstates of the harmonic oscillator	61
6 Multi-Particle Systems	62
6.1 Introduction	62
6.2 Fundamental concepts	62
6.3 Non-Interacting Particles	62
6.4 Two-Particle Systems	62
6.5 Identical particles.	63
Exercises. (N.B. Neglect spin in the following questions.)	66
Exercise 6.1 Two non-interacting particles and three states	66
Exercise 6.2 Two non-interacting particles and the harmonic oscillator potential	67

Exercise 6.3 Two non-interacting particles in a box.....	68
Exercise 6.4 Two particles in a one-dimensional box.....	70
7 Three-Dimensional Quantum Mechanics.....	70
7.1 Introduction.....	70
7.2 Fundamental concepts	70
7.3 Particle in a box	71
7.4 Degenerate Electron Gases	71
7.5 White-Dwarf Stars	71
Exercises	71
Exercise 7.1 A particle in a three-dimensional isotropic harmonic oscillator	71
Exercise 7.2 Fermi energy for the relativistic case	72
Exercise 7.3 The density of states of an electron gas in a box of volume L^3	72
Exercise 7.4 The density of states in a square L^2	73
Exercise 7.5 The Fermi energy for free electrons in copper	73
Exercise 7.6 Fermi energy of an electron in a white dwarf star.....	73
8 Orbital Angular momentum	74
8.1 Introduction.....	74
8.2 Angular Momentum Operators.....	74
8.3 Representation of Angular Momentum	75
8.4 Eigenstates of Angular Momentum	75
8.5 Eigenvalues of L_z	75
8.6 Eigenvalues of L^2	75
8.7 Spherical Harmonics.....	76
Exercises	76
Exercise 8.1 Expectation values of momentum operators.....	76
Exercise 8.2 The eigenvalues and eigenfunctions of L_x	78
Exercise 8.3 The probabilities of the results of the measurements of the momentum operators	79
Exercise 8.4 Eigenvalues of the Hamiltonian of an axially symmetric rotator	81
9 Central Potentials	81
9.1 Introduction.....	81
9.2 Derivation of Radial Equation.....	81
9.3 Infinite Potential Well.....	81
9.4 Hydrogen atom.....	82

9.5 Rydberg Formula	83
Exercises	83
Exercise 9.1 The ground-state of a particle in a spherical well	83
Exercise 9.2 The three-dimensional harmonic oscillator	84
Exercise 9.3 About the wavefunction for the ground-state of a hydrogen-like atom	86
Exercise 9.4 Decay of the nucleus of a tritium atom.....	88
Exercise 9.5 Wavelengths of emitted photons.....	88
Exercise 9.6 About hydrogen's recoil energy emitting a photon	88
10 Spin Angular Momentum	89
10.1 Introduction.....	89
10.2 Spin Operators.....	89
10.3 Spin space	90
10.4 Eigenstates of S_z and S^2	90
10.5 Pauli Representation	90
10.6 Spin Precession.....	91
Exercises	91
Exercise 10.1 The Pauli representations of S_x , S_y and S_z for spin-1 particle.....	91
Exercise 10.2 Pauli representation of normalized states S_x and S_y for a spin-1/2 particle.....	92
Exercise 10.3 A spin-1/2 particle and the probabilities of a measurement of S_z	93
Exercise 10.4 An electron spin-state: normalizing, values of S_z , S_x and S_y . Probabilities.	94
Exercise 10.5 a spin-1/2 system represented by a normalized spinor. Probability of S_y	96
Exercise 10.6 An electron at rest in an oscillating magnetic field.....	97
11 Addition of Angular Momentum	99
11.1 Introduction.....	99
11.2 General principles.....	99
11.3 Angular momentum in the Hydrogen Atom.	100
11.4 Two Spin One-Half Particles	104
Exercises.	105
Exercise 11.1 . An electron in a hydrogen atom occupies the combined spin(angular and spin) and position state.....	105
Exercise 11.2 The Potential Energy of a Proton-Neutron System.....	106
Exercise 11.3 Two Electrons in a Spin Singlet State	109
Intermezzo singlet state.	109

12 Time-Independent Perturbation Theory	111
12.1 Introduction.....	111
12.2 Improved Notation	111
12.3 Two-State system.	111
12.4 Non-Degenerate Perturbation Theory	113
12.5 Quadratic Stark Effect	114
12.6 Degenerate Perturbation Theory	115
12.7 Linear Stark Effect.	115
12.8 Fine Structure of Hydrogen	116
12.9 Zeeman Effect.....	122
12.10 Hyperfine Structure	125
No Exercises.....	126
13 Time-dependent Perturbation Theory	126
13.1 Introduction.....	126
13.2 Preliminary Analysis	126
13.3 Two-State System.....	127
13.4 Spin Magnetic Resonance	127
13.5 Perturbation Expansion	128
13.6 Harmonic Perturbations	128
13.7 Electromagnetic Radiation	129
13.8 Electric Dipole Approximation.....	130
13.9 Spontaneous Emission.....	131
13.10 Radiation from a Harmonic Oscillator.....	131
13.11 Selection Rules	131
13.12 $2P \rightarrow 1S$ Transitions in Hydrogen	132
13.13 Intensity Rules	133
13.14 Forbidden Transitions.....	134
No Exercises.....	134
14 Variational Methods.....	134
14.1 Introduction.....	134
14.2 Variational principle	134
14.3 Helium atom	134
14.4 Hydrogen Molecule Ion	134

No Exercises.....	135
15 Scattering Theory.	135
15.1 Introduction.....	135
15.2 Fundamentals.....	135
15.3 Born Approximation	136
Intermezzo: Yukawa Potential and Bound States	136
15.4 Partial Waves.....	137
15.5 Determination of Phase-Shifts	137
15.6 Hard Sphere Scattering.....	138
15.7 Low Energy Scattering.	138
15.8 Resonances.....	139
No exercises.....	139
End of the under-graduate course.	139
Literature	139

1.Introduction

In the introduction the intended audience, major sources, aim of course and outline of the course are given.

2. Probability Theory.

2.1 Introduction

A brief introduction of probability theory is presented.

2.2 What is probability?

Attention is given to the scientific definition of probability.

2.3 Combining Probabilities.

Two possible combination are presented:

- a combination of two mutually exclusive outcomes X and Y . The probability of the outcome X or the outcome Y is the sum of the individual probabilities.
- a combination of statistically independent observations. The probability of the outcomes X and Y is the product of the individual probabilities.

2.4 Mean, Variance and Standard Deviation.

In this section the entities as mean etc are defined.

Remark: On page 10 Fitzpatrick writes: “The variance of u (the general variable) is proportional to the square of the scatter of u around its mean value”. I suppose the proportionality factor to be the probability $P(u_i)$

2.5 Continuous Probability Distributions.

In this section the variable u can take a continuous range of possible values.

Exercises.

Exercise 2.1 About Russian Roulette

This exercise is about Russian roulette, a rough start for an undergraduate course.

In this game a player inserts a single cartridge into the drum of a revolver, leaving the other five chambers empty. The player then spins the drum and pulls the trigger.

Remark: I assume the drum is spun each time the trigger is pulled. This assumption is based on playing the game N times. Otherwise N max is 5 and ‘game over’ for $N = 6$.

a) what is the probability of the player still being alive after playing the game N times.

The probability to get killed is $1/6$. So the probability of staying alive is $5/6$.

After playing N times, the probability of staying alive is: $(5/6)^N$ and being dead is $1 - (5/6)^N$.

b) what is the probability of the player surviving $N - 1$ turns in this game, and then being shot the N th time the trigger is pulled.

The probability to get killed is $1/6$. So the probability to survive the $N - 1$ round and to get killed in the N th round is: $\frac{1}{6} (5/6)^{N-1}$.

what is the mean number of times the player gets to pull the trigger?

The mean number or expectation value is:

$$E(N) = \langle N \rangle = \sum_{n=1}^{\infty} \left(\frac{5}{6}\right)^n n. \quad (C2.1)$$

We subtract the series $\frac{5}{6} E(N)$ from Eq. (C2.1) and obtain

$$\left(1 - \frac{5}{6}\right) E(N) = \frac{5}{6} + \left(\frac{5}{6}\right)^2 + \left(\frac{5}{6}\right)^3 + \dots \quad (C2.2)$$

$$\text{For } n \rightarrow \infty \text{ the sum is: } \lim_{n \rightarrow \infty} \frac{5}{6} \left(\frac{1 - \left(\frac{5}{6}\right)^n}{1 - \frac{5}{6}}\right). \quad (C2.3)$$

$$\text{Hence } \langle N \rangle = \sum_{n=1}^{\infty} \left(\frac{5}{6}\right)^n, n = 30.$$

So a drum with more chambers is preferable.

Now a few remarks without spinning of the drum after pulling the trigger.

After one round the probability of survival is, as in the above case, $5/6$.

After two rounds, since one chamber has been used, the probability of survival is $4/5$, etc.

Consequently, the probability of being dead after the third round is $\frac{5}{6} \times \frac{4}{5} \times \frac{1}{4}$. But that is not the whole story. You have to add the probabilities of the preceding two rounds.

The probability of death after the first round: $\frac{1}{6}$,

The probability of death after the second round: $\frac{5}{6} \times \frac{1}{5}$,

The probability of death after the third round: $\frac{5}{6} \times \frac{4}{5} \times \frac{1}{4}$.

So the probability of being dead after the third round is the sum of the three above probabilities: $\frac{1}{2}$.

This equals the number of rounds times $\frac{1}{6}$.

In this case the answer to the question of being dead after playing the game $N(N \leq 5)$ times is $N \times \frac{1}{6}$. So being alive equals: $1 - N \times \frac{1}{6}$.

Exercise 2.2 About the speed of a car

Suppose the probability density for the speed s of a car on a road is given by:

$$P(s) = As \cdot \exp\left(-\frac{s}{s_0}\right),$$

where $0 \leq s \leq \infty$. Here, A and s_0 are positive constants. $P(s)ds$ is the probability of finding the car's speed in the interval between s and $s + ds$.

a) Determine A in terms of s_0 .

$$\text{So } \int_0^{\infty} A s \exp\left(-\frac{s}{s_0}\right) ds = 1.$$

Integration by parts gives: $A = s_0^{-2}$.

b) What is the mean value of the speed? With $A = s_0^{-2}$ the mean value is:

$$\langle s \rangle = \int_0^{\infty} A s^2 \exp\left(-\frac{s}{s_0}\right) ds, \text{ gives } \langle s \rangle = 2s_0.$$

c) What is the "most probable" speed: *i.e.*, the speed for which the probability density has a maximum?

$$\text{With } A = s_0^{-2}, P(s) = s_0^{-2} s \cdot \exp\left(-\frac{s}{s_0}\right).$$

Now $\frac{dP}{ds} = 0$ gives: $s = s_0$.

d) What is the probability that a car has a speed more than three times as large as the mean value? The mean value is $2s_0$.

This means to determine the integral $\int_{6s_0}^{\infty} s_0^{-2} s \exp\left(-\frac{s}{s_0}\right) ds$.

Again, integration by parts results into the probability to be $2e^{-6s_0}$.

Exercise 2.3 About the probability of decay

A radioactive atom has a uniform decay probability per unit time w : *i.e.* the probability of decay in a time interval dt is $w dt$. Let $P(t)$ be the probability of the atom not having decayed at time t , given that it was created at time $t = 0$. Demonstrate that

$$P(t) = e^{-wt}.$$

The probability P_d of having decayed should be

$$P_d = 1 - e^{-wt}.$$

Hence $\lim_{t \rightarrow \infty} P_d = 1$. So $P(t) = e^{-wt}$ seems to be correct. A demonstration, not a proof.

What is the mean lifetime of the atom?

By definition: $\langle t \rangle = \int_0^\infty t e^{-wt} dt$.

Integration by parts: $\langle t \rangle = \frac{1}{w}$.

3 Wave-Particle Duality

3.1 Introduction

Fitzpatrick examines in this chapter how wave-particle duality shapes the general features of quantum mechanics.

3.2 Wavefunctions

The wave functions are defined. The general features of wavefunctions are discussed.

3.3 Plane Waves

The plane wave is introduced by the one-dimensional wave. The three-dimensional plane wave function is presented.

3.4 Representation of Waves via Complex Functions

Instead of the cos function the exponential is used.

3.5 Classical Light Waves

The classical electromagnetic wave theory is presented. The physical electric field is given and the energy density of a light wave.

Remark:

On page 16 Fitzpatrick gave the formula:

$$e^{i\phi} \equiv \cos \phi + i \sin \phi$$

and denoted this expression as *de Moivre's theorem*. I assume this expression to be *Euler's Formula*.

de Moivre's theorem is

$$(\cos \phi + i \sin \phi)^n = \cos n\phi + i \sin n\phi.$$

3.6 Photoelectric Effect.

In this section Fitzpatrick presented the photoelectric effect. He also mentioned photoelectrons. I do not know these kinds of beasts. May be this is shorthand for emitted electrons by action of photons.

3.7 Quantum Theory of Light

In this subsection the energy and momentum of photons is presented.

Expression to be remembered:

$$E = \hbar\omega, (3.34),$$

$$p = \frac{E}{c}, (3.35),$$

and

$$p = \hbar k, (3.36).$$

3.8 Classical Interference of Light Waves

With help of the double-slit interference experiment, Figure 3.5, the width of the equally spaced light and dark bands has been derived.

The slits are a distance d apart. The light is projected on a screen a distance D behind the slits.

A point on the screen, a distance y from the centre-line, is chosen at a distance x_1 behind one slit and a distance x_2 behind the other slit.

To find Eq. (3.37) we have two equations:

$$\left(y - \frac{d}{2}\right)^2 + D^2 = x_1^2,$$

and

$$\left(y + \frac{d}{2}\right)^2 + D^2 = x_2^2.$$

Subtracting both equations leads to $\Delta x \equiv x_2 - x_1 = \frac{2yd}{x_1 + x_2}$.

With $d \ll D$ and $x_1 + x_2 \cong 2D$, the expression for $\Delta x \cong \frac{d}{D}y$ (Eq. (3.37)).

Eq. (3.41) is obtained by using:

$$|\psi(y, t)|^2 = |e^{ikx_1} + e^{ikx_2}|^2 = (\cos kx_1 + \cos kx_2)^2 + (\sin kx_1 + \sin kx_2)^2 =$$

$$2(1 + \cos k\Delta x) = 4\cos^2 \frac{k\Delta x}{2}.$$

Set $\Delta x = \lambda$ in Eq. (3.37) and Eq. (3.42) is found.

3.9 Quantum Interference of Light

The double slit experiment is considered from a quantum mechanical point of view.

3.10 Classical Particles

Fitzpatrick mentioned to concentrate on non-relativistic particles of non-zero mass.

Expressions to be remembered:

$$v = \frac{p}{m}, \quad (3.45),$$

and

$$E = \frac{p^2}{2m}, \quad (3.46).$$

3.11 Quantum Particles

In this section the relation between momentum and wave number for a quantum particle is presented.

The de Broglie wave length for an electron has been presented (Eq.3.48).

Remark: I assume this to be the wave length of a non-relativistic particle, since in section 3.10 Fitzpatrick mentioned in this course to concentrate on the behaviour of non-relativistic particles.

Fitzpatrick derived the phase velocity and found it to be half of the classical particle velocity.

In section 3.12 Fitzpatrick looks more closely into this.

3.12 Wave Packets

In this section it follows the phase velocity to be half of the classical particle velocity. This does not have any real physical consequences.

Fitzpatrick showed an important property of wave packets:

- to construct a wave packet which is localized in x -space, you need a wide range of k -values.
- to combine plane waves with a small range of k -values, the resulting wave packet is smeared out in x -space.

3.13 Evolution of Wave Packets

The question to be answered in this section is: how does the wavefunction evolve in time?

Remark: in Eq. (3.73) dk is missing, a typo.

Eq. (3.79) : $\alpha = \frac{d^2 \omega(k_0)}{dk^2}$. This is a bit confusing. I prefer: $\alpha = \frac{d^2 \omega(k)}{dk^2}$.

With Eq. (3.53), $\omega = \frac{\hbar k^2}{2m}$, we have $\alpha = \frac{\hbar}{m}$.

Eq. (3.87) represents the wave packet as a function of time and position.

In this expression you will find the function $\sigma(t)$ represented by Eq.(3.86). This expression is related to the denominator in the wave function $\psi(x, t)$, Eq. (3.85) :

$$\sqrt{1 + i2\alpha(\Delta k)^2}.$$

To calculate the probability density it is convenient to write the denominator $\sqrt{1 + i2\alpha(\Delta k)^2}$ in polar representation. After multiplying with the complex conjugate, the resulting expression for the denominator is:

$$\sqrt{1 + (4\alpha)^2(\Delta k)^4 t^2}.$$

We learned, Eq. (3.70), $\Delta x \Delta k = \frac{1}{2}$. Plug this into $\sqrt{1 + (2\alpha)^2(\Delta k)^4 t^2}$ and we have:

$$\frac{1}{\Delta x} \sqrt{(\Delta x)^2 + \frac{\alpha^2 t^2}{4(\Delta x)^2}}. \text{ This equal } \frac{1}{\Delta x} \sigma(t).$$

Since Fitzpatrick presented the probability density, Eq. (3.87) proportional to a function of x and t , I assume the number Δx to be absorbed in the proportionality factor. Δx is a scaling factor for the width of the *Gaussian* distribution (page 27).

At the bottom of page 31 Fitzpatrick writes: "...the group velocity, $v_g = d\omega/dt$." In Eq. (3.89) $v_g = d\omega/dk$. This is the correct expression.

At the top of page 32, Fitzpatrick gave the characteristic time for a wave packet of original width Δx to double in spatial extent, Eq. (3.91). The probability distribution, Eq. (3.86) is Gaussian of characteristic width:

$$\sigma = \sqrt{(\Delta x)^2 + \left(\frac{\hbar}{m}\right)^2 \frac{t^2}{4(\Delta x)^2}}, \text{ where use has been made of } \alpha = \frac{\hbar}{m}.$$

So to double σ in spatial extension, $\Delta x \rightarrow 2\Delta x$, we plug into the expression for $\sigma = 2\Delta x$:

$$3(\Delta x)^2 = \left(\frac{\hbar}{m}\right)^2 \frac{t^2}{4(\Delta x)^2}, \text{ and we obtain } t \sim \frac{m}{\hbar} (\Delta x)^2.$$

3.14 Heisenberg's Uncertainty Principal.

Fitzpatrick derived Heisenberg's uncertainty principle using $\Delta x \Delta k \geq \frac{1}{2}$.

Keep in mind Δx to be the initial value, a number, of the characteristic width of the wave packet. So, as Fitzpatrick mentioned, the wave packet stays the same in k -space.

On page 33 the equation of the special extent σ large t , Eq. (3.94), is given.

As obtained in 3.13, $\sigma = \sqrt{(\Delta x)^2 + \left(\frac{\hbar}{m}\right)^2 \frac{t^2}{4(\Delta x)^2}}$. For large t , σ can be approximated by

$$\sigma \sim \frac{\hbar t}{m \Delta x}, \text{ with } \frac{\hbar t}{m \Delta x} \gg \Delta x.$$

On page 33 and 34 Fitzpatrick described the Heisenberg's microscope. With this microscope the scattering of a photon by an electron.

By the change in the x - component of the wave vector the uncertainty principle is derived.

Use has been made of $\Delta x = \frac{\lambda}{2\alpha}$ and $k = \frac{2\pi}{\lambda}$. Here α , assumed to be small, is the half-angle subtended by the lens at the electron.

3.15 Schrödinger's Equation

In this subsection Schrödinger's equation is derived.

This is done by balancing the time derivative and the second position derivative of the wave function of a free particle.

Fitzpatrick gave in addition the Schrödinger's equation for a particle moving in a potential.

3.16 Collapse of the Wave Function.

The theoretical part of chapter 3 concluded with the measurement of the particle's position and the collapse of the wave function.

Exercises.

Exercise 3.1 About a He-Ne laser

A He-Ne laser emits radiation of wavelength $\lambda = 633$ nm. How many photons are emitted per second by a laser with a power W of 1 mW? What force does such laser exert on a body which completely absorbs its radiation?

The energy of the n photons per second emitted by the laser for the given wave length is:

$$nE,$$

where the energy of the photon

$$E = \frac{2\pi\hbar c}{\lambda}.$$

$$\text{Hence } n \frac{2\pi\hbar c}{\lambda} = W, \text{ and } n = \frac{\lambda W}{2\pi\hbar c}.$$

Now we have a beam of photons n photons per second hitting an object. The object perfectly adsorbs photons.

The amount of momentum imparted to the object per unit of time $\frac{dp}{dt}$, the force F , equals the momentum of the photons $n\hbar k$:

$$\frac{dp}{dt} = n2\pi\hbar k.$$

So the force exerted on the object is:

$$F = n2\pi\hbar k = \frac{\lambda W}{2\pi\hbar c} 2\pi\hbar k .$$

With $k = \frac{2\pi}{\lambda}$, we finally obtain for the force $F = 2\pi \frac{W}{c}$.

A cheque on dimensions: $[F] = \left[\frac{W}{c}\right] = \left[\frac{Nm/sec}{m/sec}\right] = [N]$.

Exercise 3.2 The Ionization of a Hydrogen atom

The ionization energy of a hydrogen atom in its ground state is $E_{ion} = 13.6$ eV (1 eV is the energy acquired by an electron accelerated through a potential difference of 1 V). Calculate the frequency, wavelength, and wave number of the electromagnetic radiation which will just ionize the atom.

$$E = 2\pi\hbar\nu .$$

$$\text{Furthermore } \nu = \frac{\omega}{2\pi} = \frac{kc}{2\pi} ,$$

$$\text{In addition } k = \frac{2\pi}{\lambda} .$$

So we have :

$$\nu = \frac{E}{h}, \lambda = \frac{c}{\nu}, \text{ and } k = \frac{2\pi}{\lambda} .$$

$$1 \text{ eV} = 1.60218 \cdot 10^{-19} \text{ J},$$

and

$$J = 1 \text{ Nm}.$$

Exercise 3.3 Planck's constant and the Work Function

The maximum energy of photoelectrons(?) from aluminium is 2.3 eV for radiation of wavelength 2000 Å, and 0.90 eV for radiation of wavelength 2580 Å . Use this data to calculate Planck's constant, and the work function of aluminium.

So this is about the photoelectric effect.

The work function W is the energy required by the electron to be emitted from the surface of a solid. The formula we will use is given by Eq. (3.33):

$$K = 2\pi\hbar\nu - W ,$$

where K is the kinetic energy of the electron.

Given are two energy levels and two wavelengths. Now we know two points of the straight line represented by $K = 2\pi\hbar\nu - W$.

After some algebra we obtain:

$$2\pi\hbar = \frac{K_1 - K_2}{\nu_1 - \nu_2} .$$

With $\nu = \frac{c}{\lambda}$, we rewrite the expression for Planck's constant:

$$2\pi\hbar = \frac{\lambda_1 \lambda_2 (K_1 - K_2)}{c(\lambda_2 - \lambda_1)} .$$

On the right hand side of the latter expression for \hbar , all the quantities are given.

$$\text{With } 1 \text{ eV} = 1.60218 \cdot 10^{-19} \text{ J and } 1 \text{ Å} = 10^{-10} \text{ m}.$$

$$\text{Then we find for } 2\pi\hbar = 6.651 \cdot 10^{-34} \text{ Js}.$$

Now the work function. We use 1 of the given points on the line $K = 2\pi\hbar\nu - W$:

$$W = 2\pi\hbar \frac{c}{\lambda_1} - K_1 .$$

With the known quantities on the right hand side of the expression for W we find:

$$W = 3.9 \text{ eV}.$$

www.Wikipedia.org gives for Al: 4.06-4.26 eV.

Exercise 3.4 de Broglie Wavelength

Show that the de Broglie wave length of an electron accelerated from rest across a potential difference V is given by:

$$\lambda = 1.29 \times 10^{-9} V^{-1/2} \text{ m},$$

where V is measured in Volts.

In section 3.11 on *Quantum Particles* Fitzpatrick presented the *de Broglie wavelength*:

$$\lambda = \frac{2\pi\hbar}{p} .$$

In addition Fitzpatrick introduced the wave length of an electron with the electron energy E measured in electron-volts (eV):

$$\lambda_e = 1.2 \times 10^{-9} [E(\text{eV})]^{-1/2} \text{ m}. \quad (3.48)$$

The energy obtained by the electron due to acceleration from rest across a potential difference V equals V . So I don't understand the different factors 1.2 and 1.29.

The derivation of the de Broglie wave length can be found in textbooks on Physics.

The final velocity u obtained by the electron in crossing the potential difference V is found from:

$$V = \frac{1}{2} mu^2 . \text{ (Remark: } u \text{ is the particle velocity.)}$$

de Broglie equated mu^2 with $\hbar v$, the energy given in Planck's equation .

Furthermore, for the electron we have $v = \frac{u}{\lambda}$ (Remark: u in the expression $v = \frac{u}{\lambda}$ represents the phase velocity. Except for photons the phase velocity differs from the group velocity or particle velocity).

So, we have:

$$mu^2 = 2\pi\hbar \frac{u}{\lambda} . \text{ (Remark: on the left-hand side we have } mu^2 . \text{ In deriving the de Broglie wave length apparently, } u \text{ on the left hand side is also considered to be the phase velocity.)}$$

With the expression for the potential $V = \frac{1}{2} mu^2$, we arrive at the expression for the wave length to be:

$$\lambda = \frac{2\pi\hbar}{mu} = \frac{2\pi\hbar}{(2m)^{1/2}} (V)^{-1/2} \text{ m}.$$

Remark: in this expression for the de Broglie wave length the particle and the phase velocity are the same. I do not consider this to be correct. When I set in $E = mu^2$ and in $V = \frac{1}{2} mu^2$, the velocity u equal to the particle or group velocity, I would have found the de Broglie wave length half the wave length given by $\lambda = \frac{2\pi\hbar}{mu} = \frac{2\pi\hbar}{(2m)^{1/2}} (V)^{-1/2} \text{ m}$. See Eqs. (3.53)-(3.55).

Here we assume $u \ll c$; the non-relativistic approach.

Now we plug in some numbers:

$$m = 9.109 \times 10^{-31} \text{ kg},$$

$$\hbar = 1.0546 \times 10^{-34} \text{ Js}.$$

$$\text{Keep in mind to use eV: } 1\text{J} = \frac{1}{1.602} \times 10^{19} \text{ eV}.$$

Hence:

$$\lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.109 \times 10^{-31}}} \frac{1}{\sqrt{V \times 1.602 \times 10^{-19}}} = 1.23 \times 10^{-9} (V)^{-1/2} \text{ m},$$

and V given in eV.

The number 1.23 is in the range of 1.2 and 1.29 .

Remark: Do we have an idea for which value of V the non-relativistic approach to be acceptable?

A textbook of physics gives us the relativistic mass to be:

$$m = \frac{m_0}{\sqrt{1 - \left(\frac{u}{c}\right)^2}}, \text{ where } m_0 \text{ represents the rest mass.}$$

An expansion of the square root with respect to $\left(\frac{u}{c}\right)^2$ gives:

$$m = m_0 \left(1 + \frac{1}{2} \left(\frac{u}{c}\right)^2 + \frac{3}{8} \left(\frac{u}{c}\right)^4 + \dots \right).$$

Assume $\left(\frac{u}{c}\right)^2$ to be of $O(0.1)$.

Then we have $u^2 \cong .1 \times c^2$. Multiply both sides of this expression with $m/2$, use the approximation for m and include only the first term of the expansion:

we find:

$$\frac{1}{2} m u^2 = V \cong \frac{m_0 c^2}{20} \left(1 + \frac{1}{20} \right).$$

Now we plug in some numbers and use eV, we obtain the potential difference to be of the order:

$$V = 10 \text{ kV}.$$

This number for V can be found in www.hyperphysics.phy.astr.gsu.edu : “Thresholds for Relativistic Effects”.

Exercise 3.5 Electron Diffraction from a Crystal

If the atoms in a regular crystal are separated by $3 \times 10^{-10} \text{ m}$, demonstrate that an accelerating voltage of about 1.5 kV would be required to produce an electron diffraction pattern from the crystal.

On page 25 Fitzpatrick writes:

“In general, in order to perform an effective interference experiment, the spacing of the slits must not be too much greater than the wave length of the (particle) wave. Hence, particle interference experiments require either extremely low energy particles (since $\lambda \propto E^{-1/2}$), or very closely spaced slits. Usually the “slits” consist of crystals, which act a bit like diffraction gratings with a characteristic spacing of the inter-atomic spacing (which is generally about 10^{-9} m).”

We have for the particle(electro) wave length:

$$\lambda_e = 1.2 \times 10^{-9} [E(\text{eV})]^{-1/2} \text{ m (Eq. 3.48)}.$$

Now the accelerating voltage of 1.5 kV gives the electron an energy of 1500 eV

Plugging this value into Eq. (3.48) gives

$$\lambda_e = \frac{1.2}{\sqrt{15}} \times 10^{-9} \text{ m.}$$

Or $\lambda_e \cong .3 \times 10^{-9} \text{ m}$. This comes close to the inter-atomic spacing.

Exercise 3.6 Group and Phase Velocities

The relationship between wavelength and frequency for electromagnetic waves in a waveguide is:

$$\lambda = \frac{c}{\sqrt{v^2 - v_0^2}},$$

where c is the velocity of light in vacuum. What are the group and phase velocities of such waves as functions of v_0 and λ ?

Well, in *Feynman's Lectures on Physics*, chapter 24 Vol. II, a lot more about Waveguides can be found.

To start with, we rewrite the equation for the wave length in terms of wavenumber and angular frequency:

$$k = \pm \sqrt{\left(\frac{\omega}{c}\right)^2 - \left(\frac{\omega_0}{c}\right)^2}.$$

This expression for the wavenumber comes pretty close to Eq. (24.20), Feynman.

ω_0 is the cut-off frequency of the wave guide.

Here we choose the right going wave.

Now, we derive the dispersion relation from the expression for the wave number.

So,

$$\omega = \sqrt{k^2 c^2 + \omega_0^2}.$$

For the phase velocity we obtain:

$$v_p = \frac{\omega}{k} = \sqrt{c^2 + (\lambda v_0)^2}.$$

The phase velocity is greater than the speed of light.

As is explained in the *Feynman Lectures*, "... that phase velocities greater than light are possible, because it is just the nodes of the wave which are moving and not energy or information."

To find out about how fast signals will travel we need the group velocity:

$$v_g = \frac{d\omega}{dk}.$$

Differentiating the dispersion relation $\omega = \sqrt{k^2 c^2 + \omega_0^2}$, and rewriting the resulting equation in terms of wave length and frequency, we have:

$$v_g = \frac{c^2}{\sqrt{c^2 + (\lambda v_0)^2}}.$$

Or with the expression for the phase velocity $v_p = \sqrt{c^2 + (\lambda v_0)^2}$:

$$v_p v_g = c^2.$$

Completely similar to Eq. (24.28) in Feynman.

Exercise 3.7 Application of the Uncertainty Principle

Nuclei, typically of size 10^{-14} m, frequently emit electrons with energies of 1-10 MeV

Use the uncertainty principle to show that electrons of energy 1MeV could not be contained in the nucleus before decay.

Remark: What is the meaning of: “*electrons of energy 1MeV could not be contained in the nucleus before decay*”? Is Fitzpatrick saying the electrons with this amount of energy are emitted? Well, I could imagine this to be called decay: beta-decay for example. However, then this exercise makes no sense to me.

On the other hand electrons of energy are non-relativistic? In Exercise 3.4, I found the non-relativistic approach no longer feasible for energy levels of the order of 10 keV (and higher). So, what to do?

Let us find some numbers.

$$1 \text{ MeV} = 1.60218 \times 10^{-13} \text{ J} = E = \hbar\omega.$$

$$\omega = 2\pi\nu = \frac{2\pi u_{ph}}{\lambda}. \text{ In this expression } u_{ph} \text{ is the phase velocity.}$$

For the wave length λ we plug in the de Broglie wavelength(Eq. (3.48)) with $E = 1\text{MeV}$:

$\lambda = 1.2 \times 10^{-9} \times 10^{-3} = 1.2 \times 10^{-12}$ m. This number is 100 times the size of the nuclei. Wait a moment. This de Broglie wavelength is based on non-relativistic quantum mechanics. So, what is the meaning of this? I will come back to this question later on.

With $\hbar\omega = h\nu = 1.60218 \times 10^{-13}$ we have :

$$\nu = 2.418 \times 10^{20} \text{ (1/sec).}$$

The de Broglie wavelength and this frequency we find for the phase velocity:

$$u_{ph} = \frac{\omega}{k} = \lambda\nu = 2.9 \times 10^8 \text{ m/sec,}$$

pretty close to c .

What do we obtain for the particle velocity, i.e. the group velocity?

Well, using the non-relativistic dispersion relation Eq. (3.53), the result is:

$$u_g = \frac{d\omega}{dk} = \frac{\hbar k}{m} = 2u_{ph}.$$

So the particle, wave packet velocity, is $\approx 2c$.

This leads us to the relativistic approach, www.pa.uky.edu , for a particle with a speed u_g .

For the phase velocity we have: $u_{ph} = \frac{\omega}{k} = \lambda\nu$.

$$\text{Energy: } E = h\nu = mc^2 = \gamma m_0 c^2.$$

$$\text{Hence } \nu = \frac{\gamma m_0 c^2}{h},$$

$$\text{where } m_0 \text{ is the rest mass and } \gamma = \frac{1}{\sqrt{1 - (\frac{u_g}{c})^2}}.$$

For momentum we have

$$p = \gamma m_0 u_g = \frac{h}{\lambda}.$$

$$\text{Hence } \lambda = \frac{h}{\gamma m_0 u_g}.$$

Now we have the ingredients for the phase velocity:

$$u_{ph} = \lambda v = \frac{h}{\gamma m_0 u_g} \frac{\gamma m_0 c^2}{h} = \frac{c^2}{u_g}.$$

Nota bene: this expression for the relation between phase velocity, group velocity and c we also found in Exercise 3.5 on wave guides.

We know $u_g < c$, so $u_{ph} > c$.

The group velocity:

To find the group velocity use is made of the relation between phase velocity, angular frequency and the wavenumber.

We have with the phase velocity $u_{ph} = \frac{\omega}{k} = \frac{c^2}{u_g}$:

$$u_g = \frac{kc^2}{\omega}.$$

In addition the dispersion relation can be found.

Let's start with the energy:

$$E = h\nu = \hbar\omega = mc^2 = \gamma m_0 c^2.$$

Substitute the expression $\gamma = \frac{1}{\sqrt{1-(\frac{u_g}{c})^2}}$ into the expression for $E = \hbar\omega = \gamma m_0 c^2$, use

$u_g = \frac{kc^2}{\omega}$, hence we have for the dispersion relation:

$$\omega = \sqrt{(kc)^2 + \left(\frac{m_0 c^2}{\hbar}\right)^2}.$$

As a cheque you can differentiate the dispersion relation with respect k giving:

$$\frac{d\omega}{dk} = \frac{kc^2}{\omega}, \text{ the group velocity.}$$

The question remains: how to relate the non-relativistic- and the relativistic dispersion relation?

More can be said about that, however I strictly focus now on the Fitzpatrick undergraduate course.

Now, back to the exercise: "Use the uncertainty principle to show that electrons of energy 1MeV could not be contained in the nucleus before decay."

The Heisenberg's uncertainty principle, Eq.(3.92) or (3.93):

$$\Delta x \Delta k > 1/2 \text{ or } \Delta x \Delta p > \hbar/2.$$

Well, the only thing I can say here is when we could find the contradiction $\Delta x \Delta k < 1/2$.

What we know is Δx to be given for a wave packet "*which is initially localized around x_0 in some region whose width is of order Δx* ", page 28/29.

Furthermore, Eq.(3.68), $\Delta k = 1/2\Delta x$. The width of the wave packet Δx is of the order of the wavelength. So Δk is of the order of the reciprocal value of the wavelength. I could not learn from the text what "*before decay*" means.

Another approach with the uncertainty principle is with energy and time. Then we have:

$$\Delta E \Delta t \geq \hbar/2,$$

with $\Delta E = O(1\text{MeV})$ we have $\Delta t \geq O(10^{-21}\text{sec})$. In addition, this means $\Delta v \geq O(10^{21}\text{1/sec})$.

Citing Fitzpatrick, page 32, : "*Evidently, particle wave packets (for free moving particles) spread very rapidly.*"

Exercise 3.8 Potential Energy

A particle of mass m has a wave function

$$\psi(x, t) = A \exp\left[-a\left(\frac{mx^2}{\hbar} + it\right)\right],$$

where A and a are positive real constants. For what potential $V(x)$ does ψ satisfy the Schrödinger equation?

By plugging the above expression for the wave function into the Schrödinger equation, Eq. (3.110), we find for the potential:

$$V(x) = 2ma^2x^2,$$

the potential of the harmonic oscillator.

4 Fundamentals of Quantum Mechanics

4.1 Introduction

In this chapter the basic concepts of quantum mechanics are examined systematically. This is done for the one-dimensional systems.

4.2 Schrödinger's Equation.

In this section the evolution of the wave function is given by Schrödinger's equation (4.1).

The probability density, finding a particle in an infinite interval dx and the probability of finding a particle in a finite interval $[b, a]$ are presented.

4.3 Normalization of the Wavefunction

The normalization of the wavefunction is presented. Fitzpatrick started with the example of the normalization of a Gaussian wave packet with no time dependency. I do not know why there is no time dependency included, may be for the following reason(?):

the time dependence part of a wave function is in most(all?) cases

$$e^{-i\omega t}. \text{ So, with } |\psi|^2 \rightarrow e^{-i\omega t} e^{i\omega t} = 1, \text{ see Eq.(4.20).}$$

Furthermore, it is demonstrated that if a wavefunction is initially normalized, it stays normalized.

On page 41 Fitzpatrick mentioned the probability P of a measurement of the displacement giving a result between a and b (where $a < b$) is given by, Eq.(4.18), a sort of continuity equation (Mahan):

$$\frac{dP_{x \in [a, b]}}{dt} + j(b, t) - j(a, t) = 0,$$

$j(x, t)$ is the probability current (Mahan denoted $j(x, t)$ to be the particle current) given in Eq. (4.19). $j(x, t)$ is real since, Eq.(4.15), $\frac{\partial}{\partial t}(\psi^* \psi)$ is real.

With a Gaussian wave packet you will find for $j(x, t)$ and Eq. (4.19): $j = 0$.

Remark: I just follow the notation of Fitzpatrick. However, I could imagine $\frac{\partial}{\partial t}$ to be better than $\frac{d}{dt}$.

Fitzpatrick mentioned Eq.(4.18) to be found by similar analysis for the proof of the time independency of the normalization condition.

The only difference is the change of integration interval: $\int_{-\infty}^{\infty} \rightarrow \int_a^b$.

Eqs. (4.12), (4.15) and (4.19) can be combined as

$$\int_{-\infty}^{\infty} \left[\frac{\partial}{\partial t} |\psi|^2 + \frac{\partial j}{\partial x} \right] dx = 0.$$

We learned from Eq.(4.16):

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial t} |\psi|^2 dx = 0 \text{ and } \int_{-\infty}^{\infty} \frac{\partial j}{\partial x} dx = 0 .$$

Furthermore, it is assumed in this lecture all wave functions to be square-integrable and normalized, unless stated otherwise.

4.4 Expectation Values and Variances.

In chapter 2, expectation value and variance has been introduced.

The expectation value of displacement x , $\langle x \rangle$, is analysed.

4.5 Ehrenfest's Theorem

Eq. (4.35) is found by substituting the probability density $|\psi|^2 = \frac{dP}{dx}$ into Eq. (4.18).

Or Euler meeting Leibniz for a small interval Δx :

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial t} \int_x^{x+\Delta x} |\psi|^2 dx = \frac{\partial}{\partial t} |\psi|^2 \Delta x ,$$

and

$$j(x + \Delta x, t) - j(x, t) = \frac{\partial j}{\partial x} \Delta x .$$

Hence with $\frac{dP_{x \in a:b}}{dt} + j(b, t) - j(a, t) = 0$, Eq. (4.18), we have

$$\frac{\partial}{\partial t} |\psi|^2 + \frac{\partial j}{\partial x} = 0 , \text{ Eq.(4.35).}$$

At the bottom of page 43 the particle current j has been used to evaluate the expectation value of momentum $\langle p \rangle$.

With integrating by parts Eq. (4.37), the expression for $\langle p \rangle$ has been found. With $|\psi|^2$ to be zero since $|\psi| \rightarrow 0$ as $|x| \rightarrow \infty$ (Eq. (4.17)).

No remark is made about the possible outcome from integrating by parts for $\langle p \rangle$ to be:

$$\langle p \rangle = i\hbar \int_{-\infty}^{\infty} \psi \frac{\partial \psi^*}{\partial x} dx. \text{ Does it matter?}$$

Take note for a Gaussian wave packet $\psi(x, t)$ as given in Eq. (3.85) and using Eq. (4.38) $\langle p \rangle$ to be: $\langle p \rangle = \hbar k_0$.

To find Eq.(4.39) we need partial integration of $-i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial^2 \psi}{\partial t \partial x} dx$:

$$-i\hbar \left[\psi^* \frac{\partial \psi}{\partial t} \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial t} dx \right].$$

The first term in this expression is 0. Consequently you will obtain Eq. (4.39).

Fitzpatrick substituted Schrödinger's equation into Eq. (4.39) and simplifying means:

$$-\frac{\hbar^2}{2m} \left(\frac{\partial \psi}{\partial x} \frac{\partial^2 \psi^*}{\partial x^2} + \frac{\partial \psi^*}{\partial x} \frac{\partial^2 \psi}{\partial x^2} \right) = -\frac{\hbar^2}{2m} \left(\frac{\partial}{\partial x} \left(\frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x} \right) \right) . \text{ Then you find Eq. (4.40).}$$

Furthermore Fitzpatrick integrated Eq.(4.40) by parts.

However, as far as I do understand integration by parts, there is not much to integrate by parts.

Since $\int_{-\infty}^{\infty} \frac{\partial}{\partial x} \left(\frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x} \right) dx = \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x} \Big|_{-\infty}^{\infty}$ is set equal to 0, and the integral of the derivative of the potential is the only integral left.

4.6 Operators

In this section operators are introduced and particularly the Hermitian operator. This section starts with the mathematical definition of an operator.

With (4.50), non-commutating of operators is illustrated.

Eq. (4.57) represents the constraint which needs to be satisfied for an operator to be Hermitian:

$$\int_{-\infty}^{\infty} \psi^* (O\psi) dx = \int_{-\infty}^{\infty} (O\psi)^* \psi dx,$$

Where O represents the operator.

Fitzpatrick: the operators x and p are both Hermitian.

The operator x :

x is a real number, so,

$$\int_{-\infty}^{\infty} \psi^* (x\psi) dx = \int_{-\infty}^{\infty} (x\psi)^* \psi dx. \text{ Consequently the operator } x \text{ is Hermitian.}$$

The operator $p \equiv -i\hbar \frac{\partial}{\partial x}$:

$$\begin{aligned} \text{with the constraint, Eq. (4.57), we evaluate } \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial \psi}{\partial x} \right) dx &= -i\hbar \psi^* \psi \Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} i\hbar \psi \frac{\partial \psi^*}{\partial x} dx \\ &= - \int_{-\infty}^{\infty} \psi \left(-i\hbar \frac{\partial \psi^*}{\partial x} \right) dx = - \int_{-\infty}^{\infty} \psi \left(i\hbar \frac{\partial \psi^*}{\partial x} \right)^* dx = \int_{-\infty}^{\infty} \left(-i\hbar \frac{\partial \psi}{\partial x} \right)^* \psi dx ; \text{ QED.} \end{aligned}$$

For a non-Hermitian operator we can demonstrate the following:

$$(O^\dagger)^\dagger = O.$$

$$\text{Replace in Eq.(4.58) } O \text{ by } O^\dagger \text{ and we have } \int_{-\infty}^{\infty} ((O^\dagger)^\dagger \psi)^* \psi dx = \int_{-\infty}^{\infty} (\psi)^* (O^\dagger \psi) dx .$$

Take the complex conjugated of the latter expression to find

$$\int_{-\infty}^{\infty} (O^\dagger)^\dagger \psi \psi^* dx = \int_{-\infty}^{\infty} \psi (O^\dagger \psi)^* dx. \text{ This expression, using the righthand side of Eq.(4.58), becomes:}$$

$$\int_{-\infty}^{\infty} (O^\dagger)^\dagger \psi \psi^* dx = \int_{-\infty}^{\infty} O\psi (\psi)^* dx .$$

$$\text{Consequently } (O^\dagger)^\dagger = O.$$

Furthermore, it can be demonstrated $O + O^\dagger$ to be Hermitian:

we know an Hermitian operator to be equal to its Hermitian conjugate.

So we need to prove: $O + O^\dagger = (O + O^\dagger)^\dagger$.

The latter expression can be rewritten as $O + O^\dagger = O^\dagger + (O^\dagger)^\dagger$.

We demonstrated above $(O^\dagger)^\dagger = O$.

Hence, $O + O^\dagger = O^\dagger + O$; QED.

Fitzpatrick also introduced two operators A and B . For these operators it can be demonstrated:

$(AB)^\dagger = B^\dagger A^\dagger$. Is this expression also easily demonstrated? I assume A and B to be non-Hermitian. We use the proof by “negative contradiction”.

Assume $(AB)^\dagger = B^\dagger A^\dagger$ to be correct.

Take the conjugate of the latter expression:

$$((AB)^\dagger)^\dagger = (B^\dagger A^\dagger)^\dagger.$$

Now we use $(O^\dagger)^\dagger = O$, then $((AB)^\dagger)^\dagger = AB$,

and with the above assumption : $(B^\dagger A^\dagger)^\dagger = (A^\dagger)^\dagger (B^\dagger)^\dagger = AB$.

Hence we found $AB = AB$; QED.

Now with three operators: O_1, O_2 and O_3 .

What has been proven for two operators will be used:

$$(O_1 O_2)^\dagger = (O_2)^\dagger (O_1)^\dagger.$$

Multiply this expression on the left with $(O_3)^\dagger$:

$$(O_3)^\dagger (O_1 O_2)^\dagger = (O_3)^\dagger (O_2)^\dagger (O_1)^\dagger.$$

With the result of two operators we have:

$$(O_3)^\dagger (O_1 O_2)^\dagger = (O_1 O_2 O_3)^\dagger.$$

Hence $(O_1 O_2 O_3)^\dagger = (O_3)^\dagger (O_2)^\dagger (O_1)^\dagger$; QED.

Completely similar we have for n operators:

$$(\prod_{i=0}^n O_i)^\dagger = \prod_{i=0}^n (O_i)^\dagger.$$

We assume this to be true.

Multiply the left hand side of the latter expression with O_{n+1}^\dagger :

$$O_{n+1}^\dagger (\prod_{i=0}^n O_i)^\dagger = O_{n+1}^\dagger \prod_{i=0}^n (O_i)^\dagger.$$

And with the expression for n , we have proven the expression for $n + 1$ to be correct.

On page 47 Fitzpatrick mentioned the Hamiltonian to be Hermitian. The Hamiltonian H depends on p^2 and the potential $V(x)$. p is a Hermitian operator. So p^2 is a Hermitian operator.

$V(x)$ can be expressed as a polynomial in x , where x is a Hermitian operator. Consequently $V(x)$ is a Hermitian operator.

4.7 Momentum Representation

The momentum-space wave function equivalent to the real-space wavefunction is presented.

The Dirac delta- function (Dirac, page 48) is introduced.

In Eqs. (4.73) and (4.74) the integral representation of the Dirac delta function is found (Chisholm and Morris).

With the Eqs. (4.64) and (4.65) the workings of the integral representation of the Dirac delta function can be illustrated:

plug Eq. (4.65), after replacing the dummy variable x by x' , into Eq.(4.64). We have

$$\psi(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi(x', t) e^{-ikx'} dx' e^{ikx} dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi(x', t) e^{ik(x-x')} dx' dk.$$

Changing the order of integration:

$$\psi(x, t) = \int_{-\infty}^{\infty} \psi(x', t) \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} dk dx' = \int_{-\infty}^{\infty} \psi(x', t) \delta(x - x') dx' = \psi(x, t).$$

In Chisholm and Morris the inverse route is shown: from Dirac delta function to Fourier transform.

To find Eq. (4.80), page 49, use has been made of:

$$x e^{ipx/\hbar} = \frac{\hbar}{i} \frac{\partial}{\partial p} e^{ipx/\hbar} = -i\hbar \frac{\partial}{\partial p} e^{ipx/\hbar}.$$

To obtain Eq. (4.81), integration by parts has been used for the integral:

$$\int_{-\infty}^{\infty} \phi(p, t) (-i\hbar \frac{\partial}{\partial p} e^{\frac{ipx}{\hbar}}) dp .$$

$$\text{This leads to } -i\hbar e^{\frac{ipx}{\hbar}} \phi(p, t) |_{-\infty}^{\infty} + \int_{-\infty}^{\infty} e^{\frac{ipx}{\hbar}} \left(i\hbar \frac{\partial}{\partial p} \right) \phi(p, t) dp = \int_{-\infty}^{\infty} e^{\frac{ipx}{\hbar}} (i\hbar \frac{\partial}{\partial p}) \phi(p, t) dp ,$$

since the first term on the left hand side is zero and Eq. (4.81) is obtained.

In Eq. (4.82) Fitzpatrick writes $\phi(p)$ in stead of $\phi(p, t)$. A typo I assume.

4.8 Heisenberg's Uncertainty Principle

To arrive at the general form of the Heisenberg's uncertainty principle use has been made of the Cauchy-Schwarz inequality (Susskind, page 142).

By evaluating Eq. (4.93) we have four integrals:

$$\int_{-\infty}^{\infty} \psi^* AB\psi dx , - \int_{-\infty}^{\infty} \psi^* A\langle B \rangle \psi dx , - \int_{-\infty}^{\infty} \psi^* \langle A \rangle B\psi dx \text{ and } \int_{-\infty}^{\infty} \psi^* \langle A \rangle \langle B \rangle \psi dx .$$

Since expectations values are just numbers, Eq. (4.94),

$$z = \int_{-\infty}^{\infty} \psi^* AB\psi dx - \langle A \rangle \langle B \rangle , \text{ is found.}$$

Eq. (4.94) can also be written as:

$$z = \langle AB \rangle - \langle A \rangle \langle B \rangle .$$

Now we take the complex conjugate of z , Eq.(4.94):

$$z^* = \int_{-\infty}^{\infty} (\psi^* AB\psi)^* dx - \langle A \rangle \langle B \rangle .$$

To arrive at Eq. (4.95) we use the definition of the Hermitian conjugate of an operator,

Eq. (4.58):

$$\int_{-\infty}^{\infty} \psi^* (AB\psi) dx = \int_{-\infty}^{\infty} ((AB)^\dagger \psi)^* \psi dx .$$

So,

$$z^* = \int_{-\infty}^{\infty} (((AB)^\dagger \psi)^* \psi)^* dx - \langle A \rangle \langle B \rangle = \int_{-\infty}^{\infty} (AB)^\dagger \psi \psi^* dx - \langle A \rangle \langle B \rangle .$$

Furthermore, we use $(AB)^\dagger = B^\dagger A^\dagger$ as shown in section 4.6. In addition with A and B to be Hermitian operators we find: $(AB)^\dagger = B^\dagger A^\dagger = BA$.

Then

$$z^* = \int_{-\infty}^{\infty} (AB)^\dagger \psi \psi^* dx - \langle A \rangle \langle B \rangle = \int_{-\infty}^{\infty} \psi^* BA\psi dx - \langle A \rangle \langle B \rangle = \langle BA \rangle - \langle A \rangle \langle B \rangle .$$

This gives us for $z - z^*$, Eq.(4.94) and the above expression for z^* :

$$z - z^* = \int_{-\infty}^{\infty} \psi^* AB\psi dx - \int_{-\infty}^{\infty} \psi^* BA\psi dx = \langle AB - BA \rangle = \langle [A, B] \rangle .$$

With this analysis we find the general form of *Heisenberg's uncertainty principle* , Eq.(4.96) as given on page 51. Hence, when two observables commute, they can be measured simultaneously.

Remark:

In addition it is not so easily demonstrated since there remains the question:

$z = \langle AB \rangle - \langle A \rangle \langle B \rangle$, and the right hand side of this expression represents expectation values, i.e. measurable quantities , z is a real number. Consequently: $z = z^*$ and the uncertainty disappears as it should. Under the condition A and B being Hermitian and can be measured simultaneously.

Let us set $A = x$, $B = p$, we know the answer: $z - z^*$ is not a real number:

$$[x, p] = i\hbar.$$

$$(xp - px)\psi = -x i\hbar \frac{\partial \psi}{\partial x} + i\hbar \frac{\partial}{\partial x}(x\psi) = -x i\hbar \frac{\partial \psi}{\partial x} + i\hbar \psi + i\hbar x \frac{\partial \psi}{\partial x} = i\hbar \psi.$$

Consequently: $[x, p] = xp - px = i\hbar$, Eq.(4.98).

x and p cannot be measured simultaneously in an accurate way.

Then, are we allowed to conclude from the general Heisenberg's uncertainty principle:

Given $A \neq B$, A and B never commute? Here again a caveat. For example, $B = A^2$, $A \neq B$: A and B still commute. So $A \neq B$ is a bit imprecise. To be at the safe side, the condition should read: $B \neq f(A)$ and $f(A)$ represents a function of A , i.e. a polynomial. Is there a theorem on uncertainty and commutation?

Now what about $\langle xp \rangle$? Well, $\langle xp \rangle = -\int_{-\infty}^{\infty} \psi^* x i\hbar \frac{\partial \psi}{\partial x} dx$. Using integration by parts, the integral gives:

$\langle xp \rangle = i\hbar(1 + \int_{-\infty}^{\infty} \psi^* x \frac{\partial \psi}{\partial x} dx)$. Hence, with the integral to be a real number $\langle xp \rangle$ is an imaginary number. For a wave packet of width σ , we find for the expectation value $\langle xp \rangle$:

$$\langle xp \rangle = i\hbar(1 - \langle (\frac{x}{\sigma})^2 \rangle).$$

Let's play a bit further with the Hermitian operators A and B . In addition, we assume again AB to be a Hermitian operator.

We have $AB = A^\dagger B^\dagger = (BA)^\dagger$. Also $AB = (AB)^\dagger = B^\dagger A^\dagger = BA$. Then, with $AB = BA$ and the Hermitian operators A and B commute: $[A, B] = 0$.

Fitzpatrick paid some attention in section (4.10) on the commutation of the Hermitian operators A and B .

At the top of page 52 Fitzpatrick mentioned the minimum uncertainty (i.e., $\sigma_x \sigma_p = \hbar/2$) is only achieved by Gaussian wave packets. This statement comes as a surprise. Since, the general form of the Heisenberg's uncertainty principle does not depend on a wave function; Eq. (4.96). So, how to find out?

Fitzpatrick refers to Sect. 3.12. There he presented for a Gaussian probability distribution of characteristic width Δx in x -space and of characteristic width Δk in k -space Eq. (3.70):

$$\Delta x \Delta k = 1/2. \text{ Now we know } \Delta x = \sigma_x \text{ and } \Delta p = \hbar \Delta k = \sigma_p. \text{ Consequently } \sigma_x \sigma_p = \hbar \Delta x \Delta k = \frac{\hbar}{2}.$$

Energy and time are represented by operators which do not commute. Completely similar to $[x, p] = i\hbar$ you will find $[H, t] = i\hbar$, where use have been made of the operators $H \equiv i\hbar \partial / \partial t$. This section is concluded by Fitzpatrick that, again the minimum uncertainty principle is obtained for Gaussian wave packets, i.e. $\sigma_E \sigma_t = \hbar/2$. I suppose this is obtained completely like $\sigma_x \sigma_p = \hbar/2$ (Sect. 3.12), with the wave functions presented in the time domain (Eqs. (4.107) and (4.108)).

4.9 Eigenstates and Eigenvalues.

The general presentation for eigenstates and eigenvalues is given.

On top of page 55 Fitzpatrick introduces degenerate eigenstates. There Fitzpatrick writes: "The

above proof of the orthogonality of different eigenstates fails for degenerate eigenstates. Note, however, that any linear combination of ψ_a and ψ'_a is also an eigenstate of A corresponding to the eigenvalue a ." What I read here is a new eigenstate is created with the same eigenvalue a . Consequently, this is a new degenerated state of which the orthogonality cannot be proven. This looks like a contradiction. I will neglect this.

Furthermore Fitzpatrick writes: "Thus, even if ψ_a and ψ'_a are not orthogonal, we can always choose two linear combinations of these eigenstates which are orthogonal." Susskind, on page 66, also mentioned the possibility of two orthogonal linear combinations. Why two linear combinations? One is enough.

A linear combination of the two degenerate eigenstates are given in Eq. (4.124):

$$\psi''_a = \frac{|c|}{\sqrt{1-|c|^2}} (\psi_a - c^{-1}\psi'_a),$$

and $\int_{-\infty}^{\infty} \psi_a^* \psi'_a dx = c$ and c is in general a complex number.

Now we find out the normalization and the eigenvalue of ψ''_a .

The eigenvalue:

$A\psi''_a = a\psi''_a$? Plugging the operator A in Eq. (4.124) gives

$$\begin{aligned} A\psi''_a &= \frac{|c|}{\sqrt{1-|c|^2}} (A\psi_a - c^{-1}A\psi'_a) = \frac{|c|}{\sqrt{1-|c|^2}} (a\psi_a - c^{-1}a\psi'_a) = a \frac{|c|}{\sqrt{1-|c|^2}} (\psi_a - c^{-1}\psi'_a) = \\ &= a\psi''_a. \end{aligned}$$

The normalization of ψ''_a :

$$\int_{-\infty}^{\infty} (\psi''_a)^* \psi''_a dx = \frac{|c|^2}{1-|c|^2} \int_{-\infty}^{\infty} (\psi_a - c^{-1}\psi'_a)^* (\psi_a - c^{-1}\psi'_a) dx.$$

By evaluating the integral on the right hand side of the above expression we make use of :

$$c^{-1} = \frac{c^*}{|c|^2}, \int_{-\infty}^{\infty} (\psi'_a)^* \psi_a dx = c^* \text{ and } \int_{-\infty}^{\infty} \psi_a^* \psi'_a dx = c.$$

Then we finally obtain: $\int_{-\infty}^{\infty} (\psi''_a)^* \psi''_a dx = 1$.

What comes next is the question whether ψ''_a is perpendicular to ψ_a or ψ'_a ?

$$\int_{-\infty}^{\infty} \psi_a^* \psi''_a dx = \int_{-\infty}^{\infty} \psi_a^* \frac{|c|}{\sqrt{1-|c|^2}} (\psi_a - c^{-1}\psi'_a) dx = \frac{|c|}{\sqrt{1-|c|^2}} [\int_{-\infty}^{\infty} \psi_a^* \psi_a dx - \int_{-\infty}^{\infty} \psi_a^* c^{-1}\psi'_a dx].$$

With Eq. (4.123) and ψ_a and ψ'_a properly normalized, we find $\int_{-\infty}^{\infty} \psi_a^* \psi''_a dx = 0$.

Consequently $\int_{-\infty}^{\infty} (\psi'_a)^* \psi''_a dx \neq 0$?

$$\int_{-\infty}^{\infty} (\psi'_a)^* \frac{|c|}{\sqrt{1-|c|^2}} (\psi_a - c^{-1}\psi'_a) dx = \frac{|c|}{\sqrt{1-|c|^2}} [\int_{-\infty}^{\infty} (\psi'_a)^* \psi_a dx - \int_{-\infty}^{\infty} (\psi'_a)^* c^{-1}\psi'_a dx].$$

With $c^{-1} = \frac{c^*}{|c|^2}$ and $\int_{-\infty}^{\infty} (\psi'_a)^* \psi_a dx = c^*$ we obtain:

$$\int_{-\infty}^{\infty} (\psi'_a)^* \psi''_a dx = -\frac{c^*(1-|c|^2)}{|c|\sqrt{1-|c|^2}} \neq 0.$$

In Eq. (4.124) the numerical c appears in the denominator. Then, you may wonder what will happen for $|c| \rightarrow 1$.

Eq. (4.123):

$$\int_{-\infty}^{\infty} \psi_a^* \psi'_a dx = c \rightarrow e^{i\theta}, \text{ with } 0 \leq \theta \leq 2\pi.$$

Eq. (4.124):

$$\psi_a'' = \frac{|c|}{\sqrt{1-|c|^2}} (\psi_a - c^{-1} \psi_a') = \frac{1}{\sqrt{1-1}} (\psi_a - e^{-i\theta} \psi_a').$$

What will happen? What is the physical meaning of $c \rightarrow e^{i\theta}$?

The eigenstates of a Hermitian operator form a complete set. Fitzpatrick mentioned the proof of this to be quite difficult and he did not attempt to prove this completeness in this section. I suppose the proof is about the eigenstate to form a complete set and not about “to demonstrate”. On the other hand, Susskind writes on page 67: *“The final part of the theorem states that the eigenvectors are complete. In other words if the space is N -dimensional there will be N orthonormal eigenvectors. The proof is easy, and I will leave it to you.”* I do not know whether Susskind meant the proof of completeness to be easy. The statement by Susskind is followed by an exercise 3.1 : *“Prove the following: If a vector space is N -dimensional, an orthonormal basis of N eigenvectors can be constructed from the eigenvectors of a Hermitian operator.”*

With a complete set of eigenvectors, a general wave function ψ can be constructed of the complete set ψ_i : $\psi = \sum_i c_i \psi_i$,

Eq. (4.125). In this expression c_i represent the complex weights.

With help of the Kronecker delta-function the weights or expansion coefficients are found:

$$\int_{-\infty}^{\infty} \psi_i^* \psi dx = \int_{-\infty}^{\infty} \psi_i^* (\sum_j c_j \psi_j) dx = \sum_j \int_{-\infty}^{\infty} \psi_i^* \psi_j dx = \sum_j c_j \delta_{ij} = c_i,$$

where use has been made of the definition of the *Kronecker delta* Eq.(4.127).

With ψ properly normalized we have, using $\psi = \sum_i c_i \psi_i$,

$$\int_{-\infty}^{\infty} \psi^* \psi dx = \int_{-\infty}^{\infty} (\sum_i c_i^* \psi_i^*) (\sum_i c_i \psi_i) dx = \sum_{ij} \int_{-\infty}^{\infty} c_i^* c_j \psi_i^* \psi_j dx = \sum_{ij} c_i^* c_j \delta_{ij} = \sum_i |c_i|^2 = 1.$$

4.10 Measurement

In this section the collapse of the wave function as mentioned in section 3.16 is discussed in more detail.

We expand the wave function $\psi = \sum_i c_i \psi_i$, Eq. (4.130).

and ψ_i is an eigenstate of the operator A with eigenvalue a_i . Furthermore

$A\psi = a\psi$. Consequently $\langle A \rangle = a$.

Now

$$A^2\psi = A(a\psi) = aA\psi = a^2\psi.$$

This gives for the expectation value of A^2

$$\langle A^2 \rangle = a^2.$$

So we find $\sigma_A^2 = 0$, Eq. (4.132).

With help of the expansion of the wave function $\psi = \sum_i c_i \psi_i$:

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* A\psi dx = \int_{-\infty}^{\infty} (\sum_i c_i^* \psi_i^*) A(\sum_i c_i \psi_i) dx = \int_{-\infty}^{\infty} (\sum_i c_i^* \psi_i^*) (\sum_i a_i c_i \psi_i) dx = \sum_{ij} a_i \int_{-\infty}^{\infty} c_i^* c_j \psi_i^* \psi_j dx = \sum_i |c_i|^2 a_i.$$

In a similar way we find

$$\langle A^2 \rangle = \int_{-\infty}^{\infty} \psi^* A^2\psi dx = \sum_i |c_i|^2 a_i^2.$$

Then with $\sigma_A^2 = 0$, we obtain Eq.(4.135).

Fitzpatrick showed an example of two eigenstates. A two-dimensional case with two orthonormal wave functions: a complete set. There the collapse of the wave function is demonstrated. He mentioned the result for the 2-dimensional case can “easily be generalized” to the case where there are more than two eigen states. Well, „*da spricht man ein großes Wort gelassen aus*”. Or, he just indicated Eq. (4.135) to be the generalization. However, the point is to show the collapse of the wave function for a value of A for which one of the values of $|c_i|^2$ is unity.

Let's give it a try. We start with Eq. (4.135).

$$\sum_i a_i^2 |c_i|^2 - (\sum_i |c_i|^2 a_i)^2 = 0.$$

We rewrite the latter equation:

$$\sum_{ij} [a_i a_j |c_i| |c_j| \delta_{ij} - a_i a_j |c_i|^2 |c_j|^2] = 0.$$

$$\sum_{ij} a_i a_j |c_i| |c_j| [\delta_{ij} - |c_i| |c_j|] = 0.$$

(C.4.10.1)

With the latter equation we arrive at the conclusion, using $\sum_i |c_i|^2 = 1$,: “*It follows that a state associated with a definite value of A is one in which of the $|c_i|^2$ is unity(= δ_{ii}), and all of the others are zero. Is that what Fitzpatrick meant with ‘easily be generalized’?*” I do not know.

What I know is the statement coming after Eq. (4.137). Is that equation easily generalized?

Again, I do not know. Let us try to find out and look for the result of three eigenstates. For

convenience we set $|c_1|^2 = x$, $|c_2|^2 = y$ and $|c_3|^2 = 1 - x - y$.

Well, after some straight forward collecting and regrouping terms we arrive at :

$$(a_1 - a_3)^2 x(1 - x) + (a_2 - a_3)^2 y(1 - y) - 2(a_1 - a_3)(a_2 - a_3)xy = 0.$$

(C.4.10.2)

Alas, this expression does not easily create information about x and y , since the third term in this expression can be negative, zero or positive. Well, you could try for example $x = 1/2$, and $y = 1/2$. This would lead to a contradiction for $a_1 \neq a_2$. That's just fine but not a very strong argument for:

$$|c_1|^2 = 1, |c_2|^2 = 0 \text{ and } |c_3|^2 = 0 \text{ or}$$

$$|c_1|^2 = 0, |c_2|^2 = 1 \text{ and } |c_3|^2 = 0, \text{ or}$$

$$|c_1|^2 = 0, |c_2|^2 = 0 \text{ and } |c_3|^2 = 1.$$

When we set $a_3 = 0$, reducing **(C.4.10.2)** to the two-dimensional case or two eigen states, you will find Eq. (4.137).

With **(C.4.10.2)** you have a clue to generalize for the four eigenstates:

$$|c_1|^2 = x, |c_2|^2 = y, |c_3|^2 = z \text{ and } |c_4|^2 = 1 - x - y - z :$$

$$(a_1 - a_4)^2 x(1 - x) + (a_2 - a_4)^2 y(1 - y) + (a_3 - a_4)^2 z(1 - z) - 2(a_1 - a_4)(a_2 - a_4)xy - 2(a_1 - a_4)(a_3 - a_4)xz - 2(a_2 - a_4)(a_3 - a_4)yz = 0.$$

(C.4.10.3)

To find out whether this works, set $a_4 = 0$ and you will find the three-dimensional case or three eigenstates **(C.4.10.2)**. Again you will have the problem of only knowing the signs of the first three terms in **(C.4.10.3)**.

Now let's return to Eq. (4.135):

$$\sum_i a_i^2 |c_i|^2 - (\sum_i |c_i|^2 a_i)^2 = 0.$$

This equation can be written as:

$$\sum_i a_i^2 |c_i|^2 (1 - |c_i|^2) - \sum_{i \neq j} a_i a_j |c_i|^2 |c_j|^2 .$$

we plug into this equation $|c_i|^2 = 1 - \sum_{i \neq j} |c_j|^2$:

$$\sum_i a_i^2 \{ (1 - \sum_{i \neq j} |c_j|^2) \sum_{i \neq j} |c_j|^2 \} - \sum_{i \neq j} a_i a_j |c_i|^2 |c_j|^2 = 0 . \quad (\mathbf{C.4.10.4})$$

Since the first term between braces in **(C.4.10.4)** runs over all i this term has to be zero.

We have to analyse $\sum_{i \neq j} a_i a_j |c_i|^2 |c_j|^2 = 0$ in **(C.4.10.4)**.

Since $a_i a_j \neq 0$, the solutions are $|c_i|^2 = 0$ or $|c_j|^2 = 0$. In addition we still have $\sum_i |c_i|^2 = 1$.

So, for all $j \neq i$: $|c_j|^2 = 0$ and $|c_i|^2 = 1$.

We can also analyse **(C.4.10.1)**.

There is no need to use the Kronecker delta.

We just analyse Eq. (4.135), $\sum_i a_i^2 |c_i|^2 - (\sum_i |c_i|^2 a_i)^2 = 0$, once more:

Plug into this equation $|c_i|^2 = 1 - \sum_{i \neq j} |c_j|^2$:

$$\sum_i a_i^2 (1 - \sum_{i \neq j} |c_j|^2) - \left(\sum_i a_i (1 - \sum_{i \neq j} |c_j|^2) \right)^2 = 0 .$$

Since both summations runs over all i , $\sum_{i \neq j} |c_j|^2 = 0$ and we find $|c_i|^2 = 1$.

Note $(\sum_i |c_i|^2 a_i)^2$, due to $i \neq j$, into $\sum_i a_i^2 |c_i|^2$.

That is all we need.

In this section Fitzpatrick returned to the two Hermitian operators A and B (section 4.8). He posed the question: "*Under what circumstances is it possible to simultaneously measure these two variables (exactly)*"? The conclusion is the commuting operators to possess simultaneous eigenstates.

4.11 Continuous Eigenvalues.

In the foregoing sections Fitzpatrick assumes the operators to possess discrete eigenvalues.

On top of page 58 Fitzpatrick writes: "*Evidently, $\psi_x(x, x')$ reduces to $\delta(x - x')$ *".

Well, it took me some time to except this "*Evidently*". Since, according to Dirac (page 58), $\delta(x)$ is not a function of x according to the mathematical definition of a function.

Question: $\psi_x(x, x') = \delta(x - x')$ indicates the wave function to be a dimensionless function?

Susskind (Chapter 8) adopted a slightly different approach. Using the notation of Fitzpatrick, Eq. (4.141) can be written as

$$(x - x') \psi_x(x, x') = 0.$$

Susskind writes: "*Thus, if $x \neq x'$, then $\psi_x(x, x') = 0$. That is a strong condition. It says that for a given eigenvalue x' , the function $\psi_x(x, x')$ can be nonzero at only one point, namely at $x = x'$. For an ordinary continuous function, this condition would be deadly: no sensible function can be zero everywhere except at one point and be nonzero only at that point. But that is exactly the property of the Dirac delta function $\delta(x - x')$.*"

Furthermore Fitzpatrick writes on page 58 to derive Eq. (4.144): "*..., it is easily demonstrated..*". Then, it makes you wonder why Dirac (page 60) did verify an equation like Eq. (4.144). For

Dirac¹, when something is easily demonstrated, he certainly would not have verified it. Well, he did in Section 15 on *The δ function*.

First let's guess what Fitzpatrick mentioned with: "*Easily demonstrated*".

It is about Eq. (4.144):

$$\int_{-\infty}^{\infty} \delta(x - x') \delta(x - x'') dx = \delta(x' - x'').$$

Consider $\delta(x - x')$ to be a function $g(x)$.

Caveat: $g(x)$ is not well-defined at $x = x'$, whereas $\int_{-\infty}^{\infty} f(x) \delta(x) dx = f(0)$, is well-defined at $x = 0$.

Now use $\int_{-\infty}^{\infty} f(x) \delta(x) dx = f(0)$, replace $f(x)$ by $g(x)$ and $\delta(x)$ by $\delta(x - x'')$.

We have $\int_{-\infty}^{\infty} g(x) \delta(x - x'') dx = g(x'')$.

With $g(x) \equiv \delta(x - x')$ it is demonstrated: $\int_{-\infty}^{\infty} \delta(x - x') \delta(x - x'') dx = \delta(x' - x'')$.

How did Dirac verify Eq. (4.144)? I will use the notation of Fitzpatrick.

Dirac: "*Take any continuous function (no Caveat, Nz) of x' , $f(x')$. Then*

$$\begin{aligned} \int f(x') dx' \int \delta(x' - x) dx \delta(x - x'') &= \int \delta(x - x'') dx \int f(x') dx' \delta(x' - x) \\ &= \int \delta(x - x'') dx f(x) = (f(x'')) = \int f(x') dx' \delta(x' - x''). \end{aligned}$$

Consequently, by comparing the left hand side and the right hand side we finally reach the conclusion of Dirac: $\int_{-\infty}^{\infty} \delta(x - x') \delta(x - x'') dx = \delta(x' - x'')$.

This result gives something more (Noordzij):

The normalization condition is: $\int_{-\infty}^{\infty} \delta(x - x') \delta(x - x') dx = 1$.

The expectation value for x with the eigenfunction $\psi_x(x, x') = \delta(x - x')$ is:

$$\int_{-\infty}^{\infty} \psi_x^*(x, x') x \psi_x(x, x') dx = \int_{-\infty}^{\infty} \delta(x - x') x \delta(x - x') dx = x'.$$

Hence $\delta(x - x') \delta(x - x') \equiv \delta(x - x')$. With " \equiv " I mean identical behaviour or operates in the same way.

So we found:

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi_x^*(x, x') x \psi_x(x, x') dx = \int_{-\infty}^{\infty} \delta(x - x') x \delta(x - x') dx = x'.$$

Basically I consider this derivation not to be elegant. More or less we imply $\langle x \rangle = x'$.

Can we do better?

Let's replace x by $y + x'$:

$$\langle x \rangle = \int_{-\infty}^{\infty} \delta(y)(y + x') \delta(y) dy = \int_{-\infty}^{\infty} \delta(y) y \delta(y) dy + x' \int_{-\infty}^{\infty} \delta(y) \delta(y) dy.$$

For the first integral on the right hand side we use Dirac's toolkit, page 60- Eq. (7),:

$$y \delta(y) = 0.$$

The second integral on the right-hand side gives with the normalization condition: x' .

Consequently: $\langle x \rangle = x'$.

More concise: $\langle x \rangle = \langle y + x' \rangle = \langle y \rangle + x' = x'$.

¹ To learn more about Dirac, Graham Farmelo's book *The strangest man, the hidden life of Paul Dirac, Quantum Genius*, is very instructive to say the least.

Below Eq. (4.146), the alternative definition of the delta-function, Fitzpatrick writes: “We can thus write $\psi(x) = \int_{-\infty}^{\infty} c(x') \psi_x(x, x') dx'$.”, Eq. (4.147).

Keep in mind x' is a continuous eigenvalue and $\psi_x(x, x')$ the eigenstate to the eigenvalue x' . Can we find out about this “thus”?

We can write: $c(x) = \int_{-\infty}^{\infty} c(x') \delta(x - x') dx'$, similar to Eq. (4.146).

With Eq. (4.143): $c(x) = \int_{-\infty}^{\infty} c(x') \psi_x(x, x') dx'$.

Then Fitzpatrick(Fp) sets $c(x) = \psi(x)$ and finds:

$$\psi(x) = \int_{-\infty}^{\infty} c(x') \psi_x(x, x') dx', \text{ Eq. (4.147).}$$

Why Fp did not replace in Eq. (4.147), $c(x')$ by $\psi(x')$? I do not know. May be to show the similarity with the discrete eigenvalues?

How do we arrive at Eq. (4.148)?

Well, multiply Eq. (4.147) by $\psi_x^*(x, x'')$, use Eq.(4.145) and integrate over x :

$$\begin{aligned} \int_{-\infty}^{\infty} \psi_x^*(x, x'') \psi(x) dx &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c(x') \psi_x^*(x, x'') \psi_x(x, x') dx' dx = \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c(x') \delta(x - x'') \delta(x - x') dx dx' = \int_{-\infty}^{\infty} c(x') \delta(x' - x'') dx' = c(x''). \end{aligned}$$

So $\int_{-\infty}^{\infty} \psi_x^*(x, x'') \psi(x) dx = c(x'')$.

Replacing x'' by x' we have Eq.(4.148): $\int_{-\infty}^{\infty} \psi_x^*(x, x') \psi(x) dx = c(x')$.

Multiply the left hand side and the right hand side of Eq.(4.148) with $c(x')^*$, integrate over x' and we have:

$$\int_{-\infty}^{\infty} c(x')^* c(x') dx' = \int_{-\infty}^{\infty} c(x')^* \int_{-\infty}^{\infty} \psi_x^*(x, x') \psi(x) dx dx' . \quad (\text{C.4.11.1})$$

Then, we use the delta function representation of the position eigenstate and the equality $c(x') = \psi(x')$ in (C.4.11.1) to obtain:

$$\int_{-\infty}^{\infty} |c(x')|^2 dx' = \int_{-\infty}^{\infty} \psi^*(x') \int_{-\infty}^{\infty} \delta(x - x') \psi(x) dx dx' = \int_{-\infty}^{\infty} |\psi(x')|^2 dx' .$$

With $\psi(x)$ properly normalized we have Eq.(4.149).

Another operator with eigenvalues in a continuous range is the momentum operator p :

$$p\psi_p(x, p') = p'\psi_p(x, p') ,$$

where $\psi_p(x, p')$ is the eigenstate of the operator p with eigenvalue p' .

Then, with $p \equiv -i\hbar\partial/\partial x$, you will obtain Eq.(4.151).

Completely similar to the eigenfunction normalization of the position wave function Fp uses delta-function normalization. Before discussing the results, let us have a closer look at the Dirac delta-function. To this end we introduce the integral representation of the delta-function (Chisholm and Morris):

$$\delta(y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iky} dk .$$

Now, we change variables in this integral representation, $y = p'' - p'$, and $x = k\hbar$:

$$\delta(p' - p'') = \delta(p'' - p') = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{ix(p'' - p')/\hbar} dx . \quad (\text{C.4.11.2})$$

In the latter expression use has been made of $\delta(y) = \delta(-y)$.

We rearrange the integral in (C.4.11.2):

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\hbar}} e^{ix(-p')/\hbar} \frac{1}{\sqrt{2\pi\hbar}} e^{ix(p'')/\hbar} dx = \delta(p' - p'') . \quad (\text{C.4.11.3})$$

The Dirac δ function a magical and mysterious function indeed.²

Since with Eq. (4.151) and **(C.4.11.3)** we fulfil the normalization and orthogonality condition and obtained the constant of proportionality in Eq. (4.151):

$$\psi_p(x, p') \propto e^{ip'x/\hbar} \text{ to be } \frac{1}{\sqrt{2\pi\hbar}}.$$

Fp found the constant of proportionality using Fourier's theorem, Eq. (4.47) and Eq. (4.74).

With the Eqs. (4.66) and (4.67) respectively, which I repeat here:

$$\psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p, t) e^{ipx/\hbar} dp$$

and

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

Fp derived Eq. (4.154).

Remark: Fp tacitly ignored time dependency.

Set $p \rightarrow p'$ and $c(p') = \phi(p')$ in Eq.(4.66):

$$\psi(x) = \int_{-\infty}^{\infty} c(p') \psi_p(x, p') dp', \text{ Eq.(1.54).}$$

Using Eq. (4.67):

$$\phi(p') = c(p') = \int_{-\infty}^{\infty} \psi(x) \frac{1}{\sqrt{2\pi\hbar}} e^{-ip'x/\hbar} dx = \int_{-\infty}^{\infty} \psi(x) \psi_p^*(x, p') dx, \text{ Eq.(4.155).}$$

The probabilities are again properly normalized, Eq.(4.156), with a normalized $\psi(x)$ similar to Eq.(4.149) for the position operator.

Question: does Eq. (4.153) explains the "dimensionality" of the wave function $\psi_p(x, p')$?

4.12 Stationary States

In this section the eigenstates of the energy operator are discussed.

The eigenstate for the energy operator is obtained from Eq. (4.157), a first order differential equation the solution of which is given in Eq.(4.158).

Here, it is assumed the eigenstate of the energy operator can be presented as a product of a non-time varying wave function, $\psi_i(x)$, and the time dependent part as the general solution of the differential equation, Eq.(4.157), $e^{-iE_it/\hbar}$.

Well, this complies with the condition for the probability density not to depend on time.

Is Eq. (4.158) the only possible solution?

In this section Fp presented the results for the discrete eigenvalues.

For continuous eigenvalues we have, in real-space representation:

$$\psi(x, t) = \int_{-\infty}^{\infty} c(E) \psi(x, 0) e^{-iEt/\hbar} dE,$$

or with $E = \frac{p^2}{2m}$:

$$\psi(x, t) = \int_{-\infty}^{\infty} c(p) \psi(x, 0) e^{-ip^2t/2m\hbar} dp,$$

where $c(p)$ is

$$c(p) = \int_{-\infty}^{\infty} \psi^*(x, 0) e^{+ip^2t/2m\hbar} \psi(x, t) dx.$$

² Dirac's δ function is in the same league as Euler's equation, I think. Who am I?

See David Stipp, *A most elegant equation, Euler's formula & the beauty of mathematics*.

At the bottom of page 60, Fp made some remarks on a Hermitian operator A which commutes with H . In section 4.10 *On Measurement*, Fp dealt with subject. I will repeat the major points.

With Eq. (4.138) we have:

$$(H - E_i)A\psi_E = 0 .$$

Eq. (4.139):

$$H(A\psi_E) = E_i A\psi_E .$$

So $A\psi_E$ is an eigenstate of H with eigenvalue E_i . In other words, $A\psi_E \propto \psi_E$, or

Eq. (4.140):

$$A\psi_E = a_i \psi_E .$$

Hence ψ_E is an eigenstate of A .

$$\text{Now } \langle A \rangle = \int_{-\infty}^{\infty} \psi_E^* A\psi_E dx = \int_{-\infty}^{\infty} \psi_E^* a_i \psi_E dx .$$

With Eq. (4.158), the expression for ψ_E , :

$$\langle A \rangle = a_i , \text{ time independent indeed.}$$

Exercises.

Exercise 4.1 The spreading of wave lengths

Monochromatic light with a wavelength of 6000\AA passes through a fast shutter that opens for 10^{-9} sec. What is the subsequent spread in wave lengths of the no longer monochromatic light?

A fast shutter: how fast?

By means of the shutter a wave packet is created. A wave packet.

Well, the shutter opens for $\Delta t = 10^{-9}$ sec. For the speed of light, we take the value in vacuum:

$$c = 3 \cdot 10^8 \text{ m/sec.}$$

Hence, the length of the wave packet is .3 m.

Using the wavelength $\lambda = 6000\text{\AA} = 6 \cdot 10^{-7} \text{ m}$, we have a wave packet built up of:

$$\frac{c\Delta t}{\lambda} = 5 \cdot 10^5 \text{ wavelengths.}$$

So, we denote this wave packet a wave train.

How do we find out about the spread in wavelengths due to this shutter activity?

The shutter action can be mathematically represented by two Heaviside step functions:

- $t = 0$, the shutter opens instantaneously,

- $t = \Delta t$ the shutter close like wise.

This action can be mathematically represented in the following way:

$$\theta(t) - \theta(t - \Delta t) .$$

So far so good.

We started with monochromatic light (photons) of a specific wavelength. The spread in wave numbers is practically zero: $\Delta k \approx 0$. Then, Fp page 29, the resulting wave packet will be very extended: $\Delta x \rightarrow \infty$.

Now what about the subsequent spread in wave lengths?

Let's look for what Fp tells us about light waves, light pulses propagating in vacuum.

Fp, page 32:

“...Now, the dispersion relation (3.24) for light waves is linear in k . It follows that light pulses propagate through vacuum without spreading”.

The wave train of this exercise is a **light** pulse of .3m. So, we do not expect a spread in wave lengths.

A sort of catch exercise.

Exercise 4.2 About expectation values and the variances for a given wave function

Calculate $\langle x \rangle$, $\langle x^2 \rangle$, and σ_x , as well as $\langle p \rangle$, $\langle p^2 \rangle$, and σ_p for the normalized wavefunction

$$\psi(x) = \sqrt{\frac{2a^3}{\pi}} \frac{1}{x^2 + a^2}.$$

Use these results to find $\sigma_x \sigma_p$.

Note that $\int_{-\infty}^{\infty} \frac{dx}{x^2 + a^2} = \frac{\pi}{a}$. In addition, due to normalization of the wave function we have:

$\int_{-\infty}^{\infty} \frac{dx}{(x^2 + a^2)^2} = \frac{\pi}{2a^3}$. I suppose these two integrals are part of our toolkit. To find out about these

two integrals you could use the WolframAlpha app and investigate the step by step solutions.

An old school approach is using complex functions and calculate the residues at the singularity $-ia$ (Chisholm and Morris).

$$\psi(x) = \sqrt{\frac{2a^3}{\pi}} \frac{1}{x^2 + a^2}, \text{ a Lorentzian wave packet.}$$

A peak at $x = 0$ and $\psi(x) \rightarrow 0$ for $x \rightarrow \pm\infty$. The same character as the Gaussian wave packet. However, mathematically speaking, totally different.

Calculate $\langle x \rangle$:

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x) dx = \frac{2a^3}{\pi} \int_{-\infty}^{\infty} \frac{x}{(x^2 + a^2)^2} dx = -\frac{a^3}{\pi} \frac{1}{x^2 + a^2} \Big|_{-\infty}^{\infty} = 0.$$

This is what we expect: a peak at $x = 0$. So, the particle represented by the wave packet is most probably found at $x = 0$. Furthermore, the integrand is anti-symmetric.

Calculate $\langle x^2 \rangle$:

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^*(x) x^2 \psi(x) dx = \frac{2a^3}{\pi} \int_{-\infty}^{\infty} \frac{x^2}{(x^2 + a^2)^2} dx.$$

$$\langle x^2 \rangle = \frac{2a^3}{\pi} \int_{-\infty}^{\infty} x \frac{x}{(x^2 + a^2)^2} dx.$$

Integration by parts and using the toolkit:

$$\langle x^2 \rangle = -\frac{a^3}{\pi} \frac{1}{x^2 + a^2} \Big|_{-\infty}^{\infty} + \frac{a^3}{\pi} \int_{-\infty}^{\infty} \frac{dx}{x^2 + a^2} = a^2.$$

Calculate σ_x^2 , Eq.(4.24):

$$\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 = a^2.$$

Calculate $\langle p \rangle$:

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^*(x) \frac{\partial \psi(x)}{\partial x} dx = 0.$$

with $\psi^*(x) = \psi(x)$, you will find:

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \frac{1}{2} \frac{\partial \psi^2}{\partial x} dx = 0. \text{ So}$$

$$\langle p \rangle = 0.$$

Calculate $\langle p^2 \rangle$:

$$\langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi^*(x) \frac{\partial^2 \psi(x)}{\partial x^2} dx.$$

Which steps do we take with integration by parts in this case?

$$\langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi^*(x) \frac{\partial^2 \psi(x)}{\partial x^2} dx = -\hbar^2 \psi^*(x) \frac{\partial \psi(x)}{\partial x} \Big|_{-\infty}^{\infty} + \hbar^2 \int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x} \frac{\partial \psi(x)}{\partial x} dx.$$

Now I assumed $-\hbar^2 \psi^*(x) \frac{\partial \psi(x)}{\partial x} \Big|_{-\infty}^{\infty} = 0$ and

$$\langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi^*(x) \frac{\partial^2 \psi(x)}{\partial x^2} dx = \hbar^2 \int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x} \frac{\partial \psi(x)}{\partial x} dx.$$

This is not of much help.

So I leave the toolkit and use the WolframAlpha app.

Plug into this expression the Lorentzian wave packet and we find by using the WolframAlpha app:

$$\langle p^2 \rangle = \frac{\hbar^2}{a^2}.$$

Calculate σ_p^2 :

$$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2 = \frac{\hbar^2}{a^2}.$$

Now the last question of this exercise:

Calculate $\sigma_x \sigma_p$:

With the above results we have

$$\sigma_x \sigma_p = \hbar.$$

Hence $\sigma_x \sigma_p \geq \frac{\hbar}{2}$, as it should be.

Exercise 4.3 One-dimensional particle in a box

Classically, if a particle is not observed then the probability of finding it in a one-dimensional box of length L , which extends from $x = 0$ to $x = L$, is a constant $1/L$ per unit length. Show that the classical expectation value of x is $L/2$, the expectation value of x^2 is $L^2/3$, and the standard deviation of x is $L/\sqrt{12}$.

This is about a continuous uniform probability distribution with probability density $1/L$.

Calculate $\langle x \rangle$:

$$\langle x \rangle = \int_0^L x \frac{1}{L} dx = \frac{L}{2}.$$

Calculate $\langle x^2 \rangle$:

$$\langle x^2 \rangle = \int_0^L x^2 \frac{1}{L} dx = \frac{L^2}{3}.$$

Calculate σ_x :

$$\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{L^2}{3} - \left(\frac{L}{2}\right)^2 = \frac{L^2}{12}.$$

Hence $\sigma_x = L/\sqrt{12}$.

Exercise 4.4 A one-dimensional bound particle and its momentum expectation value

Demonstrate that if a particle in a one-dimensional stationary state is bound then the expectation value of its momentum must be zero.

In section 4.12 stationary states are mentioned: Eq. (4.158). So far so good. In addition, here, the bound state is mentioned. However, in the preceding text the bound state is not even

mentioned or defined. What to do? The only place I found something on a trapped particle in a potential well is page 20, section 3.6, on the photoelectric effect.

Of course, we can search literature on bound states. See Mahan page 15 and 16. It is about a particle in a square well. A similar subject can be found in Chapter 5 of Fp.

Alas, we studied so far Chapter 4.

We give it a try.

A bound particle? That is a particle not able to move and with $v = 0$, momentum is 0.

Well, this is a bit more poetical than physical. We should think about a vibrating particle, represented in the one-dimensional case by a string. Or, in the language of chapter 4, the particle current $j = 0$; j given by Eq.(4.19).

Furthermore, $\langle p \rangle$ can be expressed in terms of the particle current, Eq. (4.36):

$$\langle p \rangle = m \int j dx.$$

The range of integration being dependent on the width of the potential well by which the particle is bound.

With $j = 0$, we have:

$$\langle p \rangle = m \int j dx = 0.$$

Exercise 4.5 About a complex potential

Suppose $V(x)$ is complex. Obtain an expression for $\partial P(x, t)/\partial t$ and $d/dt \int P(x, t) dx$ from Schrödinger's equation. What does this tell us about a complex $V(x)$?

Now $V(x)$ is complex. We can represent complexity by $V(x)^* \neq V(x)$ and/or by $V(x) = V_R(x) + iV_I(x)$, where $V_R(x)$ and $V_I(x)$ are real functions of x .

We start with the probability density.

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial t} |\psi|^2 = \frac{\partial}{\partial t} \psi^* \psi = \frac{\partial \psi^*}{\partial t} \psi + \psi^* \frac{\partial \psi}{\partial t}.$$

With Schrödinger's equation (4.1) and the analysis of section 4.3, we arrive at:

$$\frac{\partial P}{\partial t} = \frac{i\hbar}{2m} \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right) - \frac{i}{\hbar} (\psi^* V \psi - \psi V^* \psi^*)$$

or

$$\frac{\partial P}{\partial t} = \frac{i\hbar}{2m} \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right) + \frac{2}{\hbar} V_I |\psi|^2.$$

Let's use the expression for the particle current, Eq. (4.19):

$$\frac{\partial P}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial j}{\partial x} - \frac{i}{\hbar} (V - V^*) |\psi|^2$$

or

$$\frac{\partial P}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial j}{\partial x} + \frac{2}{\hbar} V_I |\psi|^2.$$

The next expression to be analysed is the integral $d/dt \int P(x, t) dx$.

So, with $\frac{\partial P}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial j}{\partial x} - \frac{i}{\hbar} (V - V^*) |\psi|^2$,

$$\frac{d}{dt} \int_{-\infty}^{\infty} P dx = \int_{-\infty}^{\infty} \frac{i\hbar}{2m} \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right) dx - \int_{-\infty}^{\infty} \frac{i}{\hbar} (V - V^*) |\psi|^2 dx,$$

or

$$\frac{d}{dt} \int_{-\infty}^{\infty} P dx = \int_{-\infty}^{\infty} \frac{i\hbar}{2m} \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right) dx + \int_{-\infty}^{\infty} \frac{2}{\hbar} V_I |\psi|^2 dx.$$

Then with the particle current we find:

$$\frac{d}{dt} \int_{-\infty}^{\infty} P dx = -\frac{i\hbar}{2m} j|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{i}{\hbar} (V - V^*) |\psi|^2 dx,$$

or

$$\frac{d}{dt} \int_{-\infty}^{\infty} P dx = -\frac{i\hbar}{2m} j|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{2}{\hbar} V_I |\psi|^2 dx.$$

Now we have to say something about the complex potential.

The expressions for $\frac{\partial P}{\partial t}$ and $\frac{d}{dt} \int_{-\infty}^{\infty} P dx$ with the complex potential included differ from the expressions in Eqs. (4.3), (4.4), (4.16) and (4.18). This is hardly a surprising statement.

By the way we also learn $\frac{2}{\hbar} V_I = -\frac{i}{\hbar} (V - V^*)$.

Are we still allowed to state: $\frac{d}{dt} \int_{-\infty}^{\infty} P dx = 0$?

If so, then the complex potential changes the particle current.

Exercise 4.6 About degeneracy

$\psi_1(x)$ and $\psi_2(x)$ are normalized eigenfunctions corresponding to the same eigenvalue.

If $\int_{-\infty}^{\infty} \psi_1^* \psi_2 dx = c$,

where c is real, find normalized linear combinations of $\psi_1(x)$ and $\psi_2(x)$ which are orthogonal to

(a) $\psi_1(x)$, or (b) $\psi_1(x) + \psi_2(x)$.

Note: c is real, then $c = \int_{-\infty}^{\infty} \psi_1^* \psi_2 dx = \int_{-\infty}^{\infty} \psi_2^* \psi_1 dx$.

ad (a)

We choose a third state ψ_3 to be a linear combination of $\psi_1(x)$ and $\psi_2(x)$:

$$\psi_3 = \alpha \psi_1 + \beta \psi_2,$$

where α and β represent complex numbers.

We will find α and β with the orthogonality- and normalization condition.

The orthogonality:

$$\int_{-\infty}^{\infty} \psi_3 \psi_1^* dx = 0.$$

So

$$\int_{-\infty}^{\infty} (\alpha \psi_1 + \beta \psi_2) \psi_1^* dx = \alpha + c\beta = 0,$$

$$\text{and } \beta = -\frac{\alpha}{c}.$$

Normalization

$$\int_{-\infty}^{\infty} \psi_3^* \psi_3 dx = 1,$$

then

$$\int_{-\infty}^{\infty} \alpha^* (\psi_1^* - \frac{1}{c} \psi_2^*) \alpha (\psi_1 - \frac{1}{c} \psi_2) dx = 1,$$

hence, with orthogonality:

$$|\alpha|^2 = \frac{c^2}{1-c^2},$$

for $|c| \neq 1$.

We have for α :

$$|\alpha| = \frac{|c|}{\sqrt{1-c^2}}.$$

Since $|\alpha| > 0 \rightarrow |c| < 1$.

Here we give an answer to the question with respect to “What about $|c| = 1$?”.

Please note: starting with α and β to be real numbers we would have found:

$$\alpha = \pm \frac{c}{\sqrt{(1-c^2)}}, \text{ with } |c| < 1.$$

Since $\beta = -\frac{\alpha}{c}$, it does not matter to choose $+$ or $-$.

With α and β to be complex numbers we find for α :

$$\alpha = |\alpha|e^{i\phi},$$

where ϕ represents the phase shift. We know such a phase shift to be irrelevant.

Finally, the linear combination:

$$\psi_3 = \frac{|c|}{\sqrt{(1-c^2)}}(\psi_1 - \frac{1}{c}\psi_2),$$

and we did obtain Eq. (4.124).

ad (b)

We choose a third state ψ_3 to be a linear combination of $\psi_1(x)$ and $\psi_2(x)$:

$$\psi_3 = \alpha\psi_1 + \beta\psi_2,$$

where α and β represent complex numbers.

We will find α and β with the orthogonality- and normalization condition.

The orthogonality:

$$\int_{-\infty}^{\infty} \psi_3(\psi_1^* + \psi_2^*)dx = 0.$$

So

$$\int_{-\infty}^{\infty} (\alpha\psi_1 + \beta\psi_2)(\psi_1^* + \psi_2^*)dx = \alpha(1+c) + \beta(1+c) = 0,$$

and

$$\alpha = -\beta, \text{ for } c \neq -1.$$

Normalization

$$\int_{-\infty}^{\infty} \psi_3^* \psi_3 dx = 1,$$

then

$$\int_{-\infty}^{\infty} \alpha^*(\psi_1^* - \psi_2^*)\alpha(\psi_1 - \psi_2)dx = 1,$$

hence

$$|\alpha|^2 = \frac{1}{2(1-c)} \text{ and for } c < 1 \text{ and } c \neq -1.$$

We have for α :

$$|\alpha| = \frac{1}{\sqrt{2(1-c)}},$$

and $c < 1, c \neq -1$.

With the similar reasoning as given above, we could have chosen α and β to be real numbers.

Finally for the linear combination we find:

$$\psi_3 = \frac{1}{\sqrt{2(1-c)}}(\psi_1 - \psi_2),$$

where we left the phase shift out of account.

Remark:

What is the physical meaning of $|c| = 1$?

To start with : $\int_{-\infty}^{\infty} \psi_1^* \psi_2 dx = 1$.

Well, we know this integral represents a, sort of, inner product.

Then, we may conclude $\psi_1 = \psi_2$. So, $c = 1$ represents a one-dimensional system, with one wave function.

Next $\int_{-\infty}^{\infty} \psi_1^* \psi_2 dx = -1$. This again represents the inner product: ψ_2 “opposing” ψ_1 . Hence, there is nothing left. A system complete at rest.

Exercise 4.7 Proof the momentum operator to be a Hermitian operator

Demonstrate that $p = -i\hbar\partial/\partial x$ is a Hermitian operator. Find the Hermitian conjugate of $a = x + ip$.

As Fitzpatrick(Fp) writes: *x and p are both Hermitian*, page 46.

Eq. (4.57) represents the constraint which needs to be satisfied:

$$\int_{-\infty}^{\infty} \psi^* (O\psi) dx = \int_{-\infty}^{\infty} (O\psi)^* \psi dx,$$

Where O represents the operator.

Now the operator x :

x is a real number, so $\int_{-\infty}^{\infty} \psi^* (x\psi) dx = \int_{-\infty}^{\infty} (x\psi)^* \psi dx$. Consequently the operator x is Hermitian.

The operator $p \equiv -i\hbar \frac{\partial}{\partial x}$:

$$\begin{aligned} \text{with the constraint, Eq. (4.57), we evaluate } \int_{-\infty}^{\infty} \psi^* (-i\hbar \frac{\partial \psi}{\partial x}) dx &= -i\hbar \psi^* \psi |_{-\infty}^{\infty} + \int_{-\infty}^{\infty} i\hbar \psi \frac{\partial \psi^*}{\partial x} dx \\ &= - \int_{-\infty}^{\infty} \psi (-i\hbar \frac{\partial \psi^*}{\partial x}) dx = - \int_{-\infty}^{\infty} \psi \left(i\hbar \frac{\partial \psi}{\partial x} \right)^* dx = \int_{-\infty}^{\infty} \left(-i\hbar \frac{\partial \psi}{\partial x} \right)^* \psi dx ; \text{ QED.} \end{aligned}$$

The Hermitian conjugate of $a = x + ip$:

$$a^\dagger = (x + ip)^\dagger = x^\dagger + (ip)^\dagger.$$

With x and p both Hermitian:

$$a^\dagger = x - ip.$$

$a \neq a^\dagger$ and a is not Hermitian.

Exercise 4.8 About the collapse of the wave function

An operator A , corresponding to a physical quantity α , has two normalized eigenfunctions $\psi_1(x)$ and $\psi_2(x)$, with eigenvalues a_1 and a_2 . An operator B , corresponding to another physical quantity β , has normalized eigenfunctions $\phi_1(x)$ and $\phi_2(x)$, with eigenvalues b_1 and b_2 . The eigenfunctions are related via:

$$\psi_1(x) = (2\phi_1(x) + 3\phi_2(x))/\sqrt{13},$$

and,

$$\psi_2(x) = (3\phi_1(x) - 2\phi_2(x))/\sqrt{13}.$$

α is measured and the value of a_1 is obtained. If β is then measured and then α again, show the probability of obtaining a_1 a second time is 97/169.

Notice $\psi_1(x)$ and $\psi_2(x)$ to be linear combinations of $\phi_1(x)$ and $\phi_2(x)$.

Consequently, $\phi_1(x)$ and $\phi_2(x)$ are linear combinations of $\psi_1(x)$ and $\psi_2(x)$:

$$\phi_1(x) = [2\psi_1(x) + 3\psi_2(x)]/\sqrt{13},$$

and

$$\phi_2(x) = [3\psi_1(x) - 2\psi_2(x)]/\sqrt{13}.$$

To do this exercise, it is of help to read section 4.10. It is about the definite value of an operator after the measurement and the probability of a measurement of the operator (page 56 and 57).

Remark:

For me it became clear when thinking of the metaphor: Throwing the die. A priori, before throwing the die, the probability of throwing a number is 1/6 (The probability of a measurement). Posteriori, after throwing the die, we obtain a definite value (The result of a measurement, one of the 6 states associated with the operation of throwing the die): probability is 1. Sort of “collapse of the dice (Dice: The wave function)”.

Now, α is measured and the value of a_1 is obtained.

The system has collapsed into $\psi_1(x)$ and the probability of finding a_1 is 1.

Next, β is measured. So the operator B acts on $\psi_1(x) = [2\phi_1(x) + 3\phi_2(x)]/\sqrt{13}$.

In what state is this system after the measurement?

We know

$$\langle B \rangle = |c_1|^2 b_1 + |c_2|^2 b_2, \quad \text{Eq. (4.133),}$$

$$|c_1|^2 + |c_2|^2 = 1, \quad \text{Eq. (4.136).}$$

With $\psi_1(x) = [2\phi_1(x) + 3\phi_2(x)]/\sqrt{13}$ and (4.130): $c_1 = \frac{2}{\sqrt{13}}$, and $c_2 = \frac{3}{\sqrt{13}}$. So,

$$\langle B \rangle = |c_1|^2 b_1 + |c_2|^2 b_2 = (4b_1 + 9b_2)/13.$$

Which state do we find after the operation of B ?

We do not know, since B is not executed. It is about probabilities and not an actual measurement, I assume. The metaphor of the dice was of great help.

Fp did not give a statement about the states. So, we have two routes to follow.

Are we allowed to say that the probability to be in $\phi_1(x)$ and finding a_1 is 4/13 and the probability to be in $\phi_2(x)$ and finding a_1 is 9/13? Yes, we are. So, in the end we must combine probabilities of the two routes.

Finally, we “measure” α again. The operator A acts on $\phi_1(x)$ or $\phi_2(x)$, since we do not know in which state the system is. It is again about probabilities. Then we have two probabilities for finding a_1 . The square of the coefficients of $\psi_1(x)$ in the expressions for $\phi_1(x)$ and $\phi_2(x)$ gives us the probabilities. These are 4/13 and 9/13.

Now we must combine probabilities of the two routes.

Assume we have “measured” $\phi_1(x)$, with operating B , the probability is 4/13. With this probable wave function, we enter the probable measurement of α by operating A on $\phi_1(x)$. The probability to find a_1 is again 4/13.

Hence the total probability becomes: $\frac{4}{13} \times \frac{4}{13} = \frac{16}{169}$.

Keep in mind: this probability is found by following one route.

The other route is by the probable measurement of a_1 by using the wave function $\phi_2(x)$. With operating B , the probability is 9/13. With this probable wave function, we enter the probable

measurement of α by operating A on $\phi_2(x)$. The probability to find a_1 is again $9/13$.

Hence the total probability of this route becomes: $\frac{9}{13} \times \frac{9}{13} = \frac{81}{169}$.

We have followed two routes. So, we must add the two total probabilities in order to find the probability of obtaining a_1 :

$$\frac{16}{169} + \frac{81}{169} = \frac{97}{169} .$$

Exercise 4.9 About commutation

Demonstrate that an operator which commutes with the Hamiltonian, and contains no explicit time dependence, has an expectation value which is constant in time.

At the bottom of page 60 Fp made some remarks on a Hermitian operator A which commutes with H . In section 4.10 *On Measurement*, Fp dealt with subject matter of simultaneous eigenstates.

With Eq. (4.138), section 4.10, we have:

$$(H - E_i)A\psi_E = 0 .$$

Eq. (4.139):

$$H(A\psi_E) = E_i A\psi_E .$$

So $A\psi_E$ is an eigenstate of H with eigenvalue E_i . In other words, $A\psi_E \propto \psi_E$, or

Eq. (4.140):

$$A\psi_E = a_i \psi_E .$$

Hence ψ_E is an eigenstate of A , and $[A, H] = 0$.

$$\text{Now } \langle A \rangle = \int_{-\infty}^{\infty} \psi_E^* A\psi_E dx = \int_{-\infty}^{\infty} \psi_E^* a_i \psi_E dx .$$

With Eq. (4.158), section 4.12, the expression for ψ_E ,

$$\langle A \rangle = a_i , \text{ time independent indeed.}$$

Exercise 4.10 About commutation and time dependency

For a certain system, the operator to the physical quantity A does not commute with the Hamiltonian. The eigen values of the operator A are a_1 and a_2 , corresponding to properly normalized eigenfunctions:

$$\phi_1 = \frac{u_1 + u_2}{\sqrt{2}} ,$$

$$\phi_2 = \frac{u_1 - u_2}{\sqrt{2}} ,$$

where u_1 and u_2 are properly normalized eigenfunctions of the Hamiltonian with eigenvalues E_1 and E_2 . If the system is in state $\psi = \phi_1$ at time $t = 0$, show that the expectation value of A at time t is

$$\langle A \rangle = \left(\frac{a_1 + a_2}{2} \right) + \left(\frac{a_1 - a_2}{2} \right) \cos\left(\frac{[E_1 - E_2]t}{\hbar} \right) .$$

Let us start with the comment of Fp at the end of section 4.10 *On Measurements*: "We conclude that if A and $B(= H)$ commute then they possess simultaneous eigen states. And are thus simultaneously measurable (exactly)."

So $[H, A] \neq 0$:

$$\phi_1 \neq u_1 \text{ and } \phi_1 \neq u_2 ,$$

and

$$\phi_2 \neq u_1 \text{ and } \phi_2 \neq u_2 .$$

The wave function of the system.

With Eq. (4.158) we have for the two eigenfunctions, $j = 1, 2$:

$$u_j = u_j(x, 0)e^{-\frac{iE_j t}{\hbar}} .$$

For the wave function $\psi(x, t)$ of the system:

$$\psi(x, t) = c_1 u_1(x, t) + c_2 u_2(x, t) .$$

At time $t = 0$:

$$\psi(x, 0) = \phi_1 .$$

$$\text{Then } \psi(x, 0) = c_1 u_1(x, 0) + c_2 u_2(x, 0) = \phi_1(x, 0) = \frac{[u_1(x, 0) + u_2(x, 0)]}{\sqrt{2}} .$$

$$\text{So } c_1 = \frac{1}{\sqrt{2}} \text{ and } c_2 = \frac{1}{\sqrt{2}} .$$

Hence for the wave function of the system we find:

$$\psi(x, t) = \frac{1}{\sqrt{2}} \left[u_1(x, 0)e^{-\frac{iE_1 t}{\hbar}} + u_2(x, 0)e^{-\frac{iE_2 t}{\hbar}} \right] .$$

Remark:

In Susskind you can find a slightly different approach to obtain $\psi(x, t)$.

$$\text{Again, } \psi(x, t) = c_1(t)u_1(x) + c_2(t)u_2(x) .$$

u_1 and u_2 are the eigenfunctions constituting the vector space of the wave function $\psi(x, t)$.

These are time independent. So, the coefficients $c_j(t)$ are functions of t .

With the time dependent Schrödinger equation we have:

$$\sum_j \frac{d}{dt} [c_j(t)u_j(x)] = -\frac{i}{\hbar} \sum_j c_j(t) E_j u_j(x) .$$

Hence

$$c_j(t) = c_j(0)e^{-\frac{iE_j t}{\hbar}} ,$$

and

$$c_j(0) = \int_{-\infty}^{\infty} u_j^*(x) \psi(x, 0) dx = \int_{-\infty}^{\infty} u_j^*(x) \phi_1(x, 0) dx = \frac{1}{\sqrt{2}} .$$

Now, we collect the expressions needed to find $\langle A \rangle$.

The expectation value $\langle A \rangle$:

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* A \psi dx .$$

We express $u_1(x, t)$ and $u_2(x, t)$ into $\phi_1(x, t)$ and $\phi_2(x, t)$:

$$u_1(x, t) = \frac{[\phi_1(x, t) + \phi_2(x, t)]}{\sqrt{2}} ,$$

and

$$u_2(x, t) = \frac{[\phi_1(x, t) - \phi_2(x, t)]}{\sqrt{2}} .$$

Then

$$\psi(x, t) = \frac{1}{\sqrt{2}} \left\{ \frac{1}{\sqrt{2}} [\phi_1(x, 0) + \phi_2(x, 0)] e^{-\frac{iE_1 t}{\hbar}} + \frac{1}{\sqrt{2}} [\phi_1(x, 0) - \phi_2(x, 0)] e^{-\frac{iE_2 t}{\hbar}} \right\} .$$

The operator A :

$$A\phi_1(x, t) = a_1\phi_1(x, t),$$

and

$$A\phi_2(x, t) = a_2\phi_2(x, t).$$

The goniometric relation:

$$\frac{1}{2} \left\{ e^{\frac{i(E_1-E_2)t}{\hbar}} + e^{-\frac{i(E_1-E_2)t}{\hbar}} \right\} = \cos\left(\frac{[E_1-E_2]t}{\hbar}\right)$$

This completes the set of ingredients we need to find $\langle A \rangle$.

Using the wavefunction $\psi(x, t)$ of the system, the normalisation and orthogonality conditions and the operation of A , we finally obtain after straightforward bookkeeping:

$$\langle A \rangle = \left(\frac{a_1+a_2}{2} \right) + \left(\frac{a_1-a_2}{2} \right) \cos\left(\frac{[E_1-E_2]t}{\hbar}\right).$$

So $\langle A \rangle$, now a function of time, fluctuates between a_1 and a_2 .

Remarks:

This above result for $\langle A \rangle$ could lead you to conclude: no collapse. Then it is of some help to read section 4.10 *On Measurement* again. There you find, in general, Eq. (4.132):

$$\sigma_A^2 = \langle A^2 \rangle - \langle A \rangle^2 = 0.$$

Here $\langle A \rangle$ can be a function of time. I assume. Eq. (4.136) still holds. So, with an actual measurement we will arrive at the collapse of the wave function. Will we?

Let's find out about $\langle A^2 \rangle$.

With the expression for the wave function of the system $\psi(x, t)$ expanded into $\phi_1(x, 0)$ and $\phi_2(x, 0)$, we find for $\langle A^2 \rangle$:

$$\langle A^2 \rangle = \left(\frac{a_1^2+a_2^2}{2} \right) + \left(\frac{a_1^2-a_2^2}{2} \right) \cos\left(\frac{[E_1-E_2]t}{\hbar}\right).$$

$$\text{Then } \sigma_A^2 = \langle A^2 \rangle - \langle A \rangle^2 = \left(\frac{a_1-a_2}{2} \right)^2 \sin^2\left(\frac{[E_1-E_2]t}{\hbar}\right).$$

For σ_A^2 to be 0, the sin function has to be 0.

So,

$$\frac{[E_1-E_2]t}{\hbar} = k\pi, \text{ with } k = 0, 1, 2, 3, \dots.$$

Or $E_1 - E_2 = \frac{\hbar k\pi}{t}$, eigenvalues dependent on time and ultimately becoming a degenerate system.

The above exercise is about a wavefunction $\psi(x, t) = \phi_1(x, 0)$ at $t = 0$. So, the system is prepared in the eigenstate $\phi_1(x, 0)$. You could guess, the system remains in that situation.

However, the problem does not go away:

$$\sigma_A^2 = \langle A^2 \rangle - \langle A \rangle^2 = \left(\frac{a_1}{2} \right)^2 \sin^2\left(\frac{[E_1-E_2]t}{\hbar}\right).$$

In section 4.10 Fp dealt with a two dimensional system.

Translate Eq. (4.137) for this exercise 4.10, then:

$$(a_1 - a_2)^2 |c_1|^2 |c_2|^2 = \left(\frac{a_1-a_2}{2} \right)^2 \sin^2\left(\frac{[E_1-E_2]t}{\hbar}\right),$$

where

$$c_1(t) = \int_{-\infty}^{\infty} \phi_1^*(x, 0) \psi(x, t) dx,$$

and

$$c_2(t) = \int_{-\infty}^{\infty} \phi_2^*(x, 0) \psi(x, t) dx .$$

So we need to expand $\psi(x, t)$ in the eigenstates $\phi_1(x, 0)$ and $\phi_2(x, 0)$.

We did that already. After some regrouping:

$$\psi(x, t) = \frac{1}{2} \phi_1(x, 0) \{e^{-\frac{iE_1 t}{\hbar}} + e^{-\frac{iE_2 t}{\hbar}}\} + \frac{1}{2} \phi_2(x, 0) \{e^{-\frac{iE_1 t}{\hbar}} - e^{-\frac{iE_2 t}{\hbar}}\}.$$

Then

$$c_1(t) = \frac{1}{2} \{e^{-\frac{iE_1 t}{\hbar}} + e^{-\frac{iE_2 t}{\hbar}}\},$$

and

$$c_2(t) = \frac{1}{2} \{e^{-\frac{iE_1 t}{\hbar}} - e^{-\frac{iE_2 t}{\hbar}}\}.$$

These two expressions give us

$$|c_1|^2 = \frac{1}{2} [1 + \cos(\frac{[E_1 - E_2] t}{\hbar})]$$

and

$$|c_2|^2 = \frac{1}{2} [1 - \cos(\frac{[E_1 - E_2] t}{\hbar})].$$

Both expressions represent the probabilities of finding the eigenvalues a_1 and a_2 respectively as a function of time.

Obviously, $|c_1|^2 + |c_2|^2 = 1$.

Could we still speak of the collapse of the wave function?

Finally, the commutator $[H, A] \neq 0$.

What do we find by simultaneously measuring H and A ?

For the wave function of the system I now use an expansion in the eigenfunctions u_1 and u_2 :

$$\psi(x, t) = d_1 u_1 + d_2 u_2 .$$

Above we found:

$$\psi(x, t) = \frac{1}{\sqrt{2}} \left[u_1(x, 0) e^{-\frac{iE_1 t}{\hbar}} + u_2(x, 0) e^{-\frac{iE_2 t}{\hbar}} \right].$$

Now:

$$d_1(t) = e^{-\frac{iE_1 t}{\hbar}} / \sqrt{2} ,$$

and

$$d_2(t) = e^{-\frac{iE_2 t}{\hbar}} / \sqrt{2} .$$

Obviously, $|d_1|^2 + |d_2|^2 = 1$.

What about:

$$(HA - AH)\psi(x, t) \neq 0?$$

For the analysis we use the expression for ϕ_1 and ϕ_2 in terms of u_1 and u_2 and vice versa.

I just give the result:

$$(HA - AH)\psi(x, t) = -\frac{1}{2\sqrt{2}} (E_1 - E_2) (a_1 - a_2) (d_1 - d_2) (\phi_1 - \phi_2) \neq 0 ,$$

or:

$$(HA - AH)\psi(x, t) = -\frac{1}{2\sqrt{2}}(E_1 - E_2)(a_1 - a_2)(e^{-\frac{iE_1 t}{\hbar}} - e^{-\frac{iE_2 t}{\hbar}})u_2 \neq 0.$$

We can do the same analysis with one eigenfunction, u_1 say.

The result is:

$$(HA - AH)u_1 = -\frac{1}{2}(E_1 - E_2)(a_1 - a_2)u_2 \neq 0.$$

That is what we should find.

5. One-Dimensional Potentials

5.1 Introduction

In this chapter Fp investigates the interaction of a particle with a potential $V(x)$.

Stationary solutions are analysed. So, the eigenfunction given in Eq. (4.158) can be used. The time-independent Schrödinger equation is given by Eq. (4.159).

5.2 Infinite Potential Well.

A particle of mass m and energy E is considered.

Eq.(5.5) is the equation to be solved.

Fp mentioned there are no solutions for $E < 0$. The physical reasoning is presented. The mathematical reasoning is the following.

Proof:

The Schrödinger equation (5.5) is: $\left(\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + E\right) \psi = 0$.

For the boundary conditions:

$$\psi(x) = 0, \text{ at } x = 0 \text{ and } \psi(x) = 0 \text{ at } x = a.$$

The mathematics are:

for $E < 0$, the solution of the above wave equation is:

$$\psi(x) = C_3 e^{-\alpha x} + C_4 e^{\alpha x},$$

$$\text{where } \alpha^2 = -\frac{2mE}{\hbar^2}.$$

So for $x = 0$,

$$C_3 = -C_4 \text{ and}$$

$$\text{for } x = a, : C_3(e^{-\alpha a} - e^{\alpha a}) = 0.$$

With $\alpha \neq 0$, $C_3 = 0 \rightarrow \psi(x) = 0$: no solution for $E < 0$.

End of proof.

Pug (5.7) into (5.10), and the value $A_n = \sqrt{2/a}$ is obtained.

At the end of section 5.2 Fp presented the coefficients of the linear superposition of the stationary solutions, eigenfunctions, Eq. (5.13):

$$c_n = \int_0^a \psi_n(x) \psi(x, 0) dx.$$

In section 4.12 on stationary states the similar equation is given:

$$c_i = \int_{-\infty}^{\infty} \psi_i^*(x) \psi(x, 0) dx.$$

So there is a typo in Eq. (5.13) : the complex conjugate sign is missing.

Furthermore, I prefer the approach by Susskind:

$$c_n(t) = c_n(0) e^{-iE_n t/\hbar} = \int_0^a \psi_n^*(x) \psi(x, t) dx.$$

5.3 Square Potential Barrier

In this section we deal with incoming particles, reflected particles and transmitted particles.

On page 65 Fp referred to the probability current [particle current (4.19)]:

$$j(x, t) = \frac{i\hbar}{2m} \left(\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right).$$

Substitute the general expression for the wave function to the left of the barrier, (5.16), into the expression for $j(x, t)$ and you will find Eq. (5.17).

Pug (5.18) into (4.19) \rightarrow (5.19).

At the bottom of page 65 Fp investigated the results inside the potential barrier. There Fp writes: “...consider the case where $E > V_0$ ” Well, this I don’t think inside the barrier but inside the barrier range $0 < x < a$. Inside the barrier I assume $E < V_0$.

On page 66 Fp obtained Eqs. (5.28) and (5.29) after considerable algebra indeed.

Fp discussed the comparison of the quantum mechanical probabilities and the results derived from classical physics.

At the bottom of page 66 Fp referred to the de Broglie wavelength:

$$\lambda_B = \frac{2\pi\hbar}{p}. \text{ Keep in mind } p \equiv q.$$

In the final part of this section Fp discussed the case $E < V_0$.

Again Fp compared the quantum mechanical probabilities with those from classical physics.

The phenomenon of tunneling is mentioned.

5.4 WKB Approximation

In this section Fp discussed approximate solutions for the wave equation when exact solutions cannot be obtained. A particle moving slowly through some slowly varying potential $V(x)$.

A solution of the form:

$$\psi(x) = \psi_0 \exp\left[\int_0^x ik(x') dx'\right],$$

is used.

Before going any further let’s make a detour to Mahan.

Mahan presented WKBJ(what’s in a name) as a perturbation expansion the small parameter being \hbar . Indeed a bit weird in a mathematical sense: a dimensional parameter.

The first term of the expansion presented by Mahan is

$$\psi(x) = \psi_0 \exp\left[\int_0^x ik(x') dx'\right]$$

(notation of Fp) for a particle in the positive x -direction.

Including the second term of the expansion, Mahan arrived at:

$$\psi(x) = \frac{\psi_0}{\sqrt{k(x)\hbar}} \exp\left[\int_0^x ik(x')dx'\right],$$

again in the notation of Fp.

In the expansion used by Mahan dk/dx is neglected too. The differences between Mahan and Fp are small indeed. Mahan started with a mere simple exponential function and obtained Eq. (5.40). However, by using the second term in the expansion, Mahan found the amplitude to depend on $1/\sqrt{k(x)}$. Making the wave function infinite for $k(x) \rightarrow 0$. This is discussed by Fp on page 71.

On page 70: *"In other words, the variation length-scale of $k(x)$, which is approximately the same as the variation length-scale of $V(x)$, must be much greater than the particle's de Broglie wavelength(which is of the order k^{-1})"*.

At the top of page 71, Fp writes: *"...By definition, $E < V(x)$ inside ..."*. There I agree.

At the bottom of page 71 Fp mentioned that the transmission probability must be small for the WKB to be valid. This follows from the criterion given in Eq. (5.43). Well, the exponential in Eq. (5.49) can be approximated by

$$k(x_2 - x_1).$$

So the in order to have a small probability of tunneling, we need to have

$$k(x_2 - x_1) \gg 1,$$

or

$$k^2 \gg \left| \frac{k}{(x_2 - x_1)} \right|.$$

$$\text{With } \frac{dk}{dx} = O\left(\frac{k}{(x_2 - x_1)}\right),$$

we find Eq. (5.43).

Fp mentioned the validity of the criterion to break down at the edges of the potential barrier. I would have appreciated a reference to further reading.

5.5 Cold Emission

In this section an example of transmission is presented.

It is about the photoelectric effect as presented in Sect 3.6.

Fp introduced an external electric of strength \mathcal{E} .

The electrons near the surface of the metal are trapped in a potential well of strength W .

So I think, in the absence of the electric field, the square root in Eq. (5.50) should read:

$$\sqrt{W - E}.$$

(5.52) is obtained by the substitution of: $x = \frac{W}{e\mathcal{E}}y$.

Then, in Eq. (5.53) W should be replaced by $W - E$.

The subject matter of tunneling is also dealt with by Mahan, section 3.3 on Electron Tunneling.

5.6 Alpha Decay

In this section Fp investigates the α -decay of an atomic nucleus.

This is another example of tunneling. The potential is the potential between the α -particle and the daughter nucleus.

On page 74 Fp derived the expression for the probability of the α -particle tunneling through the potential barrier: Eq. (5.61).

To find this expression the integral needs to be solved.

$$\int_1^{1/\epsilon} \left[\frac{1}{y} - \epsilon \right]^{1/2} dy ,$$

where $\epsilon = \frac{E}{E_c}$, and E_c is defined by Eq.(5.59).

Usually, Fp writes that this integration is easily done.

When you use the substitution

$$\sqrt{y} = \frac{\sin s}{\sqrt{\epsilon}} ,$$

you arrive at :

$$\frac{\pi}{2\sqrt{\epsilon}} - \frac{1}{2\sqrt{\epsilon}} \sin 2 \sin^{-1} \sqrt{\epsilon} - \frac{1}{\sqrt{\epsilon}} \sin^{-1} \sqrt{\epsilon} .$$

Now make use of $\epsilon \ll 1$ and Eq. (5.60) is found.

Having obtained by solving this integral the probability of tunneling, $|T|^2$, Fp paid attention to the decaying process. To this end Fp derived the frequency of the particle bouncing in the potential well.

I assumed Fp derived the frequency by using a mass m_p of the α -particle not given in the text.

On the internet, www.en.wikipedia.org, I obtained a number for $m_p \cong 6 \times 10^{-27}$ kg.

With $1\text{MeV}=1.6 \cdot 10^{13}$ Joule you obtain the frequency in cycles per year as given in Eq.(5.62).

Finally, Fp derived the half-live time of the α -particle and evaluated the theoretical results with experimental data.

5.7 Square Potential Well

Fp considered the unbound situation. The potential well is located in the interval

$$-a/2 \leq x \leq a/2 \text{ with } V(x) = -V_0 \text{ and elsewhere } V(x) = 0.$$

For $E > 0$ the particle is unbounded or in a continuum state.

For the potential well, replace in Eq. (5.22) V_0 through $-V_0$ and you obtain the expression for the reflection and transmission coefficients as presented in the Eqs. (5.28) and (5.29).

When the potential is symmetric, by replacing x through $-x$ it is shown that the solutions of the Schrödinger's equation are symmetric or anti-symmetric.

Fp discussed the symmetric solution: $\psi(x) = \psi(-x)$.

The solutions are presented in Eqs. (5.76)-(5.81).

The constraints: continuity of the wave function and its first derivative at $x = a/2$ gives the following set of equations:

$$\psi\left(\frac{a}{2}\right) = B \cos\left(\frac{qa}{2}\right) , \text{ inside the well,}$$

$\psi\left(\frac{a}{2}\right) = Ae^{-ka/2}$, outside the well,

$\frac{d\psi}{dx} = -Bq \sin\left(\frac{qa}{2}\right)$, inside the well,

$\frac{d\psi}{dx} = -Ake^{-ka/2}$, outside the well.

Hence we have:

$$B \cos\left(\frac{qa}{2}\right) = Ae^{-ka/2},$$

and

$$-Bq \sin\left(\frac{qa}{2}\right) = -Ake^{-ka/2}.$$

Dividing both expression we get rid of A and B :

$$q \tan\left(\frac{qa}{2}\right) = k, \rightarrow \text{Eq. (5.82)}.$$

Eq. (5.83) by rewriting Eq. (5.81):

$$E = \frac{q^2 \hbar^2}{2m} - V_0,$$

using

$$E_0 = \frac{2\hbar^2}{ma^2}, \text{ and } y = qa/2.$$

In addition Eq.(5.82) can be expressed in terms of y :

$$k = q \tan y,$$

where k is given by Eq. (5.74):

$$k^2 = \frac{2mE}{\hbar^2},$$

with $-V_0 < E < 0$.

$$\text{So } \tan y = \frac{k}{q} = \frac{\sqrt{2m|E|/\hbar^2}}{q}.$$

Given $-V_0 < E < 0$, we know $|E| = V_0 - E_0 y^2$, where E_0 is given by Eq. (5.84).

You will finally obtain:

$$\frac{\sqrt{\lambda - y^2}}{y} = \tan y, \text{ Eq.(5.85),}$$

where λ is given in Eq. (5.86).

On page 78 Fp discussed Eq. (5.85) represented in Figure 5.7 for a particular value of λ .

On page 79 Fp briefly discussed the anti-symmetric solution of Schrödinger's equation:

$$\psi(x) = -\psi(x) \rightarrow \psi(x) = D \sin(qx) \text{ inside the well.}$$

Outside the well, the wave function vanish for $|x| \rightarrow \infty$.

With the square well, we have a symmetric and an anti-symmetric solution. What will we obtain by using from the start the symmetric and anti-symmetric solution?

Since we have a linear second order differential equation, we have inside the well:

$$\psi(x) = B \cos(qx) + D \sin(qx), \tag{C.5.7.1}$$

and outside the well: $x > a/2$

$$\psi(x) = Ae^{-kx},$$

for $x < -a/2$,

$$\psi(x) = Ce^{kx}.$$

(C.5.7.1) can be written as

$$\psi(x) = F \sin(qx + \gamma) .$$

For the phase shift γ :

$$\tan \gamma = \frac{B}{D} .$$

The constraints at $x > a/2$, i.e. continuity of the wave function and its derivative, give us:

$$\tan \left[\left(\frac{qa}{2} \right) + \gamma \right] = -\frac{1}{k} . \quad (C.5.7.2)$$

From the constraints at $x < a/2$ we have:

$$\tan \left[-\left(\frac{qa}{2} \right) + \gamma \right] = \frac{1}{k} . \quad (C.5.7.3)$$

Divide (C.5.7.2) and (C.5.7.3) $\rightarrow \gamma = 0$.

We recover the anti-symmetric wave function solution.

On the other hand, we could have used another goniometric representation of (C.5.7.1):

$$\psi(x) = G \cos(qx - \gamma) \text{ and}$$

$$\tan \gamma = \frac{D}{B} .$$

Again using the constraints

at $x > a/2$:

$$\tan \left[\left(\frac{qa}{2} \right) - \gamma \right] = k , \quad (C.5.7.4)$$

at $x < a/2$:

$$\tan \left[-\left(\frac{qa}{2} \right) - \gamma \right] = -k . \quad (C.5.7.5)$$

Divide (C.5.7.4) and (C.5.7.5) $\rightarrow \gamma = 0$.

Now we obtain the symmetric wave function for the square potential well.

Let us pay attention to normalization of the symmetric wave function for the square potential well.

We need to evaluate the interval $-\infty < -a/2 < a/2 < \infty$ for three wavefunctions:

$$A_1 e^{kx} : -\infty < x < -a/2 ,$$

$$A_2 \cos qx : -\frac{a}{2} \leq x \leq a/2 \text{ and}$$

$$A_3 e^{-kx} : a/2 < x < \infty .$$

The integral to be evaluated are:

$$1 = A_1^2 \int_{-\infty}^{-a/2} e^{2kx} dx + A_2^2 \int_{-a/2}^{a/2} \cos^2(qx) dx + A_3^2 \int_{a/2}^{\infty} e^{-2kx} dx . \quad (C.5.7.6)$$

Using continuity at the edges of the well, we finally obtain with Eq. (C.5.7.6):

$$A_2 = \left[\frac{2kq}{\cos^2\left(\frac{qa}{2}\right) + akq - k \sin(qa)} \right]^{1/2} ,$$

and

$$A_1 = A_3 = A_2 e^{ka/2} \cos\left(\frac{qa}{2}\right) .$$

Let's pay some attention to the anti-symmetric case.

Then we have for the wave function:

$$\psi(x) = B \sin qx ,$$

and for the eigenvalue equation:

$$\tan\left(\frac{qa}{2}\right) = -\frac{q}{k}.$$

The argument of the tangent function is positive: the wave number is positive.

Consequently, $\frac{qa}{2} > \frac{\pi}{2}$.

With Eqs. (5.83) and (5.86) we obtain Eq. (5.85).

So, for $\frac{qa}{2} < \frac{\pi}{2}$, there are no bound states. With Eq.(5.75) and $0 < E + V_0 < V_0$, we find no bound states for

$$V_0 < \frac{\pi^2 \hbar^2}{8ma^2}.$$

The potential well is too “shallow”.

5.8 Simple Harmonic Oscillator

The classical Hamiltonian of the simple harmonic oscillator is given in Eq. (5.90).

Fp presented approximate solutions of the time-independent Schrödinger equation given by Eq. (5.96). This approximates Weber’s equation (Parabolic cylinder functions, Abramowitz and Stegun, Whittaker and Watson). You can also use your WolframAlpha App.

Fp attempts a power solution for the approximate differential equation (5.98) and equated the coefficients with the same power of the variable.

Note:

The power-law solution used is of the form:

$$h(y) = \sum_{i=0}^{\infty} c_i y^i, \text{ Eq. (5.99).}$$

Then, you have to pay attention to the second derivative in Eq.(5.98):

$$\frac{d^2 h}{dy^2} = \sum_{i=2}^{\infty} c_i i(i-2)y^{i-2}.$$

With $i = k + 2$, we find : $\frac{d^2 h}{dy^2} = \sum_{k=0}^{\infty} c_{k+2}(k+2)(k+1)y^k$.

Set $k = i$ in the expression for $\frac{d^2 h}{dy^2}$ and start equating the coefficients of y^i .

Equating the coefficients gives the recursion relation Eq. (5.101).

Fp derived ϵ to be : $\epsilon = 2n + 1$.

So, for $i = n$, $c_{n+2} = 0$. Fp explains this to be the method to prevent the wave function ψ from blowing up for $|y| \rightarrow \infty$.

Remark: what about $c_{n+1}(= -2 \cdot c_{n-1})$, $c_{n+3}(= 2 \cdot c_{n+1})$, ... $n \rightarrow \infty$? Well, it is about terminating the series in Eq.(5.102). So, though $c_{n+3} \neq 0$, this coefficient is neglected.

At the bottom of page 81 Fp introduced *zero-point energy*.

The normalized wave function of the lowest energy state is obtained by:

$$\int_{-\infty}^{\infty} \psi_0^* \psi_0 dx = 1 \text{ and } n = 0.$$

We have, with Eqs. (5.92), (5.97) and (5.99), $h(y) = c_0$,:

$$\psi_0(x) = c_0 e^{-x^2/2d^2},$$

where $d := \sqrt{\hbar/m\omega}$.

Normalization produces:

$$c_0 = \frac{1}{\pi^{1/4} \sqrt{d}}.$$

On page 82 Fp defined two operators: a_{\pm} , Eq. (5.109) and mentioned the commutation relation of these operators:

$$[a_+, a_-] = -1, \text{ Eq. (5.110).}$$

Caveat: to find the commutation relation one has to operate in the following way:

$$[a_+, a_-] \psi = a_+(a_- \psi) - a_-(a_+ \psi) = -\psi.$$

Then you will find Eq. (5.111), with Eqs. (5.108) and (5.109):

$$a_+(a_-) \psi_n = a_+ \left(\frac{d\psi_n}{dy} + y\psi_n \right) = \frac{1}{2} \left[-\frac{d^2\psi_n}{dy^2} - \psi_n + y^2\psi_n \right] = n\psi_n.$$

Below Eq. (5.112) Fp writes: "The above two equations imply that....".

Well, 'Du sprichst wieder(Nz) ein großes Wort gelassen aus', Goethe.

The theory presented so far does not give a clue to find Eqs. (5.113) and (5.114).

So, what I can do is find out whether the implication of both equations leads to a contradiction.

Assume $a_+ \psi_n = \sqrt{n+1} \psi_{n+1}$ is correct.

With this expression and Eq. (5.112):

$$a_- a_+ \psi_n = (n+1) \psi_n = a_- \sqrt{n+1} \psi_{n+1}. \text{ This expression is correct for:}$$

$$a_- \psi_{n+1} = \sqrt{n+1} \psi_n, \text{ this represents Eq. (5.114). Hence, there is no contradiction.}$$

In the same way there is no contradiction assuming Eq. (5.114) to be correct.

In Eq. (5.117) we have the operator:

$$a_+ + a_-.$$

With Eq. (5.109), this can be written as:

$$a_+ + a_- = \frac{1}{\sqrt{2}} \left[\left(-\frac{d}{dy} + y \right) + \left(\frac{d}{dy} + y \right) \right] = \sqrt{2} \cdot y.$$

Note: in Eq. (5.117) Fp uses m for the mass of the particle and the number of the quantum state.

Mahan derived the solutions for the harmonic oscillator by application of Hermite polynomials Eq.(2.108), quite similar to the above approach by Fp for large values of the dimensionless position variable y .

Susskind derived the time independent Schrödinger equation (10.44). Susskind proposed a ground state that worked and obtained the ground state energy. With help of the raising and lowering operators, the first and second excited states are found. Included the entire spectrum of harmonic oscillator energy levels.

Exercises.

Exercise 5.1 An infinite one-dimensional well

Show that the wave function of a particle of mass m in an infinite one-dimensional square well of width a returns to its original form after quantum revival time

$$T = 4ma^2/\pi\hbar.$$

Original form suggest time dependency and quantum revival time periodicity.

So we will use the time dependent solution given in Eq. (5.12):

$$\psi(x, t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}.$$

For the infinite one-dimensional square well:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, \text{ Eq. (5.9).}$$

For the wave function's return to its original form we have:

$$E_n t \rightarrow E_n T = \frac{\frac{n^2 \pi^2 \hbar^2}{2ma^2} 4ma^2}{\pi \hbar} = n^2 2\pi \hbar.$$

Hence :

$$e^{-iE_n t/\hbar} \rightarrow e^{-iE_n T/\hbar} = e^{-in^2 2\pi} = 1.$$

With $n^2 \in \mathbb{N}$, we have shown the wave function to return to its original form.

Exercise 5.2 The time evolution of the wave function

A particle of mass m moves freely in one dimension between impenetrable walls located at $x = 0$ and $x = a$. Its initial wave function is:

$$\psi(x, 0) = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi x}{a}\right).$$

What is the subsequent time evolution of the wave function?

Suppose that the initial wave function is:

$$\psi(x, 0) = \sqrt{\frac{1}{a}} \sin\left(\frac{\pi x}{a}\right) [1 + 2 \cos\left(\frac{\pi x}{a}\right)].$$

What now is the subsequent time evolution? Calculate the probability of finding the particle between 0 and $a/2$ as a function of time in each case.

As explained in Chapter 4, we can express a general wave function as a linear combination of energy eigen states, Eq. (4.162):

$$\psi(x, t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar},$$

and

$$\psi(x, 0) = \sum_n c_n \psi_n(x).$$

First:

$$\psi(x, 0) = \sum_n c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi x}{a}\right).$$

So we have for the subsequent time evolution of the wave function:

$$\psi(x, t) = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi x}{a}\right) e^{-iE_3 t/\hbar}, \quad (\text{C.E.1})$$

with

$$E_3 = \frac{9\pi^2 \hbar^2}{2ma^2}, \text{ Eq. (5.9).}$$

The probability of finding the particle between 0 and $a/2$, $P\left(0 \leq x \leq \frac{a}{2}\right)$, as a function of time:

$$P(x, t) = \int_0^{a/2} |\psi(x, t)|^2 dx.$$

With (C.E.1) we obtain for the probability $P(x, t)$:

$$P(x, t) = \int_0^{a/2} \frac{2}{a} \sin^2\left(\frac{3\pi x}{a}\right) dx = \frac{1}{2},$$

no time dependency.

Second:

$$\psi(x, 0) = \sum_n c_n \psi_n(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{\pi x}{a}\right) [1 + 2 \cos\left(\frac{\pi x}{a}\right)] = \sqrt{\frac{1}{a}} \left[\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right) \right].$$

For the time evolution of the wave function:

$$\psi(x, t) = \sqrt{\frac{1}{a}} \left[\sin\left(\frac{\pi x}{a}\right) e^{-\frac{iE_1 t}{\hbar}} + \sin\left(\frac{2\pi x}{a}\right) e^{-\frac{iE_2 t}{\hbar}} \right], \quad (\text{C.E.2})$$

with E_1 and E_2 given by Eq. (5.9).

The probability of finding the particle between 0 and $a/2$, $P\left(0 \leq x \leq \frac{a}{2}\right)$, as a function of time:

$$P(x, t) = \int_0^{a/2} |\psi(x, t)|^2 dx.$$

With (C.E.2) we obtain for the probability $P(x, t)$:

$$P(x, t) = \frac{1}{2} + \frac{2}{3\pi} \cos\left[\frac{(E_2 - E_1)t}{\hbar}\right],$$

and we find the probability with two energy levels to be time dependent.

Exercise 5.3 A particle in an infinite square well expanded suddenly

A particle of mass m is in the ground state of an infinite one-dimensional square-well of width a . Suddenly the well expands to twice its original size, as the right wall moves from a to $2a$, leaving the wave function momentarily undisturbed. The energy of the particle is now measured. What is the most probable result? What is the probability of obtaining this result? What is the next most probable result, and what is its probability of occurrence? What is the expectation value of the energy?

We assume the moment of the sudden expansion of the width of the potential well to be $t = 0$.

So at $t = 0$ we have a wave function half a cycle of:

$$\psi(x, 0) = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}, \text{ Eq. (5.11), with } 0 \leq x \leq a \quad (\text{C.E.3})$$

and

$$\psi(x, 0) = 0, \text{ with } a \leq x \leq 2a. \quad (\text{C.E.4})$$

The energy of the particle is now measured. I assume “now” to be at $t = 0$.

Well, the measured energy is the expectation value:

$$\langle E \rangle = \int_0^b \psi^* H \psi dx,$$

$$b = 2a.$$

$$k = \frac{\pi}{a} \text{ and } k = \sqrt{\frac{2m E_1}{\hbar^2}}.$$

$$\text{Then } \langle E \rangle = E_1 \int_0^b \psi^* \psi dx$$

With (C.E.3), (C.E.4) and Eq. (5.9), we find for the expectation value:

$$\langle E \rangle = E_1 = \frac{\pi^2 \hbar^2}{2ma^2}.$$

The probability of obtaining this result is, with (C.E.3) and (C.E.4) :

$$P = \int_0^b \psi^* \psi dx = 1.$$

What is the next probable result (of the energy)?

I assume “next” to mean: the wave function has evolved in time and “feels” the potential well of width $2a$.

We do not know in what state the particle will be.

What we do assume the particle in the well of width $b = 2a$ has the same energy as the particle in the well of width a .

The energy of the particle in the well of width a is:

$$E_1 = \frac{\pi^2 \hbar^2}{2ma^2}.$$

The energy of the particle in the well of width $b = 2a$ is

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mb^2}.$$

$$\text{So } E_n = \frac{n^2 \pi^2 \hbar^2}{2mb^2} = \frac{\pi^2 \hbar^2}{2ma^2}.$$

Hence:

$$n = \frac{b}{a}.$$

Consequently, the next possible result is the particle to be in the first excited state:

$$n = 2.$$

So when time evolves, the particle will accommodate to the wider potential well in the first excited state.

Now the wave function reads:

$$\psi(x, t) = \sqrt{\frac{2}{b}} \sin \frac{n\pi x}{b} e^{-iE_2 t/\hbar}. \quad (\text{C.E.5})$$

The probability to be in that state is

$$P_2 = \int_0^b \frac{2}{b} \sin^2 \frac{2\pi x}{b} dx = 1.$$

The expectation value of the energy is:

$$\langle E \rangle = E_2 = \frac{4\pi^2 \hbar^2}{2mb^2} = \frac{\pi^2 \hbar^2}{2ma^2}.$$

Exercise 5.4 A potential step. Reflection and transmission

A stream of particles of mass m and energy $E > 0$ encounter a potential step of height $W (< E)$. $V(x) = 0$ for $x < 0$ and $V(x) = W$ for $x > 0$ with the particle's incidence from $-\infty$. Show that the fraction reflected is

$$R = \left(\frac{k-q}{k+q} \right)^2,$$

where $k^2 = \left(\frac{2m}{\hbar^2} \right) E$ and $q^2 = \left(\frac{2m}{\hbar^2} \right) (E - W)$.

The solution to the Schrödinger equation for $x < 0$:

$$\psi(x) = e^{ikx} + R e^{-ikx},$$

and for $x > 0$:

$$\psi(x) = T e^{iqx}.$$

At $x = 0$: ψ and $d\psi/dx$ are continuous.

Consequently:

$$1 + R = T ,$$

and

$$k(1 - R) = Tq.$$

$$\text{Hence } R = \frac{k-q}{k+q}.$$

Remark:

The exercise is about to prove $R = \left(\frac{k-q}{k+q}\right)^2$. Well, I assume this to be a typo. See Mahan, page 23.

Exercise 5.5 A delta function potential, reflection and a bound state

A stream of particles of mass m and energy $E > 0$ encounter the delta-function potential $V(x) = -\alpha\delta(x)$, where $\alpha > 0$. Show that the refraction/refelction reflected is :

$$R = \beta^2 / (1 + \beta^2) ,$$

$$\text{where } \beta = \frac{m\alpha}{\hbar^2 k}, \text{ and } k^2 = \left(\frac{2m}{\hbar^2}\right) E.$$

Does such a potential have a bound state? If so, what is its energy?

Let us start with the delta-function potential well and $E > 0$.

The solution to the Schrödinger equation for $x < 0$:

$$\psi(x) = e^{ikx} + Re^{-ikx} ,$$

and for $x > 0$:

$$\psi(x) = Te^{iqx} .$$

At $x = 0$: ψ is continuous and $d\psi/dx$ is not due to the delta-function. In Mahan page 45 you will find the analysis of the delta-function potential. In this exercise we will apply this analysis.

So at $x = 0$: $\lim_{x \rightarrow -0} \psi(x)$ and $\lim_{x \rightarrow +0} \psi(x)$ give

$$1 + R = T .$$

For the derivative at $x = 0$ we have:

$$\left(\frac{\partial\psi}{\partial x}\right)_{x \rightarrow +0} - \left(\frac{\partial\psi}{\partial x}\right)_{x \rightarrow -0} = -\frac{2m\alpha}{\hbar^2} \psi(0) . \text{ (Mahan Eq. (2.225)).} \quad (\text{C.E.6})$$

With both wave functions (C.E.6) produces:

$$ikT - ik + ikR = -\frac{2m\alpha}{\hbar^2} \psi(0). \quad (\text{C.E.7})$$

For $\psi(0)$ we can use $\psi(0) = 1 + R$ or $\psi(0) = T$.

Well, choose $\psi(0) = T$ and subsequently substitute $T = 1 + R$ into (C.E.7) gives:

$$R = \frac{-\beta^2 + i\beta}{1 + \beta^2} .$$

In this expression for R the imaginary part represents a phase angle and does not contribute to the absolute value of R , neither does the $-$ sign.

The following question be answered is: does the delta-function potential have a bound state? It does. Mahan dealt with this case (pages 46 and 47). I will present the results:

- There is only one bound state.

- The energy of this bound state is $E = \frac{m\alpha}{2\hbar^2}$.

Exercise 5.6 Two potential wells and tunneling

Two potential wells of width a are separated by a distance $L \gg a$. A particle of mass m and energy E is in one of the wells. Estimate the time required for the particle to tunnel to the other well.

We assume a symmetrical potential $V(x)$. Furthermore we set the depth of both wells equal to $V_0 > 0$, $-V_0 < E < 0$.

$$V = 0 \text{ for } x < -\left(\frac{L}{2} + a\right) \rightarrow \psi(x) = A_1 e^{kx}$$

$$V = -V_0 \text{ for } -\left(\frac{L}{2} + a\right) < x < -\frac{L}{2} \rightarrow \psi(x) = A_3 \cos \left[q \left(x + \frac{L}{2} + \frac{a}{2} \right) \right]$$

$$V = 0 \text{ for } -\frac{L}{2} < x < \frac{L}{2} \rightarrow \psi(x) = A_4 e^{kx} + A_5 e^{-kx}$$

$$V = -V_0 \text{ for } \frac{L}{2} < x < \left(\frac{L}{2} + a\right) \rightarrow \psi(x) = T \cos \left[q \left(x - \frac{L}{2} - \frac{a}{2} \right) \right]$$

and

$$V = 0 \text{ for } x > \left(\frac{L}{2} + a\right) \rightarrow \psi(x) = A_2 e^{-kx},$$

where

$$k^2 = -\frac{2mE}{\hbar^2}, \text{ and } q^2 = \frac{2m(V_0 + E)}{\hbar^2} \text{ with } -V_0 < E < 0.$$

We need to obtain the transition coefficient T for tunneling to the other well.

From matching conditions and normalization we find an expression for $|T|^2$.

- At $x = -\left(\frac{L}{2} + a\right)$ we have

$$A_1 e^{-k\left(\frac{L}{2} + a\right)} = A_3 \cos \left[q \left(\frac{a}{2} \right) \right],$$

and

$$k A_1 e^{-k\left(\frac{L}{2} + a\right)} = q A_3 \sin \left[q \left(\frac{a}{2} \right) \right].$$

So

$$k = q \tan \left[q \left(\frac{a}{2} \right) \right].$$

- At $x = -\frac{L}{2}$ we have

$$A_4 e^{-\frac{kL}{2}} + A_5 e^{\frac{kL}{2}} = A_3 \cos \left[q \left(\frac{a}{2} \right) \right],$$

and

$$k A_4 e^{-\frac{kL}{2}} - k A_5 e^{\frac{kL}{2}} = -q A_3 \sin \left[q \left(\frac{a}{2} \right) \right].$$

- At $x = \frac{L}{2}$ we have

$$A_4 e^{\frac{kL}{2}} + A_5 e^{-\frac{kL}{2}} = T \cos \left[q \left(\frac{a}{2} \right) \right],$$

and

$$k A_4 e^{\frac{kL}{2}} - k A_5 e^{-\frac{kL}{2}} = q T \sin \left[q \left(\frac{a}{2} \right) \right].$$

- At $x = \left(\frac{L}{2} + a\right)$ we have

$$A_2 e^{-k(\frac{L}{2}+a)} = T \cos \left[q \left(\frac{a}{2} \right) \right],$$

and

$$k A_2 e^{-k(\frac{L}{2}+a)} = q T \sin \left[q \left(\frac{a}{2} \right) \right].$$

Normalization gives us an additional equation:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1.$$

After a lot of algebra we find $|T|^2$ expressed in terms of k, q, L and a . In addition, we have a relation for k, q , and a :

$$k = q \tan \left[q \left(\frac{a}{2} \right) \right].$$

This relation is found by dividing the matching condition at the left hand side of the well for $x < 0$ or dividing the matching condition at the right hand side of the well for $x > 0$.

With help of this expression, and the matching results at $x = -L/2$ and $x = L/2$ respectively, we find $A_4 = 0, A_5 \neq 0$ and $A_4 \neq 0, A_5 = 0$. Hence $A_3 = 0$. So there is no solution.

What would we find when we choose:

$$\text{For } x < 0 \quad \psi(x) = A_3 \cos qx,$$

$$\text{and for } x > 0 \quad \psi(x) = T \cos qx.$$

The only possible non zero solutions are obtained for $qL = n\pi$ with $n \in \mathbb{N} | n \neq 0$.

Now what?

We introduce a sin and cos function for the potential well and represent both by, in general:

$\psi(x) \sim \sin(x + \gamma)$, where γ represents a phase shift.

So for $x < 0$, the expression for the wave function is chosen to be:

$$\psi(x) =$$

$$A_3 \sin \left[q \left(x + \frac{L}{2} + \frac{a}{2} \right) + \gamma_1 \right], \quad (\text{C.E.8})$$

and for $x > 0$:

$$\psi(x) = A_3 \sin \left[q \left(x - \frac{L}{2} - \frac{a}{2} \right) + \gamma_2 \right].$$

- At $x = -\left(\frac{L}{2} + a\right)$ we have

$$A_1 e^{-k(\frac{L}{2}+a)} = A_3 \sin \left[\gamma_1 - q \left(\frac{a}{2} \right) \right],$$

and

$$k A_1 e^{-k(\frac{L}{2}+a)} = q A_3 \cos \left[\gamma_1 - q \left(\frac{a}{2} \right) \right],$$

and

$$k = q \cot \left[\gamma_1 - q \left(\frac{a}{2} \right) \right].$$

- At $x = -L/2$ we have

$$A_4 e^{-kL/2} + A_5 e^{kL/2} = A_3 \sin \left[q \left(\frac{a}{2} \right) + \gamma_1 \right],$$

and

$$k A_4 e^{-kL/2} - k A_5 e^{kL/2} = q A_3 \cos \left[q(a/2) + \gamma_1 \right].$$

- At $x = L/2$ we have

$$A_4 e^{kL/2} + A_5 e^{-kL/2} = T \sin \left[\gamma_2 - q(a/2) \right],$$

and

$$kA_4e^{kL/2} - kA_5e^{-kL/2} = qT \cos[\gamma_2 - q(a/2)].$$

- At $x = \left(\frac{L}{2} + a\right)$ we have

$$A_2e^{-k\left(\frac{L}{2}+a\right)} = T \sin\left[\gamma_2 + q\left(\frac{a}{2}\right)\right],$$

and

$$-kA_2e^{-k\left(\frac{L}{2}+a\right)} = qT \cos\left[\gamma_2 + q\left(\frac{a}{2}\right)\right],$$

and

$$k = -q \cot[\gamma_2 + q\left(\frac{a}{2}\right)].$$

Now we have the relations to find the transmission coefficient T .

With the results at

$$x = -L/2$$

we express A_4 and A_5 into A_3 .

With the results at

$$x = L/2$$

we express A_4 and A_5 into T .

This gives us two expressions for A_3 and T .

Combing the results for k and q obtained at $x = \left(\frac{L}{2} + a\right)$ and $x = -\left(\frac{L}{2} + a\right)$ we have:

$$\cot\left[\gamma_1 - q\left(\frac{a}{2}\right)\right] = -\cot\left[\gamma_2 + q\left(\frac{a}{2}\right)\right],$$

and

$$\gamma_2 = -\gamma_1.$$

With the two expressions for A_3 and T and the relation $\gamma_2 = -\gamma_1$ we have a relation for A_3 and T and an equation for γ_1 :

$$A_3 = Te^{-kL} \frac{-k \tan[\gamma_1 + q\left(\frac{a}{2}\right)] + q}{k \tan[\gamma_1 + q\left(\frac{a}{2}\right)] + q}, \quad (\text{C.E.9})$$

and

$$1 = e^{-2kL} \left\{ \frac{-k \tan[\gamma_1 + q\left(\frac{a}{2}\right)] + q}{k \tan[\gamma_1 + q\left(\frac{a}{2}\right)] + q} \right\} \left\{ \frac{k \tan[\gamma_1 + q\left(\frac{a}{2}\right)] - q}{-k \tan[\gamma_1 + q\left(\frac{a}{2}\right)] - q} \right\}. \quad (\text{C.E.10})$$

Both expressions, (C.E.9) and (C.E.10), can be simplified by using $k = q \cot[\gamma_1 - q\left(\frac{a}{2}\right)]$.

Then we have for (C.E.10):

$$\sin 2\gamma_1 = e^{-kL} \sin qa. \quad (\text{C.E.11})$$

For A_3 , with (C.E.11):

$$A_3 = T. \quad (\text{C.E.12})$$

In the same way, the expressions at $x = -L/2$ for A_4 and A_5 can be written as:

$$A_4 = \frac{e^{kL/2}}{2} T \frac{\sin 2\gamma_1}{\cos[\gamma_1 - q\left(\frac{a}{2}\right)]},$$

and

$$A_5 = \frac{e^{-kL/2}}{2} T \frac{\sin qa}{\cos[\gamma_1 - q(\frac{a}{2})]} .$$

With (C.E.11): $A_4 = A_5$.

Using the normalisation procedure we will obtain an expression for $|T|^2$.

Finally we can estimate the time required for the particle to tunnel to the next well.

The velocity of the particle :

$$v = \sqrt{\frac{2E}{m}} .$$

So the time t for tunneling is about:

$$t = |T|^2 L \sqrt{\frac{m}{2E}} .$$

We could have chosen:

for $x < 0 \rightarrow \psi(x) = A_3 \sin(qx + \gamma'_1)$

(C.E.13)

and for $x > 0 \rightarrow \psi(x) = T \sin(qx + \gamma'_2)$.

I present some results:

$$\gamma'_2 = -\gamma'_1 .$$

$$e^{kL} \sin[2\gamma'_1 - q(L + a)] = \sin qa .$$

When we substitute in the latter expression

$2\gamma'_1 - q(L + a) = 2\gamma_1$, we recover (C.E.10). That is what we should expect.

Substitute in the wave function given by (C.E.12) , $2\gamma'_1 - q(L + a) = 2\gamma_1$, we obtain:

$$\psi(x) = A_3 \sin[q(x + \frac{L}{2} + \frac{a}{2}) + \gamma_1] , \text{ (C.E.8). The wave function of the potential well for } x < 0 .$$

Remark: I did not use $L \gg a$.

Exercise 5.7 Bound particle in a half-infinite well

Consider the half-infinite potential well

$$V(x) = \begin{cases} \infty & x \leq 0 \\ -V_0 & 0 < x < L , \\ 0 & x \geq L \end{cases}$$

where $V_0 > 0$.

Demonstrate that the bound states of a particle of mass m and energy $-V_0 < E < 0$ satisfy:

$$\tan[\frac{L}{\hbar} \sqrt{2m(V_0 + E)}] = -\sqrt{\frac{V_0 + E}{-E}} .$$

Mahan dealt with this exercise in Ch.2 , page 17-20.

The above expression is found from the matching condition at $x = L$.

I reproduce the results of Mahan:

$$\psi(x) = \begin{cases} 0 & x \leq 0 \\ C_1 \sin px & 0 < x < L , \\ C_3 e^{-\alpha x} & x \geq L \end{cases}$$

where

$$p^2 = \frac{2m}{\hbar^2} (V_0 + E) > 0 , \text{ and}$$

$$\alpha^2 = -\frac{2m}{\hbar^2} E \quad (\text{since } E < 0).$$

Matching results into the following two expressions:

$$C_1 \sin(pL) = C_3 e^{-\alpha L},$$

and

$$C_1 p \cos(pL) = -\alpha C_3 e^{-\alpha L}.$$

Dividing both equations gives:

$$\frac{\tan(pL)}{p} = -\frac{1}{\alpha}.$$

$$p^2 = \frac{2m}{\hbar^2} (V_0 + E) \rightarrow pL = \frac{L}{\hbar} \sqrt{2m(V_0 + E)},$$

and

$$-\frac{p}{\alpha} = -\frac{\sqrt{\frac{2m}{\hbar^2}(V_0 + E)}}{\sqrt{-\frac{2m}{\hbar^2}E}} = -\sqrt{\frac{V_0 + E}{-E}}.$$

Then, with $\frac{\tan(pL)}{p} = -\frac{1}{\alpha}$, the result is:

$$\tan\left[\frac{L}{\hbar} \sqrt{2m(V_0 + E)}\right] = -\sqrt{\frac{V_0 + E}{-E}}.$$

Exercise 5.8 About the energy eigenstates of the harmonic oscillator

Find the properly normalized first two excited energy eigenstates of the harmonic oscillator, as well as the expectation value of the potential energy in the n th energy eigenstate.

Hint: consider the raising and lowering operators a_{\pm} defined in Eq. (5.109).

The lowest energy eigenstate ($n = 0$), the ground state Eq.(5.105),

$$\psi_0 = \frac{e^{-x^2/2d^2}}{\pi^{1/4}\sqrt{d}},$$

where

$$d = \sqrt{\hbar/m\omega}, \text{ and } \omega \text{ is the oscillator's classical angular frequency.}$$

The raising and lowering operators are given by Eq. (5.109).

The first excited state is obtained by Eq. (5.113):

$$a_+ \psi_0 = \psi_1.$$

Applying the operator ($a_+ = -\frac{d}{dy} + y$) with y given in Eq. (5.92):

$$\psi_1 = \frac{y\sqrt{2}}{\pi^{1/4}\sqrt{d}} e^{-y^2/2}.$$

This state is properly normalized using $x = yd$.

the second excited state is:

$$a_+ \psi_1 = \sqrt{2} \psi_2.$$

Hence we have for

$$\psi_2 = \frac{1}{\sqrt{2}} \frac{1}{\pi^{1/4}\sqrt{d}} (2y^2 - 1) e^{-y^2/2}.$$

The expectation value of the n th energy eigenstate:

$$\langle H \rangle = \hbar\omega \int_{-\infty}^{\infty} \psi_n^* (a_+ a_- + \frac{1}{2}) \psi_n dx .$$

Then, with (5.111):

$$\langle H \rangle = \hbar\omega \left(n + \frac{1}{2} \right) \int_{-\infty}^{\infty} \psi_n^* \psi_n dx = \hbar\omega \left(n + \frac{1}{2} \right).$$

Hence,

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right).$$

6 Multi-Particle Systems

6.1 Introduction

The results for a single particle in the fore-going chapters is extended to multiple particles. The one-dimensional formulation has been chosen.

6.2 Fundamental concepts

Fp. starts with N non-relativistic particles.

The normalization condition is presented as well as the operator corresponding to momentum. The commutation relations are discussed as well as the time-dependent Schrödinger equation and the time-independent Schrödinger equation.

6.3 Non-Interacting Particles.

Fp derived the Hamiltonian,

$$H = \sum_i H_i ,$$

for the non-interacting particles.

The multi-particle wave function, the normalization constraint and the energy of the whole non-interacting system are given.

Important: "... we can generally write the total wavefunction of a many degree of freedom as a product of different system wavefunctions corresponding to each degree of freedom".

Page 88. Question: $E_1 \neq E_2 \neq \dots \neq E_N$?

6.4 Two-Particle Systems

The Hamiltonian is formulated with the particles relative position and the position of the centre of mass.

$$(6.22): x' = x_1 - x_2 .$$

$$(6.23): X = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} .$$

With these two equations:

$$\frac{\partial}{\partial x_1} = \frac{\partial}{\partial X} \frac{\partial X}{\partial x_1} + \frac{\partial}{\partial x'} \frac{\partial x'}{\partial x_1} = \frac{\partial}{\partial X} \frac{m_1}{m_1 + m_2} + \frac{\partial}{\partial x'} , (6.24),$$

and

$$\frac{\partial}{\partial x_2} = \frac{\partial}{\partial X} \frac{\partial X}{\partial x_2} + \frac{\partial}{\partial x'} \frac{\partial x'}{\partial x_2} = \frac{\partial}{\partial X} \frac{m_2}{m_1+m_2} - \frac{\partial}{\partial x'}, \quad (6.25).$$

In the centre of mass frame the system is equivalent to a single particle of reduced mass.

6.5 Identical particles.

In this section Fp infers the wavefunction to be either symmetric or anti-symmetric under change of particle labels.

Then, Fp introduces bosons with symmetric wave function, Eq. (6.41), and fermions with anti-symmetric wave function, Eq.(6.42).

The single identical particle are indicated by x_1 and x_2 . The energy levels for each particle by E_a and E_b . So, the energy of the wave function given by $\psi_E(x_1, x_2)$, (6.20),

$$E = E_a + E_b.$$

For bosons Fp mentioned the energy levels for both particles to be different. Like wise for fermions.

On top of page 91 Fp concludes: “...that it is impossible for two fermions in our system to occupy the same single-particle stationary state.”

Question: What about bosons? Well, I suppose not to face the same problem with bosons. So, E_a and E_b can be equal for bosons.

To summarize:

particle x_1 has two energy levels E_a and E_b ,

particle x_2 has two energy levels E_a and E_b .

However, there are some questions left. For example, how to derive Eq.(6.41) and Eq. (6.42) starting from the expression for Eq. (6.19) non-interacting particles? We then find for non-interacting particles:

$$\psi_E(x_1, x_2) = \psi_{E_a}(x_1)\psi_{E_b}(x_2) \equiv \psi(x_1, E_a)\psi(x_2, E_b),$$

with

$$E = E_a + E_b.$$

The next step is to introduce the particles to be identical. The result of this is, Eqs.(6.39) and (6.40), the wave function

$$\psi_E(x_1, x_2) = \psi_{E_a}(x_1)\psi_{E_b}(x_2) \equiv \psi(x_1, E_a)\psi(x_2, E_b)$$

to be symmetric or anti-symmetric.

Symmetry gives

$$\psi_E(x_1, x_2) = \psi_E(x_2, x_1),$$

with

$$\psi_E(x_2, x_1) = \psi(x_2, E_a)\psi(x_1, E_b) = \psi_E(x_1, x_2) = \psi(x_1, E_a)\psi(x_2, E_b).$$

Take a close look to this expression. After substituting this into Eq. (6.41) :

$$\psi_{E_{boson}}(x_1, x_2) = \sqrt{2}\psi(x_1, E_a)\psi(x_2, E_b).$$

Fp presented, on page 91, the stationary wave function for two particles which are somehow distinguishable. “Somehow” sounds rather mysteriously.

Question: distinguishable in what sense?

Let us start with wave function presented in Eqs.(6.19) and (6.43):

$$\psi_{E \text{ dist}}(x_1, x_2) = \psi(x_1, E_a)\psi(x_2, E_b) .$$

Question: is there something wrong with $\psi_{E \text{ dist}}(x_1, x_2) = \psi(x_1, E_b)\psi(x_2, E_a)$?

I will use Eq. (6.43). I assume “*somehow*” to mean you can distinguish particle 1 from particle 2 and you know their energy. That’s what I conclude on basis of Eq. (6.43).

Fp evaluates the variance of the distance, $x_1 - x_2$, between the two distinguishable particles:

$$\langle (x_1 - x_2)^2 \rangle_{\text{dist}} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_{E \text{ dist}}^* (x_1, x_2) (x_1 - x_2)^2 \psi_{E \text{ dist}}(x_1, x_2) dx_1 dx_2 . \quad (\text{C.6.5.1})$$

With Eq.(6.43) and the orthogonality of the single-particle states we have:

$$\langle x_1^2 \rangle = \int_{-\infty}^{\infty} \psi^* (x_1, E_a) x_1^2 \psi(x_1, E_a) dx_1 \int_{-\infty}^{\infty} \psi^* (x_2, E_b) \psi(x_2, E_b) dx_2 , \quad (\text{C.6.5.2})$$

likewise:

$$\langle x_2^2 \rangle = \int_{-\infty}^{\infty} \psi^* (x_2, E_b) x_2^2 \psi(x_2, E_b) dx_2 \int_{-\infty}^{\infty} \psi^* (x_1, E_a) \psi(x_1, E_a) dx_1 , \quad (\text{C.6.5.3})$$

$$\begin{aligned} \langle 2x_1 x_2 \rangle &= 2 \int_{-\infty}^{\infty} \psi^* (x_1, E_a) x_1 \psi(x_1, E_a) dx_1 \int_{-\infty}^{\infty} \psi^* (x_2, E_b) x_2 \psi(x_2, E_b) dx_2 = \\ &= 2 \langle x_1 \rangle \langle x_2 \rangle . \end{aligned} \quad (\text{C.6.5.4})$$

Now we have the elements of Eq.(6.44), where, with Eq.(6.45):

$$\langle x_1^2 \rangle \equiv \langle x^2 \rangle_a , \text{ particle 1 with energy } E_a ,$$

and

$$\langle x_2^2 \rangle \equiv \langle x^2 \rangle_b , \text{ particle 2 with energy } E_b ,$$

and

$$\langle 2x_1 x_2 \rangle = 2 \langle x_1 \rangle \langle x_2 \rangle \equiv 2 \langle x \rangle_a \langle x \rangle_b .$$

Next Fp evaluates $\langle (x_1 - x_2)^2 \rangle_{\text{boson}}$, two identical particles

For this evaluation we use the boson wave function given in Eq. (6.41).

So,

$$\begin{aligned} \langle (x_1 - x_2)^2 \rangle_{\text{boson}} &= \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_{E \text{ boson}}^* (x_1, x_2) (x_1 - x_2)^2 \psi_{E \text{ boson}}(x_1, x_2) dx_1 dx_2 . \end{aligned} \quad (\text{C.6.5.5})$$

The result is presented in Eq. (6.46):

$$\langle (x_1 - x_2)^2 \rangle_{\text{boson}} = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2 \langle x \rangle_a \langle x \rangle_b - 2 |\langle x \rangle_{ab}|^2 ,$$

where $\langle x \rangle_{ab}$ is given in Eq.(6.47).

Can I reproduce this result?

Plug Eq. (6.41) into (C.6.5.5), twelve integrals have to be evaluated.

The first four integrals are:

$$\begin{aligned} \langle x_1^2 \rangle &= \frac{1}{2} \iint_{-\infty}^{\infty} [\psi^* (x_2, E_b) \psi^* (x_1, E_a) + \psi^* (x_1, E_b) \psi^* (x_2, E_a)] x_1^2 \times \\ &\times [\psi(x_1, E_a) \psi(x_2, E_b) + \psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2 . \end{aligned} \quad (\text{C.6.5.6})$$

Four expressions need to be evaluated in (C.6.5.6):

$$- \iint_{-\infty}^{\infty} [\psi^* (x_2, E_b) \psi^* (x_1, E_a)] x_1^2 [\psi(x_1, E_a) \psi(x_2, E_b)] dx_1 dx_2 , \quad (\text{C.6.5.7})$$

$$- \iint_{-\infty}^{\infty} [\psi^* (x_2, E_b) \psi^* (x_1, E_a)] x_1^2 [\psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2 , \quad (\text{C.6.5.8})$$

$$- \iint_{-\infty}^{\infty} [\psi^* (x_1, E_b) \psi^* (x_2, E_a)] x_1^2 [\psi(x_1, E_a) \psi(x_2, E_b)] dx_1 dx_2 , \quad (\text{C.6.5.9})$$

and

$$- \iint_{-\infty}^{\infty} [\psi^* (x_1, E_b) \psi^* (x_2, E_a)] x_1^2 [\psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2 . \quad (\text{C.6.5.10})$$

With Eq.(6.45) which integrals contribute, can be established.

I am not so sure. However, I think (6.5.7) and (C.6.5.10):

$$\langle x_1^2 \rangle = \frac{1}{2} \langle x^2 \rangle_a + \frac{1}{2} \langle x^2 \rangle_b . \quad (\text{C.6.5.11})$$

The second set of four integrals.

Similarly for $\langle x_2^2 \rangle$, (6.5.7) and (C.6.5.10):

$$\langle x_2^2 \rangle = \frac{1}{2} \langle x^2 \rangle_b + \frac{1}{2} \langle x^2 \rangle_a . \quad (\text{C.6.5.12})$$

Then, the question is: what about (C.6.5.8) and (C.6.5.9)?

The last set of four integrals.

$$\begin{aligned} \langle 2x_1x_2 \rangle &= \frac{1}{2} \iint_{-\infty}^{\infty} [\psi^*(x_2, E_b) \psi^*(x_1, E_a) + \psi^*(x_1, E_b) \psi^*(x_2, E_a)] 2x_1x_2 \times \\ &\times [\psi(x_1, E_a) \psi(x_2, E_b) + \psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2 . \end{aligned} \quad (\text{C.6.5.13})$$

Again, four expression need to be evaluated in (C.6.5.13):

$$- \iint_{-\infty}^{\infty} [\psi^*(x_2, E_b) \psi^*(x_1, E_a)] 2x_1x_2 [\psi(x_1, E_a) \psi(x_2, E_b)] dx_1 dx_2 , \quad (\text{C.6.5.14})$$

$$- \iint_{-\infty}^{\infty} [\psi^*(x_2, E_b) \psi^*(x_1, E_a)] 2x_1x_2 [\psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2 , \quad (\text{C.6.5.15})$$

$$- \iint_{-\infty}^{\infty} [\psi^*(x_1, E_b) \psi^*(x_2, E_a)] 2x_1x_2 [\psi(x_1, E_a) \psi(x_2, E_b)] dx_1 dx_2 , \quad (\text{C.6.5.16})$$

and

$$- \iint_{-\infty}^{\infty} [\psi^*(x_1, E_b) \psi^*(x_2, E_a)] 2x_1x_2 [\psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2 . \quad (\text{C.6.5.17})$$

(C.6.5.14) and (C.6.5.17):

$$2\langle 2x_1x_2 \rangle = 2\langle x_1 \rangle \langle x_2 \rangle (\equiv 2\langle x \rangle_a \langle x \rangle_b) + 2\langle x_1 \rangle \langle x_2 \rangle (\equiv 2\langle x \rangle_a \langle x \rangle_b) . \quad (\text{C.6.5.18})$$

How to prove the existence of

$$|\langle x \rangle_{ab}|^2 ?$$

$$\langle x \rangle_{ab} = \int_{-\infty}^{\infty} \psi^*(x, E_a) x \psi(x, E_b) dx , \quad (6.47),$$

is an expectation value. So, why $||^2$?

$$\text{I suppose } (\langle x \rangle_{ab})^* = \int_{-\infty}^{\infty} \psi^*(x, E_b) x \psi(x, E_a) dx = \langle x \rangle_{ba} .$$

$$\text{Then, } (\langle x \rangle_{ab})^* \langle x \rangle_{ab} = |\langle x \rangle_{ab}|^2 .$$

Now , how to apply (6.47), with (C.6.5.15) and (C.6.5.16), to find out about $2|\langle x \rangle_{ab}|^2$?

I evaluate (C.6.5.15) as:

$$2 \int_{-\infty}^{\infty} \psi^*(x_2, E_b) x_2 \psi(x_2, E_a) dx_2 \int_{-\infty}^{\infty} \psi^*(x_1, E_a) x_1 \psi(x_1, E_b) dx_1 = 2|\langle x \rangle_{ab}|^2 . \quad (\text{C.6.5.19})$$

Similarly (C.6.5.16) $\rightarrow 2|\langle x \rangle_{ab}|^2$.

Collecting all the expressions, taking into the factor $\frac{1}{2}$ and the $-$ sign for the cross-product, I finally arrive at (6.46). Then, (C.6.5.8) and (C.6.5.9) do not contribute.

Now,

$$\begin{aligned} \langle (x_1 - x_2)^2 \rangle_{\text{fermion}} &= \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_{E \text{ fermion}}^* (x_1, x_2) (x_1 - x_2)^2 \psi_{E \text{ fermion}} (x_1, x_2) dx_1 dx_2 . \end{aligned} \quad (\text{C.6.5.19})$$

Plug Eq. (6.42) into (C.6.5.19), twelve integrals have to be evaluated.

The first four integrals are:

$$\begin{aligned} \langle x_1^2 \rangle &= \frac{1}{2} \iint_{-\infty}^{\infty} [\psi^*(x_2, E_b) \psi^*(x_1, E_a) - \psi^*(x_1, E_b) \psi^*(x_2, E_a)] x_1^2 \times \\ &\times [\psi(x_1, E_a) \psi(x_2, E_b) - \psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2 . \end{aligned} \quad (\text{C.6.5.20})$$

Four expressions need to be evaluated in (C.6.5.20):

$$- \iint_{-\infty}^{\infty} [\psi^*(x_2, E_b) \psi^*(x_1, E_a)] x_1^2 [\psi(x_1, E_a) \psi(x_2, E_b)] dx_1 dx_2, \quad (C.6.5.21)$$

$$- - \iint_{-\infty}^{\infty} [\psi^*(x_2, E_b) \psi^*(x_1, E_a)] x_1^2 [\psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2, \quad (C.6.5.22)$$

$$- - \iint_{-\infty}^{\infty} [\psi^*(x_1, E_b) \psi^*(x_2, E_a)] x_1^2 [\psi(x_1, E_a) \psi(x_2, E_b)] dx_1 dx_2, \quad (C.6.5.23)$$

and

$$- \iint_{-\infty}^{\infty} [\psi^*(x_1, E_b) \psi^*(x_2, E_a)] x_1^2 [\psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2. \quad (C.6.5.24)$$

With Eq.(6.45) which integrals contribute, can be established.

I think (6.5.21) and (C.6.5.24):

$$\langle x_1^2 \rangle = \frac{1}{2} \langle x^2 \rangle_a + \frac{1}{2} \langle x^2 \rangle_b. \quad (C.6.5.25)$$

The second set of four integrals.

Similarly for $\langle x_2^2 \rangle$, (6.5.21) and (C.6.5.24):

$$\langle x_2^2 \rangle = \frac{1}{2} \langle x^2 \rangle_b + \frac{1}{2} \langle x^2 \rangle_a. \quad (C.6.5.26)$$

The last set of four integrals.

$$\begin{aligned} \langle 2x_1 x_2 \rangle &= \frac{1}{2} \iint_{-\infty}^{\infty} [\psi^*(x_2, E_b) \psi^*(x_1, E_a) - \psi^*(x_1, E_b) \psi^*(x_2, E_a)] 2x_1 x_2 \times \\ &\times [\psi(x_1, E_a) \psi(x_2, E_b) - \psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2. \end{aligned} \quad (C.6.5.27)$$

Again, four expression need to be evaluated in (C.6.5.27):

$$- \iint_{-\infty}^{\infty} [\psi^*(x_2, E_b) \psi^*(x_1, E_a)] 2x_1 x_2 [\psi(x_1, E_a) \psi(x_2, E_b)] dx_1 dx_2, \quad (C.6.5.28)$$

$$- - \iint_{-\infty}^{\infty} [\psi^*(x_2, E_b) \psi^*(x_1, E_a)] 2x_1 x_2 [\psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2, \quad (C.6.5.29)$$

$$- - \iint_{-\infty}^{\infty} [\psi^*(x_1, E_b) \psi^*(x_2, E_a)] 2x_1 x_2 [\psi(x_1, E_a) \psi(x_2, E_b)] dx_1 dx_2, \quad (C.6.5.30)$$

and

$$- \iint_{-\infty}^{\infty} [\psi^*(x_1, E_b) \psi^*(x_2, E_a)] 2x_1 x_2 [\psi(x_2, E_a) \psi(x_1, E_b)] dx_1 dx_2. \quad (C.6.5.31)$$

(C.6.5.28) and (C.6.5.31):

$$2\langle 2x_1 x_2 \rangle = 2\langle x_1 \rangle \langle x_2 \rangle (\equiv 2\langle x \rangle_a \langle x \rangle_b) + 2\langle x_1 \rangle \langle x_2 \rangle (\equiv 2\langle x \rangle_a \langle x \rangle_b). \quad (C.6.5.32)$$

With (C.6.5.25), (C.6.5.26) and (C.6.5.32) including the factor $\frac{1}{2}$ and the $-$ sign of the cross product, the first expression on the right-hand side of (6.49), $\langle (x_1 - x_2)^2 \rangle_{dist}$, is obtained.

Simarlily to the boson case, I obtain from (C.6.5.29) and (6.5.30) the second expression in (6.49): $+2|\langle x \rangle_{ab}|^2$.

Exercises. (N.B. Neglect spin in the following questions.)

Exercise 6.1 Two non-interacting particles and three states

(Remark: how to neglect something we did not encounter so far?)

Consider a system consisting of two non-interacting particles, and three one-particle states ψ_a , ψ_b , and ψ_c . How many different two-particle states can be constructed if the particle are i) distinguishable, ii) indistinguishable bosons, or iii) indistinguishable fermions?

Two particles and three states.

Hence:

$$\psi(x_1, E_a), \psi(x_1, E_b), \psi(x_1, E_c),$$

and

$$\psi(x_2, E_a), \psi(x_2, E_b), \psi(x_2, E_c).$$

- For the distinguishable case there are, with Eq.(6.19),:

6 different two-particle states:

$$[\psi(x_1, E_a)\psi(x_2, E_b)], [\psi(x_1, E_a)\psi(x_2, E_c)], [\psi(x_1, E_b)\psi(x_2, E_a)], [\psi(x_1, E_b)\psi(x_2, E_c)], \\ [\psi(x_1, E_c)\psi(x_2, E_a)], [\psi(x_1, E_c)\psi(x_2, E_b)].$$

To visualize the way to find the boson states and the fermion states, the table below is of some help. The zero's in the table below represents states like $[\psi(x_1, E_a)\psi(x_2, E_a)]$ based on the remark by Fp made on top of page 91.

0	$\psi(x_1, E_a)\psi(x_2, E_b)$	$\psi(x_1, E_a)\psi(x_2, E_c)$
$\psi(x_1, E_b)\psi(x_2, E_a)$	0	$\psi(x_1, E_b)\psi(x_2, E_c)$
$\psi(x_1, E_c)\psi(x_2, E_a)$	$\psi(x_1, E_c)\psi(x_2, E_b)$	0

- For indistinguishable bosons there are , with Eq. (6.41),:

3 different indistinguishable bosons, where use has been made of symmetry requirement:

one boson state equals Eq. (6.41), the second is obtained by replacing in Eq.(6.41) E_b by E_c , and the third state is found by replacing in Eq. (6.41) E_a by E_c .

- For indistinguishable fermions there are , with Eq. (6.42):

3 different indistinguishable fermions, where use has been made of anti-symmetric requirements. The states are obtained in the same way as we did for the boson states:

one fermion state equals Eq. (6.42), the second is obtained by replacing in Eq.(6.42) E_b by E_c , and the third state is found by replacing in Eq. (6.42) E_a by E_c .

Exercise 6.2 Two non-interacting particles and the harmonic oscillator potential

Consider two non-interacting particles, each of mass m , in a one-dimensional harmonic oscillator potential of classical frequency ω . If one particle is in the ground-state, and the other in the first excited state, calculate $\langle (x_0 - x_1)^2 \rangle$ assuming that the particles are, (i) distinguishable , (ii) indistinguishable bosons, or (iii) indistinguishable fermions.

See also Exercise 8 of chapter 5 (page 55 of this document).

for the ground state we have, Eq. (5.105):

$$\psi_0(x) = \frac{e^{-x^2/2d^2}}{\pi^{1/4}\sqrt{d}}, \quad (C.6.E.1)$$

where

$$d = \sqrt{\frac{\hbar}{m\omega}}. \quad (C.6.E.2)$$

Furthermore we will use Eq.(5.113)

$$\psi_1(x) = a_+ \psi_0(x) .$$

With the results of Exercise 8 (page 55 of this document):

$$\psi_1(x) = \frac{x\sqrt{2}e^{-x^2/2d^2}}{\pi^{1/4}d\sqrt{d}} . \quad (\text{C.6.E.3})$$

With Eq. (6.43) we have:

$$\psi_{Edist} = \psi_0(x) \psi_1(x) = \frac{xe^{-x^2/d^2}}{\pi^{1/2}d^2} . \quad (\text{C.6.E.4})$$

$$\text{Now } \langle (x_0 - x_1)^2 \rangle_{dist} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_{Edist}^* (x_0 - x_1)^2 \psi_{Edist} dx_0 dx_1$$

We have to evaluate, Eqs. (6.44) and (6.45) ,:

$$\langle (x_0 - x_1)^2 \rangle_{dist} = \langle x^2 \rangle_0 + \langle x^2 \rangle_1 - 2\langle x \rangle_0 \langle x \rangle_1 . \quad (\text{C.6.E.5})$$

With (C.6.E.1):

$$\langle x^2 \rangle_0 = \int_{-\infty}^{\infty} \psi_0^* x^2 \psi_0 dx = \frac{\hbar}{2m\omega} , \quad (\text{C.6.E.6})$$

where use have been made of $\int_{-\infty}^{\infty} \psi_1^* \psi_1 dx = 1$.

With (C.6.E.3)

$$\langle x^2 \rangle_1 = \int_{-\infty}^{\infty} \psi_1^* x^2 \psi_1 dx = \frac{3\hbar}{4m\omega} , \quad (\text{C.6.E.7})$$

where use have been made of $\int_{-\infty}^{\infty} \psi_0^* \psi_0 dx = 1$.

The last expression of (C.6.E.5) does not contribute. The integral of the ground state is anti-symmetric.

Hence , with (C.6.E.6) and (C.6.E.7),:

$$\langle (x_0 - x_1)^2 \rangle_{dist} = \frac{5\hbar}{4m\omega} . \quad (\text{C.6.E.8})$$

To obtain $\langle (x_0 - x_1)^2 \rangle_{boson}$ we need to evaluate ,using Eq. (6.47),

$$2|\langle x \rangle_{01}|^2 = 2\left(\int_{-\infty}^{\infty} \psi_0^* x \psi_1 dx\right)^2 .$$

With (C.6.E.1) and (C.6.E.3)

$$2|\langle x \rangle_{01}|^2 = 2\left(\int_{-\infty}^{\infty} \psi_0^* x \psi_1 dx\right)^2 = \frac{\hbar}{2m\omega} . \quad (\text{C.6.E.9})$$

Then with (C.6.E.8) and (C.6.E.9):

$$\langle (x_0 - x_1)^2 \rangle_{boson} = \langle (x_0 - x_1)^2 \rangle_{dist} - 2|\langle x \rangle_{01}|^2 = \frac{3\hbar}{4m\omega} . \quad (\text{C.6.E.10})$$

Finally $\langle (x_0 - x_1)^2 \rangle_{fermion}$? With the results just obtained, Eq. (6.49) can be evaluated:

$$\langle (x_0 - x_1)^2 \rangle_{fermion} = \langle (x_0 - x_1)^2 \rangle_{dist} + 2|\langle x \rangle_{01}|^2 = \frac{7\hbar}{4m\omega} .$$

Exercise 6.3 Two non-interacting particles in a box

Two non-interacting particles, with the same mass m , are in a one-dimensional box of length a . What are the four lowest energies of the system? What are the degeneracies of these energies if the two particles are (i) distinguishable, (ii) indistinguishable bosons, or (iii) indistinguishable fermions?

I suppose the box to represent the infinite potential well. See section 5.2.

The wave function for a particle, Eq. (5.11):

$$\psi_n = \sqrt{\frac{2}{a}} \sin(n\pi \frac{x}{a}). \quad (\text{C.6.E.11})$$

The eigenvalues, Eq.(5.),:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, \quad (\text{C.6.E.12})$$

where $n = 1, 2, 3, \dots$.

We have 4 energy levels. So the four lowest energies are, with (C.6.E.12),:

$$E_1 = \frac{\pi^2 \hbar^2}{2ma^2}, E_2 = \frac{4\pi^2 \hbar^2}{2ma^2}, E_3 = \frac{9\pi^2 \hbar^2}{2ma^2}, \text{ and } E_4 = \frac{16\pi^2 \hbar^2}{2ma^2}.$$

- What are the degeneracies of distinguishable particles?

With four energy levels and two particles there are 16 combinations. As in exercise 1, we do not allow for the particles to have the same energy levels. So, we drop four combinations and we must consider the resulting twelve.

I collect the combinations in the Table E1. There I use a shorthand representation of the combinations. For example:

$\psi(x_1, E_1)\psi(x_2, E_2) \equiv \psi_{1,1}\psi_{2,2}$. In addition we add to these distinguishable states the total energy level given by Eq. (6.20). Keep in mind, the numbers to be multiplied by: $\frac{\pi^2 \hbar^2}{2ma^2}$.

Table E1 Distinguishable states +energy levels

0	$\psi_{1,1}\psi_{2,2}, 5$	$\psi_{1,1}\psi_{2,3}, 10$	$\psi_{1,1}\psi_{2,4}, 17$
$\psi_{1,2}\psi_{2,1}, 5$	0	$\psi_{1,2}\psi_{2,3}, 13$	$\psi_{1,2}\psi_{2,4}, 20$
$\psi_{1,3}\psi_{2,1}, 10$	$\psi_{1,3}\psi_{2,2}, 13$	0	$\psi_{1,3}\psi_{2,4}, 25$
$\psi_{1,4}\psi_{2,1}, 17$	$\psi_{1,4}\psi_{2,2}, 20$	$\psi_{1,4}\psi_{2,3}, 25$	0

So, we have 12 distinguishable states of degeneracy two.

-Indistinguishable bosons.

Similar to exercise 1, we have 6 boson states.

For example, using Eq. (6.41), and shorthand notation of table E1:

$$\psi_{E_{boson1}} = \frac{1}{\sqrt{2}} [\psi_{1,1}\psi_{2,2} + \psi_{1,2}\psi_{2,1}], \quad (\text{C.6.E.13})$$

and with Eqs. (6.12) and (6.20):

$$H\psi_{E_{boson1}} = (E_{boson1}) \psi_{E_{boson1}}.$$

$$E_{boson1} = (5 + 5) \frac{\pi^2 \hbar^2}{2ma^2}.$$

The number 1 in $\psi_{E_{boson1}}$ indicates one of the six boson states.

From Table E1 it is clear there are no degenerate boson states.

-Indistinguishable fermions.

Replace the + sign in (C.6.E.13) and you have one of the fermion states:

$$\psi_{E_{fermion1}} = \frac{1}{\sqrt{2}} [\psi_{1,1}\psi_{2,2} - \psi_{1,2}\psi_{2,1}] . \quad (C.6.E.14)$$

From Table E1 it is again clear there are no degenerate fermion states.

Exercise 6.4 Two particles in a one-dimensional box.

Two particles in a one-dimensional box of length a occupy the $n = 4$ and $n' = 3$ states. Write the properly normalized wave function if the particles are (i) distinguishable, (ii) indistinguishable bosons, or (iii) indistinguishable fermions.

For the one-dimensional box we have, using the shorthand notation of exercise 3,:

$$\psi_{1,3} = \sqrt{\frac{2}{a}} \sin(3\pi \frac{x_1}{a}) ,$$

$$\text{and } E_3 = \frac{9\pi^2 \hbar^2}{2ma^2} .$$

$$\psi_{2,4} = \sqrt{\frac{2}{a}} \sin(4\pi \frac{x_2}{a}) ,$$

$$\text{and } E_4 = \frac{16\pi^2 \hbar^2}{2ma^2} .$$

The wave function for distinguishable particles:

$$\psi_{Edist} = \psi_{1,3}\psi_{2,4} = \frac{2}{a} \sin(3\pi \frac{x_1}{a}) \sin(4\pi \frac{x_2}{a}) .$$

The wave function for indistinguishable bosons:

$$\psi_{Eboson} = \frac{\sqrt{2}}{a} [\sin(3\pi \frac{x_1}{a}) \sin(4\pi \frac{x_2}{a}) + \sin(3\pi \frac{x_2}{a}) \sin(4\pi \frac{x_1}{a})] .$$

The wave function for indistinguishable fermions:

$$\psi_{Efermion} = \frac{\sqrt{2}}{a} [\sin(3\pi \frac{x_1}{a}) \sin(4\pi \frac{x_2}{a}) - \sin(3\pi \frac{x_2}{a}) \sin(4\pi \frac{x_1}{a})] .$$

7 Three-Dimensional Quantum Mechanics

7.1 Introduction

The non-relativistic three-dimensional theory will be derived by extending the one-dimensional formulation.

7.2 Fundamental concepts

The three-dimensional theory is derived by extending the one-dimensional case in cartesian coordinates. See also Section 4.5

At the bottom of page 95 Fp mentioned Eq. (7.8) to be easily derivable from Eq. (7.21). Well, in section 4.3 the one- dimensional case has been derived. Completely similar Eq. (7.8) can be found.

7.3 Particle in a box

The solutions are obtained similarly to the one-dimensional case presented in section 5.2. The solution in 3-D are based on the separability of the wave function.

7.4 Degenerate Electron Gases

Fp considers electrons in a cubic box and derived the Fermi energy. The electrons are treated as non-interacting particles.

From this degenerate electron gases Fp derived an expression for the bulk modulus, i.e. the resistance to compression.

7.5 White-Dwarf Stars

An interesting example is discussed in this section: the possible collapse of a burnt-out star.

Exercises

Exercise 7.1 A particle in a three-dimensional isotropic harmonic oscillator

Consider a particle of mass m moving in a three-dimensional isotropic harmonic oscillator potential of force constant k . Solve the problem via the separation of variables, and obtain an expression for the allowed values of the total energy of the system (in a stationary state).

The wave equation is, in a cartesian frame,:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m \omega^2 (x^2 + y^2 + z^2) \right] \psi = E \psi,$$

where $\omega = \sqrt{k/m}$.

We use separation of variables as illustrated in section 7.3.

So Eq.(7.27):

$\psi(x, y, z) = X(x)Y(y)Z(z)$. Plug this expression for the wave function into the Wave equation and we find for the x -coordinate:

$$\frac{d^2 X}{dx^2} = \frac{2m}{\hbar^2} \left(\frac{1}{2} m \omega^2 x^2 - E_x \right) X.$$

Similarly you will obtain the expressions for $Y(y)$ and $Z(z)$.

With help of the analyses of section 5.8 , The Simple Harmonic Oscillator, we find:

$$E_x = \left(n_x + \frac{1}{2} \right) \hbar \omega .$$

Furthermore:

$$E = E_x + E_y + E_z ,$$

Consequently:

$$E = \left(n_x + n_y + n_z + \frac{1}{2} \right) \hbar \omega ,$$

where n_x, n_y and n_z are non-negative integers.

We define $N = n_x + n_y + n_z$.

With help of the expression for N you can find a general expression for the order of degeneracy g_N .

For $N = 0$ there is one eigenvalue and one eigen state,

For $N = 1$ there is one eigenvalue and three eigen states, etc.

Exercise 7.2 Fermi energy for the relativistic case

Repeat the calculation of the Fermi energy of a gas of fermions by assuming that the fermions are massless(relativistic), so that the energy-momentum relation is $E = pc$.

Massless Fermions?

What about the wave equation?

What does the Hamiltonian looks like?

I suppose F_p indicates to repeat the analysis of section 7.4: in this case massless Fermions in a box a dimension a .

Now we make use of the analysis of section 7.3 and 7.4. Like Eq.(7.38) we find from the latter wave equation:

$$E = \frac{l\pi}{a} \hbar c ,$$

where $l = l_x + l_y + l_z$.

Using the analysis of page 98, Eq.(7.41), we find for the Fermi energy:

$$E_F = \frac{l_F \pi}{a} \hbar c = \frac{\pi \hbar c}{a} l_F .$$

With the number of massless Fermions N and Eq. (7.41) we obtain for the Fermi energy:

$$E_F = \frac{\pi \hbar c}{a} \left(\frac{3N}{\pi} \right)^{1/3} .$$

Exercise 7.3 The density of states of an electron gas in a box of volume L^3

Calculate the density of states of an electron gas in a cubic box of volume L^3 , bearing in mind that there are two electrons per energy state. In other words, calculate the number of electron states in the interval E to $E + dE$. This number can be written $dN = \rho(E)dE$, where ρ is the density of states.

So $\rho = \frac{dN}{dE}$ or $\rho' = \frac{1}{L^3} \frac{dN}{dE}$.

With Eq. (7.42) we have

$$E = \frac{\pi^2 \hbar^2}{2mL^2} \left(\frac{3N}{\pi} \right)^{2/3} .$$

From this equation we derive:

$$\frac{dN}{dE} = \frac{1}{\pi^2} \left(\frac{L}{\hbar} \right)^3 \sqrt{2} m^{3/2} \sqrt{E} .$$

Hence $\rho = \frac{dN}{dE} = \frac{1}{\pi^2} \left(\frac{L}{\hbar} \right)^3 \sqrt{2} m^{3/2} \sqrt{E}$,

or $\rho' = \frac{1}{L^3} \frac{dN}{dE} = \frac{\sqrt{2}}{\pi^2} \left(\frac{1}{\hbar} \right)^3 m^{3/2} \sqrt{E}$.

Exercise 7.4 The density of states in a square L^2

Repeat the above calculation for a two-dimensional electron gas in a square box of area L^2 .

Now we need to derive a similar expression for Eq. (7.42) in two dimensions.

The wave numbers are given by Eqs. (7.35) and (7.36),

the energy by Eq.(7.38).

Then with the similar analysis for 3 dimensions, we find for two dimensions:

$$N = 2 \times \frac{1}{4} \times \pi l_F^2, \quad (\text{C.7.E.1})$$

Here the factor $\frac{1}{4}$ is to take into account the energy levels occupy a quadrant of the circle with radius l_F .

So

$$l_F = \left(\frac{2N}{\pi}\right)^{1/2}. \quad (\text{C.7.E.2})$$

With Eq. (7.38) we find, using (C.7.E.2),:

$$E_F = \frac{\pi \hbar^2}{m L^2} N. \quad (\text{C.7.E.3})$$

From (C.7.E.3) we derive:

$$\frac{dN}{dE} = \frac{m L^2}{\pi \hbar^2}.$$

$$\text{Hence } \rho' = \frac{1}{L^2} \frac{dN}{dE} = \frac{m}{\pi \hbar^2}.$$

(C.7.E.3) can be written as:

$$E_F = \frac{\pi \hbar^2}{m} n,$$

where $n = N/L^2$ is the number of electrons per unit square.

Exercise 7.5 The Fermi energy for free electrons in copper

Given the number density of free electrons in copper is $n = 8.5 \times 10^{28} \text{ m}^{-3}$, calculate the Fermi energy in electron volts, and the velocity of an electron whose kinetic energy is equal to the Fermi energy.

Given the number density, Eq. (7.43) is practical to use:

$$E_F = \frac{\pi^2 \hbar^2}{2m} \left(\frac{3n}{\pi}\right)^{2/3}.$$

With $1 \text{ eV} = 1.6022 \times 10^{-19} \text{ J}$,

the Fermi energy is:

$$E_F = 7.1 \text{ eV}.$$

The velocity of an electron with this amount of kinetic energy is

$$v = \sqrt{\frac{2E_F}{m}} = \sqrt{\frac{2 \times 1.13 \times 10^{-18}}{9.11 \times 10^{-31}}} = 1.57 \times 10^6 \text{ m/sec}.$$

Exercise 7.6 Fermi energy of an electron in a white dwarf star.

Obtain an expression for the Fermi energy (in eV) of an electron in a white dwarf star as a function of the stellar mass (in solar masses). At what mass does the Fermi energy equal the

rest mass energy?

With Eq. (7.52) we have the expression for the Fermi energy in a white dwarf star:

$$E_F = \frac{\pi^2 \hbar^2}{2m_e} \left(\frac{3N}{\pi V} \right)^{2/3}, \quad (C7.E.4)$$

where N is the number of electrons and V the volume of the star.

Eq. (7.53) gives us the relation between the mass M of the star and the number of electrons. The mass of the protons and neutrons are almost equal and the mass of the electrons can be neglected.

The equilibrium radius of the star, R_* , is given by Eq. (7.58) or expressed in solar radius and solar mass by Eq. (7.59).

For the volume of the star we have with Eq. (7.59):

$$V = \frac{4}{3} \pi R_*^3 = \frac{4}{3} \pi 10^{-6} R_\odot^3 \frac{M_\odot}{M}. \quad (C7.E.5)$$

where M_\odot is the solar mass.

In Eq. (C7.E.4) we replace, with Eq. (7.53), N by

$$N = \frac{M}{2m_p}$$

and V as given in (C7.E.5):

$$E_F = \frac{\pi^2 \hbar^2}{2m_e R_\odot^2} 10^4 \left(\frac{9M^2}{M_\odot} \right)^{2/3}. \quad (C7.E.6)$$

In (C7.E.6) we have the Fermi energy in Joule.

In eV Fermi energy is

$$E_F = \frac{\pi^2 \hbar^2}{2m_e R_\odot^2} 10^4 \left(\frac{9M^2}{M_\odot} \right)^{2/3} \frac{1}{1.6022} 10^{19}.$$

Equating the Fermi energy to the rest mass energy

$E_F = m_e c^2$ we obtain from this expression and (C7.E.6):

$$M = \frac{4 \times 10^{-3}}{3\pi} \left[\sqrt{2} \left(\frac{m_e}{\hbar} \right)^3 m_p M_\odot R_\odot^3 \right]^{1/2}.$$

8 Orbital Angular momentum

8.1 Introduction

The role of angular momentum in the quantum mechanical description.

8.2 Angular Momentum Operators

The classical momentum vectors are translated into quantum mechanical operators. The commutation relations are derived.

The quantum mechanical momentum operator is Hermitian:

$$L_x = y p_z - z p_y (= -i\hbar y \frac{\partial}{\partial z} + i\hbar z \frac{\partial}{\partial y}),$$

and

$$\begin{aligned} L_x^\dagger &= (y p_z)^\dagger - (z p_y)^\dagger = (p_z)^\dagger (y)^\dagger - (p_y)^\dagger (z)^\dagger = p_z y - p_y z = \\ &= [p_z, y] + y p_z - [p_y, z] - z p_y = L_x, \end{aligned}$$

since the momentum operator and the position operator are Hermitian and the various position and momentum operators commute (See Eq. 7.17, Fp).

Remark: I do not see the need in Eq. (8.5) of the second expression in the first line. After careful bookkeeping you will arrive at once at the second line of Eq. (8.5).

On page 104 Eq. (8.10):

$$[A^2, B] = AAB - BAA = A(AB - BA) + ABA - (BA - AB)A - ABA = A[A, B] + [A, B]A.$$

In Eq.(8.11) use has been made of $[L_x^2, L_x] = 0$.

Eq. (8.14) is obtained by using the angular momentum operators to be Hermitian.

Eq. (8.15) is obtained by using the Eqs. (8.6) and (8.9).

8.3 Representation of Angular Momentum

This section is about the representation by spatial operators.

Fp conclude that all angular momentum operators can be represented as differential operators.

8.4 Eigenstates of Angular Momentum

In this section Fp obtained the eigenstates of L_z and L^2 .

The representation of these operators are given by Eqs. (8.28) and (8.29).

In Eqs. (8.31) and (8.32) Fp introduces the eigenstates and eigen values of both operators.

To derive Eq. (8.35), use has been made of Eq. (8.19).

Eq. (8.38) is obtained with Eqs. (8.16) and (8.32).

On page 107 Fp presented Eq. (8.42), with the remark Eqs. (8.40) and (8.41) are satisfied when Eq. (8.42) is correct.

Let's have a look for $c_{l,m}^+ = [l(l+1) - m(m+1)]^{1/2}\hbar$ of Eq.(8.42).

Replace in this expression m through $m - 1$ Then:

$$c_{l,m-1}^+ = [l(l+1) - m(m-1)]^{1/2}\hbar.$$

Multiply $c_{l,m}^-$, Eq. (8.42), and $c_{l,m-1}^+$. The result is Eq. (8.41).

Now let's have a look for $c_{l,m}^- = [l(l+1) - m(m-1)]^{1/2}\hbar$ of Eq.(8.42).

Replace in this expression m through $m + 1$ Then:

$$c_{l,m+1}^- = [l(l+1) - m(m+1)]^{1/2}\hbar.$$

Multiply $c_{l,m}^+$, Eq. (8.42), and $c_{l,m+1}^-$. The result is Eq. (8.40).

8.5 Eigenvalues of L_z

The eigenvalues of the differential operator L_z are obtained: $m\hbar$, where m is an integer. The normalized eigenstate of L_z is derived and presented in Eq. (8.50).

8.6 Eigenvalues of L^2

In this section Fp derived a relation between m and l .

To find this relation Fp did use Eq.(4.58). The definition of the Hermitian conjugate, one dimensional:

$$\int_{-\infty}^{\infty} \psi^* (O\psi) dx = \int_{-\infty}^{\infty} (O^\dagger \psi_1)^* \psi_1 dx, \text{ Eq. (4.58),}$$

where O represents an operator.

Now Fp considers the angular wavefunction $\psi(\theta, \phi) = L_+ Y_{l,m}(\theta, \phi)$. This is plugged into

Eq. (8.51). This equation is about normalization with the operator L_+ twice in the integrand. So in what way can we use Eq. (4.58)?

I think we do need Eq. (4.57) and the generalization Eq.(4.86):

$$\int_{-\infty}^{\infty} (O\psi_2)^* \psi_3 dx = \int_{-\infty}^{\infty} \psi_2^* O^\dagger \psi_3 dx , \quad (\text{C8.6.1})$$

where O is a non-Hermitian operator like L_+ .

In (C8.6.1) let $\psi_2 = Y_{l,m}$, $\psi_3 = L_+ Y_{l,m}$ and $O = L_+$.

With Eq.(8.14) we find Eq.(8.52).

At the bottom of page 108 Fp writes “(8.31)-(8.33)”. I think this should be Eq.(8.36).

Finally we arrive at the two constraints Eqs.(8.54) and (8.56).

l is assumed to be non-negative. With the proof by contradiction,

$$m > l \text{ and } m < -l ,$$

we find from both constraints, Eqs.(8.54) and (8.56), Eq.(8.57):

$$-l \leq m \leq l .$$

8.7 Spherical Harmonics

The simultaneous eigenstates $Y_{l,m}(\theta, \phi)$ of L^2 and L_z are derived.

Exercises

Exercise 8.1 Expectation values of momentum operators

A system in state $\psi(\theta, \phi) = Y_{l,m}(\theta, \phi)$. Calculate $\langle L_x \rangle$ and $\langle L_x^2 \rangle$.

$$\langle L_x \rangle = \oint \psi^* L_x \psi d\Omega .$$

L_x is given by Eq.(8.26) and the wave function is the spherical harmonic. So, we can do the job. I also assume the eigenstates of L_z and L^2 are given by Eqs.(8.31) and (8.32). This remark is made since the real world does not depend on a coordinate system and L_x could be considered to represent L_z .

With Eq.(8.13) we have:

$$L_x = \frac{L_+ + L_-}{2} .$$

We know how the raising and lower operators act on the spherical harmonic: Eqs.(8.43) and (8.44).

Then $\langle L_x \rangle$ becomes, with Eqs.(8.42), (8.43), (8.44), and orthogonality:

$$\begin{aligned} \langle L_x \rangle &= \oint \psi^* (L_+ + L_-) \frac{1}{2} \psi d\Omega = \\ &= \frac{1}{2} [\oint c_{l,m}^+ Y_{l,m}^* Y_{l,m+1} d\Omega + \oint c_{l,m}^- Y_{l,m}^* Y_{l,m-1} d\Omega] = 0 . \end{aligned}$$

So, $Y_{l,m}(\theta, \phi)$ not to be an eigenfunction of L_x .

That is a surprise, since $[L^2, L_x] = 0$ and consequently $Y_{l,m}(\theta, \phi)$ is an eigenfunction of L_x .

Now $\langle L_x^2 \rangle$.

$$L_x^2 = \frac{1}{4} (L_+^2 + L_+ L_- + L_- L_+ + L_-^2) .$$

We need to investigate $L_+ L_-$ and $L_- L_+$. The other two terms in L_x^2 do not contribute.

First $L_+ L_-$, with Eqs.(8.42), (8.43) and (8.44),:

$$\oint \psi^* (L_+ L_-) \frac{1}{4} \psi d\Omega = \frac{1}{4} c_{l,m}^- c_{l,m-1}^+ .$$

Then $L_- L_+$, with Eqs.(8.42), (8.43) and (8.44):

$$\oint \psi^* (L_- L_+) \frac{1}{4} \psi d\Omega = \frac{1}{4} c_{l,m}^+ c_{l,m+1}^- .$$

$$\text{Hence } \langle L_x^2 \rangle = \frac{1}{4} (c_{l,m}^- c_{l,m-1}^+ + c_{l,m}^+ c_{l,m+1}^-) .$$

With Eqs.(8.15) and (8.16):

$$L_+ L_- + L_- L_+ = 2(L^2 - L_z^2) ,$$

we again find the above result for $\langle L_x^2 \rangle$.

With Eqs.(8.31) and (8.32) or with Eq.(8.42):

$$\langle L_x^2 \rangle = \frac{1}{4} (c_{l,m}^- c_{l,m-1}^+ + c_{l,m}^+ c_{l,m+1}^-) = \frac{1}{2} (l(l+1)\hbar^2 - m^2\hbar^2) .$$

Let's play a little bit further. Eq.(8.9):

$$L^2 = L_x^2 + L_y^2 + L_z^2 .$$

Then

$$\langle L_x^2 + L_y^2 \rangle = \langle L^2 - L_z^2 \rangle , \text{ and}$$

with Eqs(8.31) and (8.32) :

$$\langle L_x^2 + L_y^2 \rangle = l(l+1)\hbar^2 - m^2\hbar^2 ,$$

and by definition of the expectation value:

$$\langle L_x^2 \rangle + \langle L_y^2 \rangle = l(l+1)\hbar^2 - m^2\hbar^2 .$$

Consequently, with the above value for $\langle L_x^2 \rangle = \frac{1}{2} (l(l+1)\hbar^2 - m^2\hbar^2)$:

$$\langle L_y^2 \rangle Y_{l,m} = \frac{1}{2} (l(l+1)\hbar^2 - m^2\hbar^2) Y_{l,m} .$$

This is also found from:

$$L_y = -\frac{i}{2} (L_+ - L_-) \text{ and } L_y^2 = L_y^* L_y .$$

Now the results of section 4.10, page 57.

$Y_{l,m}$ is an eigenfunction of L^2 and $l(l+1)\hbar^2 (\equiv a_{l,m})$ is the eigenvalue of L^2 .

L_x and L^2 commute, Eq. (8.11).

$$(L^2 L_x - L_x L^2) Y_{l,m} = (L^2 L_x - L_x a_{l,m}) Y_{l,m} = 0 .$$

Hence

$$(L^2 - a_{l,m}) L_x Y_{l,m} = 0 , \text{ or}$$

$$L^2 L_x Y_{l,m} = a_{l,m} L_x Y_{l,m} .$$

Consequently $L_x Y_{l,m}$ is an eigenstate of L^2 with eigenvalue $a_{l,m}$.

Then $L_x Y_{l,m} \propto Y_{l,m}$.

This can be written as

$$L_x Y_{l,m} = b_{l,m} Y_{l,m} ,$$

where $b_{l,m}$ is a constant of proportionality. Hence, $Y_{l,m}$ is an eigenstate of L_x .

So far section 4.10.

Did we run into a contradiction? I think we did. Since we found $Y_{l,m}$ not to be an eigenstate of L_x .

Is $L_x Y_{l,m}$ an eigenstate of L^2 with eigenvalue $a_{l,m}$?

$$L_x Y_{l,m} = \frac{1}{2} (c_{l,m}^+ Y_{l,m+1} + c_{l,m-1}^- Y_{l,m-1}) .$$

Operating L^2 on this expression yields the eigenvalue $a_{l,m}$.

So, we run into trouble with $L_x Y_{l,m} = b_{l,m} Y_{l,m}$.

This can be demonstrated by $l = 1, m = 0$ and the Eqs.(8.92) and(8.93):

$$L_x Y_{1,0} = \frac{L_+ + L_-}{2} Y_{1,0} = \frac{\sin \theta}{\cos \theta} \sin \phi e^{-i\pi/2} Y_{1,0}.$$

What is the meaning of this relation?

Exercise 8.2 The eigenvalues and eigenfunctions of L_x

Find the eigenvalues and eigenfunctions of L_x .

Exercise 1 teaches us the spherical harmonic $Y_{l,m}(\theta, \phi)$ not to be an eigenfunction of L_x . On the other hand, I learned in Chapter 8, section 8.2, :

$$[L^2, L_x] = 0.$$

How to find the eigenfunctions and eigenvalues?

I assume the eigenfunction of L_x to be a function of θ and ϕ . Fp on page 113: “any function of θ and ϕ can be represented as a superposition of spherical harmonics.” The question arises: superposition over m, l , or m and l or what? The other question is: given $Y_{l,m}(\theta, \phi)$ not to be an eigenfunction of L_x , a superposition of spherical harmonics is?

Let’s go en route and find out.

We denote the eigenfunction of L_x : $X(\theta, \phi)$.

$$\text{Hence } X(\theta, \phi) = \sum_{m=-l}^{m=l} a_m Y_{l,m}(\theta, \phi). \quad (\text{C.8.E.1})$$

Then,

$$L_x X(\theta, \phi) = \frac{1}{2} (L_+ + L_-) \sum_{m=-l}^{m=l} a_m Y_{l,m}(\theta, \phi). \quad (\text{C.8.E.2})$$

With Eqs.(8.36) and (8.37) , (C.8.E.2) gives:

$$L_x X(\theta, \phi) = \frac{1}{2} \sum_{m=-l}^{m=l} a_m [c_{l,m}^+ Y_{l,m+1}(\theta, \phi) + c_{l,m}^- Y_{l,m-1}(\theta, \phi)]. \quad (\text{C.8.E.3})$$

Caveat: in the summation $Y_{l,l+1}(\theta, \phi) = 0$ and $Y_{l,-l-1}(\theta, \phi) = 0$.

To find the eigenvalues, I define the eigenvalue equation to be

$$L_x X(\theta, \phi) = \hbar A X(\theta, \phi) = \hbar A \sum_{m=-l}^{m=l} a_m Y_{l,m}(\theta, \phi), \quad (\text{C.8.E.4})$$

where A represents the factor for the eigenvalues.

First I analyse (C.8.E.3).The result is:

$$L_x X(\theta, \phi) = \frac{1}{2} a_{l-1} \hbar \sqrt{2l} Y_{l,l} + \sum_{m=-l+1}^{m=l-1} \frac{1}{2} (a_{m+1} c_{l,m}^+ + a_{m-1} c_{l,m}^-) Y_{l,m} + \frac{1}{2} a_{-l+1} \hbar \sqrt{2l} Y_{l,-l}, \quad (\text{C.8.E.5})$$

where use have been made of (8.40) and (8.41).

The next step is to equate the coefficients of $Y_{l,m}$ in (C.8.E.4) and (C.8.E.5):

$$A a_l = \frac{1}{2} a_{l-1} \sqrt{2l},$$

$$A a_{l-1} = \frac{1}{2} (\sqrt{2l} a_l + \sqrt{4l-2} a_{l-2}),$$

$$A a_{l-2} = \frac{1}{2} (\sqrt{4l-2} a_{l-1} + \sqrt{6l-6} a_{l-3}),$$

.....

$$A a_0 = \frac{\sqrt{l(l+1)}}{2} (a_1 + a_{-1}),$$

$$Aa_{-l+1} = \frac{1}{2}(\sqrt{4l-2}a_{-l+2} + \sqrt{2l}a_{-l}),$$

$$Aa_{-l} = \frac{1}{2}a_{-l+1}\sqrt{2l}.$$

These are $2l - 1$ expressions and with $-l \leq m \leq l$, the eigenvalues are found.

Exercise 8.3 The probabilities of the results of the measurements of the momentum operators
Consider a beam of particles with $l = 1$. A measurement of L_x yields the result \hbar . What values will be obtained by a subsequent measurement of L_z and with which probabilities? Repeat the calculation for the cases in which the measurement of L_x yields the result 0 and $-\hbar$.

With Exercise 8.2, the eigenfunction of L_x for $l = 1$ is obtained.

The eigenvalue equation is

$$L_x X(\theta, \varphi) = \frac{1}{2}(L^+ + L^-)X(\theta, \varphi) = \frac{1}{2}(L^+ + L^-) \sum_{m=-1}^1 a_m Y_{1,m} = A\hbar \sum_{m=-1}^1 a_m Y_{1,m},$$

where $A\hbar$ is the eigenvalue.

So, A and a_m need to be evaluated.

With (C.8.E.5)

$$\frac{1}{2}(L^+ + L^-) \sum_{m=-1}^1 a_m Y_{1,m} = \frac{1}{2}\sqrt{2}(a_0 Y_{1,1} + a_{-1} Y_{1,0} + a_1 Y_{1,0} + a_0 Y_{1,-1})\hbar. \quad (\text{C.8.E.6})$$

Equate the coefficients of the spherical harmonics in

$$\frac{1}{2}(L^+ + L^-) \sum_{m=-1}^1 a_m Y_{1,m} = \hbar A \sum_{m=-1}^1 a_m Y_{1,m} \text{ with those in (C.8.E.6):}$$

The result is

$$Aa_1 = \frac{1}{2}\sqrt{2}a_0,$$

$$Aa_0 = \frac{1}{2}\sqrt{2}(a_1 + a_{-1}), \text{ and}$$

$$Aa_{-1} = \frac{1}{2}\sqrt{2}a_0.$$

The resulting equation for A :

$$A(A^2 - 1) = 0.$$

Then: $A = 0, A = \pm 1$.

Consequently, 3 eigenvalues are found:

$$0, \pm\hbar.$$

By plugging A into the above 3 equations for a_m , the coefficients a_0, a_{-1} expressed in a_1 for the 3 eigenfunctions are obtained.

The eigenfunctions for $A = \pm 1$ are

$$X(\theta, \varphi) = a_1 Y_{1,1} + a_1 \sqrt{2} Y_{1,0} + a_1 Y_{1,-1}. \quad (\text{C.8.E.7})$$

and

$$X(\theta, \varphi) = -a_1 Y_{1,1} + a_1 \sqrt{2} Y_{1,0} - a_1 Y_{1,-1}, \quad (\text{C.8.E.8})$$

with eigenvalues $\pm\hbar$.

The eigenfunction for $A = 0$ is

$$X(\theta, \varphi) = a_1 Y_{1,1} - a_1 Y_{1,-1}. \quad (\text{C.8.E.9})$$

a_1 for $A = \pm 1$ and $A = 0$ are found by normalization of $X(\theta, \varphi)$ in (C.8.E.7) or (C.8.E.7) and (C.8.E.9):

$$\int_0^{2\pi} \int_0^\pi X^* X \sin \theta d\theta d\varphi .$$

Plug $X(\theta, \varphi)$ into this integral :

$$\text{for } A = \pm 1 : a_1 = \frac{1}{2}\sqrt{2} ,$$

and

$$\text{for } A = 0 : a_1 = 1.$$

Hence for the eigenfunction $X(\theta, \varphi)$, $A = \pm 1$, the following series of spherical harmonics is found:

$$X(\theta, \varphi) = \frac{1}{2}\sqrt{2}Y_{1,1} + Y_{1,0} + \frac{1}{2}\sqrt{2}Y_{1,-1}.$$

and

$$X(\theta, \varphi) = \frac{1}{2}\sqrt{2}Y_{1,1} - Y_{1,0} + \frac{1}{2}\sqrt{2}Y_{1,-1}.$$

The eigenfunction $F(\theta, \varphi)$, $A = 0$, the following series of spherical harmonics is found:

$$X(\theta, \varphi) = Y_{1,1} - Y_{1,-1}.$$

The eigenvalues of L_x are: $0, \pm\hbar$ respectively.

I used the $l = 1$ spherical harmonics as presented in (8.92) and (8.93) in *The Undergraduate Course*(Fp).

Conclusion

$$L_x X(\theta, \varphi) = \hbar(\frac{1}{2}\sqrt{2}Y_{1,1} + Y_{1,0} + \frac{1}{2}\sqrt{2}Y_{1,-1}),$$

$$L_x X(\theta, \varphi) = -\hbar(\frac{1}{2}\sqrt{2}Y_{1,1} - Y_{1,0} + \frac{1}{2}\sqrt{2}Y_{1,-1})$$

and

$$L_x X(\theta, \varphi) = 0.$$

The commutator

$$[L_x, L_z] \neq 0 .$$

So, Y_{1m} is not an eigenfunction of L_x .

For L_z we have:

$$L_z Y_{1m} = m\hbar Y_{1m}$$

and

$$m = 1, 0, -1 . \text{ These are the eigenvalues to be obtained by a subsequent measurement of } L_z.$$

Furthermore:

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos \theta \text{ and } Y_{1,\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\varphi}.$$

These expression are given in Section 8.7 on Spherical Harmonics.

The probability for $Y_{1,0}$ is 50% and the probabilities for $Y_{1,\pm 1}$ are 25% respectively

Repeat the calculations in which the measurement of L_x yields the results 0 and $-\hbar$.

The question: "What values will be obtained by a subsequent measurement of L_z , and with what probabilities?" , does lead to the same answer for $-\hbar$. These probabilities are obtained from the square of the amplitudes in (C.8.E.7) and (C.8.E.8).

For the eigenvalue 0, $Y_{1,\pm 1}$ are obtained with probabilities of 50% each.

Exercise 8.4 Eigenvalues of the Hamiltonian of an axially symmetric rotator

The Hamiltonian for an axially symmetric rotator is given by

$$H = \frac{L_x^2 + L_y^2}{2I_1} + \frac{L_z^2}{2I_2}.$$

What are the eigenvalues of H ?

I assume the spherical harmonics to be eigenfunctions of the Hamiltonian operator.

Rewrite H :

$$H = \frac{L^2 - L_z^2}{2I_1} + \frac{L_z^2}{2I_2}.$$

So,

$$H = \frac{L^2}{2I_1} + \frac{L_z^2(I_1 - I_2)}{2I_1 I_2}.$$

Hence

$$H Y_{l,m} = \left(\frac{L^2}{2I_1} + \frac{L_z^2(I_1 - I_2)}{2I_1 I_2} \right) Y_{l,m}.$$

With Eqs.(8.31) and (8.32), the eigenvalues are:

$$\frac{\hbar^2 l(l+1)}{2I_1} + \frac{(\hbar m)^2 (I_1 - I_2)}{2I_1 I_2}.$$

9 Central Potentials

9.1 Introduction

The interaction of a non-relativistic particle with central potentials dependent on the coordinate r is investigated.

9.2 Derivation of Radial Equation

The radial component of momentum is given by Eq. (9.4).

Fp: “.....it is easily demonstrated....”.

So, it is about p_r , with (8.20)-(8.25),

$$\frac{\partial}{\partial r} = \frac{\partial}{\partial x} \frac{\partial x}{\partial r} + \frac{\partial}{\partial y} \frac{\partial y}{\partial r} + \frac{\partial}{\partial z} \frac{\partial z}{\partial r} = \frac{x}{r} \frac{\partial}{\partial x} + \frac{y}{r} \frac{\partial}{\partial y} + \frac{z}{r} \frac{\partial}{\partial z}.$$

Multiply $\frac{\partial}{\partial r}$ with $-i\hbar$:

$$-i\hbar \frac{\partial}{\partial r} = \frac{1}{r} \left(-xi\hbar \frac{\partial}{\partial x} - yi\hbar \frac{\partial}{\partial y} - zi\hbar \frac{\partial}{\partial z} \right) = \frac{1}{r} (xp_x + yp_y + zp_z) = \frac{\mathbf{p} \cdot \mathbf{r}}{r} \equiv p_r. \quad (\text{C.9.1})$$

In Eq.(9.25) the differential equation for the radial variation of the wavefunction is given.

9.3 Infinite Potential Well

The radial part of the differential equation representing the wavefunction is solved by means of spherical Bessel functions.

At the bottom of page 120 Fp mentioned it to be easily demonstrated the Bessel functions are mutually orthogonal. Well, at least for $l = 0$, I found it to be easy.

9.4 Hydrogen atom

The radial part of the eigenfunction is obtained.

On page 122 Fp looked for a power-law solution and obtained the recursion relation given in Eq.(9.51). From this recursion relation the lowest possible value of the power, k_{min} , in the power-law is obtained. This k is an integer, not a wave number.

An alternative way (Mahan) to find the lowest possible value of k is to solve the differential equation Eq.(9.48) for $z \rightarrow 0$. The differential equation can be approximated by:

$\left[\frac{d^2}{dz^2} - \frac{l(l+1)}{z^2} \right] Z = 0$. The solution is: $Z = z^{l+1}$. Consequently, for the power-law solution, the lowest value of k , $k_{min} = l + 1$.

On the same page Fp mentioned that for large z the ratio of successive coefficients in the power series given in Eq. (9.49), follows from Eq.(9.51):

$$\frac{c_k}{c_{k-1}} = \frac{2}{k}.$$

Using Eq. (9.51) I find:

$$\frac{c_k}{c_{k-1}} = \frac{2(k-1)-\zeta}{k(k-1)-l(l+1)}.$$

Obviously, for $z \rightarrow \infty$ the largest contribution in the power-law solution stems from large values of k and

$$\frac{c_k}{c_{k-1}} = \frac{2}{k}.$$

In Eq.(9.50) z is present and the dominant term for $z \rightarrow \infty$ is z^{k-1} yielding $\zeta = 2k$. The same result is obtained for a physically acceptable behaviour of the wavefunction for $r \rightarrow \infty$.

Set $k = n$ results into Eq.(9.54).

Note: Fp referred to Eq.(9.51) and not to Eq.(9.50).

In my notes on *The Graduate Course*(Fp) §4.6 *Energy Levels of Hydrogen Atom*, I demonstrated a different approach giving the maximum value for k (www.leennoordzij.me).

On page 124 Fp presented the first radial wave functions for the hydrogen atom.

Let's look into $R_{1,0}(r)$.

At the bottom of page 121:

$$R_{n,l}(r) = Z \left(\frac{r}{a} \right) \exp\left(-\frac{r}{a}\right) / \left(\frac{r}{a} \right).$$

With $n = 1$ and $l = 0$, Eq.(9.49):

$$Z \left(\frac{r}{a} \right) = \sum_{k_{min}}^n \left(\frac{r}{a} \right)^k,$$

results into

$$Z \left(\frac{r}{a} \right) = c_1 \frac{r}{a}, \text{ and}$$

$R_{1,0} = c_1 \exp\left(-\frac{r}{a}\right)$. With help of normalisation and applying twice integration by parts Eq.(9.65) is found.

In Eq.(9.77), the total number of degenerate states for a given value of n is presented. This equation can be proven by induction.

Mahan obtained the radial part of the Hydrogen Eigenfunctions, section 5.4.3, with confluent hypergeometric functions and the, identical, associated Laguerre polynomials.

9.5 Rydberg Formula

The Rydberg formula is presented in Eq.(9.79)

Exercises

Exercise 9.1 The ground-state of a particle in a spherical well

A particle of mass m is placed in finite spherical potential well:

$$V(r) = -V_0 \text{ for } r \leq a,$$

and

$$V(r) = 0 \text{ for } r > a.$$

with $V_0 > 0$ and $a > 0$.

Find the ground-state by solving the radial equation with $l = 0$.

Show there is no ground-state if $V_0 a^2 < \pi^2 \hbar^2 / 8m$.

See Mahan, Chapter 5 Exercise 3.

The equation to be solved is given in Eq.(9.28).

There, (9.28):

$$k^2 = \frac{2m(E+V_0)}{\hbar^2}, \quad (\text{C.9.E1})$$

and

$$-V_0 < E < 0 \text{ with } r \leq a.$$

So for $l = 0$

$$R_{n,0} = A \frac{\sin kr}{kr}, \text{ Eq.(9.33).}$$

The constant A is found by normalisation.

What about $r > a$?

Well, $V(r) = 0$. Consequently k in (C.9.E.1) is imaginary.

Then we have :

$$R_{n,0} = B \frac{\sinh \alpha r}{\alpha r}, \quad (\text{C.9.E.2})$$

where,

$$\alpha^2 = -\frac{2mE}{\hbar^2}. \text{ However, } R_{n,0} \text{ diverges for } r \rightarrow \infty.$$

What to do? We would expect a function more like

$$e^{-\alpha r} / \alpha r.$$

From Abramowitz and Stegun (10.2) we know

$$R_{n,0} \propto \left(\frac{\cosh \alpha r}{\alpha r} - \frac{\sinh \alpha r}{\alpha r} \right) \text{ to be a solution. This can be written as:}$$

$$R_{n,0} \propto \frac{e^{-\alpha r}}{\alpha r}. \text{ This will work.}$$

In order to find out about the eigenvalue we have to match the values of the wavefunctions and their derivatives at $r = a$.

The wave functions:

$$A \frac{\sin ka}{ka} = B \frac{e^{-\alpha a}}{\alpha a}. \quad (\text{C.9.E.3})$$

The derivatives:

$$A \left[\frac{\cos ka}{a} - \frac{\sin ka}{ka} \right] = B \left[\frac{e^{-\alpha a}}{a} + \frac{e^{-\alpha a}}{\alpha a^2} \right] \quad (\text{C.9.E.4})$$

Now we divide both equations (C.9.E.3) and (C.9.E.4) and obtain:

$$\frac{\tan ka}{k} = -\frac{1}{\alpha}. \quad (\text{C.9.E.5})$$

We rewrite (C.9.E.5):

$$\tan \sqrt{\frac{2m(E+V_0)a^2}{\hbar^2}} = -\sqrt{\frac{E+V_0}{-E}}. \quad (\text{C.9.E.6})$$

This equation gives us the eigenvalue of the ground-state $l = 0$.

As shown in Mahan Chapter 2, (C.9.E.6) is equal to the one-dimensional case.

(C.9.E.6) shows the minus sign of the tangent function. Consequently $\sqrt{\frac{2m(E+V_0)a^2}{\hbar^2}} > \frac{\pi}{2}$,

$$\text{or } (E + V_0) > \frac{\pi^2 \hbar^2}{8ma^2}.$$

Furthermore $0 < E + V_0 < V_0$.

So, for $V_0 = \frac{\pi^2 \hbar^2}{8ma^2}$, we cannot find a bound-state.

This analysis I presented in the discussion of the square potential well in section 5.7.

Now substitute (here I follow Mahan):

$$g^2 = \frac{2mV_0a^2}{\hbar^2}, \text{ and } E = -\varepsilon V_0 \text{ into (C.9.E.6):}$$

$$\tan \sqrt{g^2(1-\varepsilon)} = -\sqrt{\frac{1-\varepsilon}{\varepsilon}}, \quad (\text{C.9.E.7})$$

and with $-V_0 < E < 0$ we have $1 > \varepsilon > 0$.

For example $g^2 = 3$ we find $\varepsilon \approx .02$.

The ground-state is $E = -.02V_0$.

The value of g^2 has been chosen on basis of the analysis presented by Mahan, page 20.

The value of ε is obtained with WolframAlpha.

Exercise 9.2 The three-dimensional harmonic oscillator

Consider a particle of mass m in the three-dimensional harmonic oscillator potential

$V(r) = m\omega^2 r^2/2$. Solve the problem by separation of variables in spherical polar coordinates, and, hence, determine the energy eigenvalues of the system.

After separation of variables the differential equation to be solved is presented in Eq.(9.25). The spherical harmonics part is already available.

The equation to start with, Eq.(9.25):

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} - \frac{m^2 \omega^2}{\hbar^2} r^2 + \frac{2m}{\hbar^2} E \right] R_{n,l} = 0. \quad (\text{C.9.E.8})$$

Now I will use the analysis of section 5.8 Simple Harmonic Oscillator.

Making use of Eqs.(5.92) and (5.93), and $x \rightarrow r$, (C.9.E.8) becomes:

$$\left[\frac{d^2}{dy^2} + \frac{2}{y} \frac{d}{dy} - \frac{l(l+1)}{y^2} - y^2 + \epsilon \right] R_{n,l} = 0. \quad (\text{C.9.E.10})$$

For $y \rightarrow \infty$, (C.9.E.10) can be approximated by

$$\left[\frac{d^2}{dy^2} - y^2 \right] R_{n,l} \cong 0.$$

The approximate solution of this equation is:

$$R_{n,l} \cong e^{-y^2/2} . \quad (\text{C.9.E.11})$$

Then, for $y \rightarrow 0$, (C.9.E.10) can be approximated by

$$R_{n,l} \sim y^{l+1} . \quad (\text{C.9.E.12})$$

Another possibility of an approximate solution could be for $y \rightarrow 0$:

$$R_{n,l} \sim y^l , \text{ with the condition } l \geq 2 .$$

First, we use $R_{n,l} \sim y^{l+1}$.

Now for the general solution we write, like Eq.(5.97),

$$R_{n,l} = y^{l+1} h(y) e^{-y^2/2} . \quad (\text{C.9.E.13})$$

Where $h(y)$ can be expected to be an algebraic function.

Now we substitute (C.9.E.13) into (C.9.E.10).

$\frac{d}{dy} R_{n,l}$, gives

$$(l+1)y^l h(y) e^{-y^2/2} + y^{l+1} \frac{dh}{dy} e^{-y^2/2} - y^{l+2} h(y) e^{-y^2/2} . \quad (\text{C.9.E.14})$$

The expression for $\frac{d^2}{dy^2} R_{n,l}$ consists of 9 terms.

I will not present them.

Here I present the differential equation of $h(y)$:

$$\frac{d^2 h}{dy^2} + 2[(l+2)y^{-1} - y] \frac{dh}{dy} + [2(l+1)y^{-2} - (2l+5) + \epsilon] h = 0 . \quad (\text{C.9.E.15})$$

Plug into (C.9.E.15) the power-law solution:

$$h(y) = \sum_{i=0}^{\infty} c_i y^i , \text{ Eq.(5.99).}$$

Insert this into (C.9.E.15), equate the coefficients of y^i . This results into:

$$c_{i+2} = \frac{(2i-\epsilon+2l+5)}{(i+1)(i+2)+2(il+3l+4)} c_i . \quad (\text{C.9.E.16})$$

Now in the limit for $y \rightarrow \infty$, the recursion relation in (C.9.E.16) becomes:

$$c_{i+2} \cong \frac{2}{i} c_i .$$

Fp: hence, at large y , when the higher powers of y dominate, we have

$$h(y) \sim C e^{y^2} .$$

So for large y , $R_{n,l} = y^{l+1} h(y) e^{-y^2/2}$ varies as: $R_{n,l} = y^{l+1} e^{y^2/2}$. Consequently, the series represented in Eq.(5.99) need to terminate at some value of $i = n$. This implies, using (C.9.E.16),

$$\epsilon = 2n + 2l + \frac{5}{2} . \quad (\text{C.9.E.17})$$

With Eq.(5.93), the eigenvalues are:

$$E = \hbar \omega (n + l + \frac{5}{2}) . \quad (\text{C.9.E.18})$$

Next we use the trial function:

$$R_{n,l} = y^l h(y) e^{-y^2/2} .$$

The we find, similar to (C.9.E.15),

$$\frac{d^2 h}{dy^2} + 2[(l+1)y^{-1} - y] \frac{dh}{dy} + [-(2l+3) + \epsilon] h = 0 .$$

Using Eq.(5.99) and equating the coefficients of y^i results into the recursion relation

$$c_{i+2} = \frac{(2i-\epsilon+2l+3)}{(i+1)(i+2)+2i(l+1)} c_i . \quad (\text{C.9.E.19})$$

Finally we have for the eigenvalues:

$$E = \hbar\omega(n + l + \frac{3}{2}). \quad (\text{C.9.E.20})$$

So, here I have two expressions for the eigenvalues: (C.9.E.18) and (C.9.E.20).

Which is the correct expression for the eigenvalues? From the literature I think the correct expression to be (C.9.E.20) with the constraint $l \geq 2$ or $i > 2$ in the power-law solution. There is no physical evidence for the latter constraint.

Which solution is correct? Is there a solution? Well, there is.

The mistake I made with the approximation for $y \rightarrow 0$ is the following:

with $R_{n,l} \approx y^{l+1}$ and neglecting $\frac{2}{y} \frac{d}{dy}$ in (C.9.E.10), $R_{n,l} \approx y^{l+1}$ is no longer an approximate solution. Consequently, we need to incorporate $\frac{2}{y} \frac{d}{dy}$ and then a better approximate solution is $R_{n,l} \approx y^{l+2}$.

For the trial function we have:

$$R_{n,l} = y^{l+2} (\sum_{i=0}^{\infty} c_i y^i) e^{-y^2/2} . \quad (\text{C.9.E.21})$$

Then, from equating the coefficients of y^i we obtain the recursion relation:

$$c_i = \frac{(2i-\epsilon+2l+3)}{i(i+2l+5)+2(2l+3)} c_{i-2} .$$

From this relation we obtain the eigenvalues presented in (C.9.E.20).

Exercise 9.3 About the wavefunction for the ground-state of a hydrogen-like atom

The normalized wavefunction for the ground-state of a hydrogen-like atom (neutral hydrogen, He^+ , Li^{++} , etc.) with nuclear charge Ze has the form:

$$\psi = A \exp(-\beta r),$$

where A and β are constants, and r is the distance between the nucleus and the electron.

Show the following:

(a) $A^2 = \beta^3/\pi$.

To find about A we need to evaluate the integral:

$$\int_0^{2\pi} \int_0^\pi \int_0^\infty A^2 \exp(-2\beta r) r^2 \sin \theta dr d\theta d\phi = 1.$$

Straightforwardly integrating over θ and ϕ and integrating by parts over r , we obtain the expression:

$$A^2 = \beta^3/\pi.$$

(b) Show $\beta = Z/a_0$, where a_0 is given by Eq.(9.58).

For the hydrogen atom we have:

$$\psi = R_{1,0} Y_{00} = 2 \frac{1}{a_0^{3/2}} \exp(-\frac{r}{a_0}) \frac{1}{\sqrt{4\pi}} . \quad (\text{C.9.E.22})$$

With Eq.(9.65) and $Y_{00} = \frac{1}{\sqrt{4\pi}}$, this gives for β :

$$\beta = 1/a_0 .$$

For the hydrogen atom $Z = 1$.

Plugging Z into the nominator of Eqs.(9.40), the potential, (9.47) and (9.57), we find:

$$\beta = Z/a_0 .$$

$$\text{Then } \psi = R_{1,0} Y_{00} = 2 \frac{Z^{3/2}}{a_0^{3/2}} \exp\left(-\frac{Zr}{a_0}\right) \frac{1}{\sqrt{4\pi}} . \quad (\text{C.9.E.23})$$

(c) Show the energy is $E = -Z^2 E_0$, where E_0 is given by Eq.(9.57).

Eq.(9.54): $\frac{\zeta}{2} = n$. With Z , this expression becomes:

$$\frac{Z\zeta}{2} = n .$$

Then, using Eq.(9.47),

$$Z \sqrt{\frac{E}{E_0}} = n . \text{ Since } E < 0 , \text{ we finally obtain:}$$

$$E = -Z^2 E_0 .$$

(d) Show the expectation values of the potential and kinetic energies are $2E$ and $-E$.

$$\langle V \rangle = \int \psi^* V \psi r^2 \sin \theta dr d\theta d\phi .$$

With Eqs.(9.40), including Z , (C.9.E.22) and (9.57), we obtain after integrating by parts,

$$\langle V \rangle = 2Z^2 E_0 .$$

Hence, with $n = 1$ and Eq.(9.55) :

$$\langle V \rangle = 2Z^2 E_0 = 2E .$$

Now the kinetic energy :

$$\langle E \rangle = -Z^2 E_0 \int \psi^* \psi r^2 \sin \theta dr d\theta d\phi = -Z^2 E_0 = E .$$

(e) Show the expectation value of $r = \left(\frac{3}{2}\right) \left(\frac{a_0}{Z}\right)$.

With Eq.(9.73), $n = 1$, $l = 0$, and $\beta = Z/a_0$ we obtain:

$$\langle r \rangle = \left(\frac{3}{2}\right) \left(\frac{a_0}{Z}\right) .$$

Obviously, with (C.9.E.23) and $\langle r \rangle = \int \psi^* r \psi r^2 \sin \theta dr d\theta d\phi$ the same result is found.

(f) Show the most probable value of $r = \left(\frac{a_0}{Z}\right)$.

Remark: is the most probable value defined?

Well, it's about the probability distribution or probability density. This is less straightforward as in the 1-D case. In the 1-D case it is the probability distribution in an interval dx , say. In the 3-D case, finding out about the probability distribution in radial direction, we must integrate the probability distribution over θ and ϕ .

Having found the probability density, differentiate with respect to r and the most probable is found. If any.

For $R_{1,0}$, the probability density looks like the solid line in Figure 9.2.

So, the probability distribution in radial direction is:

$$P(r) = R_{1,0}^* R_{1,0} r^2 \frac{1}{4\pi} \int \sin \theta d\theta d\phi .$$

Hence, we have to determine $\frac{dP}{dr}$.

$$\text{Then } P(r) = 4 \frac{Z^3}{a_0^3} r^2 \exp\left(-2 \frac{Zr}{a_0}\right) ,$$

$$\frac{dP}{dr} = 4 \frac{Z^3}{a_0^3} \left[2r - 2r^2 \frac{Z}{a_0} \right] \exp\left(-2 \frac{Zr}{a_0}\right) = 0 .$$

With $r \neq 0$, we have:

$$r = \left(\frac{a_0}{Z}\right).$$

Exercise 9.4 Decay of the nucleus of a tritium atom

An atom of tritium is in its ground-state. Suddenly the nucleus decays into a helium nucleus, via the emission of a fast electron which leaves the atom without perturbing the extranuclear electron. Find the probability that the resulting He^+ ion will be left in an $n = 1, l = 0$ state. Find the probability that it will be left in a $n = 2, l = 0$ state. What is the probability that the ion will be left in an $l > 0$ state?

He^+ and tritium are hydrogen like atoms: $Z = 1$.

“Find the probability that the resulting He^+ ion will be left in a particular state”. Has this been defined in the text?

Well, I suppose the probability is:

$$\int \psi_{tri}^* \psi_{He^+} r^2 dr \sin \theta d\theta d\phi. \quad (C.9.E.24)$$

The ground-states of tritium and the He^+ ion are given by Eq.(9.65) and spherical harmonics.

Evaluating (C.9.E.24) with these ground-states leads to a probability of 100%.

The probability of the resulting He^+ ion left in an $n = 2, l = 0$ state.

The $n = 2, l = 0$ state of the He^+ ion is given by Eq.(9.66) and the spherical harmonic Y_{00} . Plug the ground-state of tritium and the $n = 2, l = 0$ state of the He^+ ion into (C.9.E.24). The result for the probability is 0%.

Consequently, the result for the probability that the ion will be left in an $l > 0$ ($n \geq 2$), state is 0%.

Exercise 9.5 Wavelengths of emitted photons

Calculate the wavelengths of the photons emitted from the $n = 2, l = 1$ to $n = 1, l = 0$ transition in hydrogen, deuterium, and positronium.

Here we will do the job with the results of section 9.5 on the Rydberg formula.

So, we apply Eq.(9.79). The wavelength depends on the radial quantum number. The Rydberg constant (R) depends on the mass of the electron and the charge of the electron.

Hence, the wavelengths of the photons are the same in the above mentioned three cases:

$$\lambda = \frac{4}{3R},$$

where R is given by Eq.(9.80).

Exercise 9.6 About hydrogen's recoil energy emitting a photon

To conserve linear momentum, an atom emitting a photon must recoil, which means that not all the energy made available in the downward jump goes to the photon. Find a hydrogen's recoil energy when it emits a photon at in an $n = 2$ to $n = 1$ transition. What fraction of the transition energy is the recoil energy?

To calculate the recoil energy, E_r , we assume ΔE , Eq.(9.78), to be much larger than E_r .

The linear momentum of the photon, p_p , is:

$$p_p = \frac{\Delta E}{c}. \quad (C.9.E.25)$$

Conservation of momentum makes the absolute value of the momentum of the photon p_p equal to the absolute value of momentum of the hydrogen atom, $p_H = m_H v_H$.

Consequently, with (C.9.E.25),

$$(v_H)^2 = \left(\frac{\Delta E}{m_H c}\right)^2. \quad (\text{C.9.E.26})$$

Now, with (C.9.E.26),:

$$E_r = \frac{1}{2} m_H (v_H)^2 = \frac{1}{2 m_H} \left(\frac{\Delta E}{c}\right)^2. \quad (\text{C.9.E.27})$$

We can plug in some numbers.

Eq.(9.78) gives:

$$\Delta E = \frac{3}{4} E_0 \text{ and } E_0 = 1.634 \times 10^{-18} \text{ joules.}$$

Then with the speed of light c and the mass of the hydrogen atom you will find

$$E_r \ll \Delta E \text{ indeed.}$$

Since doing the proper calculations, (C.9.E.25) should read:

$$p_p = \frac{\Delta E - E_r}{c}. \quad (\text{C.9.E.28})$$

Then, the analysis gives a quadratic equation for E_r :

$$E_r = \frac{1}{2 m_H} \left(\frac{\Delta E - E_r}{c}\right)^2. \quad (\text{C.9.E.29})$$

Doing the analysis, we obtain:

$$E_r = [\Delta E + m_H c^2] \left[1 - \sqrt{1 - \frac{(\Delta E)^2}{(\Delta E + m_H c^2)^2}}\right]. \quad (\text{C.9.E.30})$$

Plugging into (C.9.E.30) the given numbers, we find $\Delta E \ll m_H c^2$ and $\frac{(\Delta E)^2}{(\Delta E + m_H c^2)^2} \ll 1$.

No assumptions being made for E_r .

Using $\frac{(\Delta E)^2}{(\Delta E + m_H c^2)^2} \ll 1$, (C.9.E.30) can be approximated as:

$$E_r \approx \frac{1}{2} \frac{(\Delta E)^2}{\Delta E + m_H c^2}. \quad (\text{C.9.E.31})$$

Now with $\Delta E \ll m_H c^2$ (C.9.E.31) gives (C.9.E.27).

10 Spin Angular Momentum

10.1 Introduction

As explained in this section the difference between classical spin and quantum mechanical spin. In quantum mechanics think of spin to be intrinsic angular momentum.

10.2 Spin Operators

The assumption is: spin to possess similar properties to orbital angular momentum.

The commutation relations for spin angular momentum operators possess analogous relations

corresponding to orbital angular momentum operators, (10.1)-(10.3).
The raising and lowering operators are presented.

10.3 Spin space

Fp introduces the complex vector space of spin vectors, the length or norm of the spin vector, orthogonality, the general spin operator, eigenvalues, normalization, and the general spin state.

10.4 Eigenstates of S_z and S^2

The similarity of orbital angular momentum and spin angular momentum is used. See section 8.6.

10.5 Pauli Representation

At the bottom of page 134 the general spin operator is discussed. There Fp writes: “*As is easily demonstrated.....*” is a bit confusing to me. I thought and think Eq.(10.44) needs not to be demonstrated. It is the definition of the Hermitian conjugate of the matrix A .

At the middle of page 135 Fp writes again: “*It is easily demonstrated*”.

Let’s have a look.

For the Pauli matrices we write:

$$\sigma_x = \begin{pmatrix} x_1 & x_2 \\ x_3 & x_4 \end{pmatrix}, \sigma_y = \begin{pmatrix} y_1 & y_2 \\ y_3 & y_4 \end{pmatrix}, \text{ and } \sigma_z = \begin{pmatrix} z_1 & z_2 \\ z_3 & z_4 \end{pmatrix}. \quad (\text{C.10.E.1})$$

With Eqs.(10.45), (10.46) and (10.51) we find for σ_z :

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \text{ Eq.(10.54).}$$

Using (C.10.E.1), Eqs.(10.49) and(10.54) we obtain:

$$\sigma_x = \begin{pmatrix} 0 & x_2 \\ x_3 & 0 \end{pmatrix}, \quad (\text{C.10.E.2})$$

and

$$y_2 = -ix_2, y_3 = ix_3. \quad (\text{C.10.E.3})$$

Using (C.10.E.1), Eqs.(10.50) and(10.54) we obtain:

$$\sigma_y = \begin{pmatrix} 0 & y_2 \\ y_3 & 0 \end{pmatrix}, \quad (\text{C.10.E.4})$$

and

$$x_2 = iy_2, x_3 = -iy_3 \text{ equal to (C.10.E.3).}$$

Now with Eq.(10.48), (C.10.E.2) and (C.10.E.4) :

$$x_2y_3 - y_2x_3 = 2i, \quad (\text{C.10.E.5})$$

and

$$x_3y_2 - y_3x_2 = -2i. \quad (\text{C.10.E.6})$$

Plugging (C.10.E.3) into (C.10.E.5) and (C.10.E.6) results in:

$$x_2x_3 = 1 \text{ and } y_2y_3 = 1. \quad (\text{C.10.E.7})$$

In addition we assume the Pauli matrices to be Hermitian:

$$x_2^*x_2 = 1 \text{ and } y_2^*y_2 = 1. \quad (\text{C.10.E.8})$$

For (C.10.E.3) we write:

$$y_2 = -ix_2, y_2^* = ix_2^*. \quad (\text{C.10.E.9})$$

From (C.10.E.8) and (C.10.E.9) we conclude some ambiguity whether to choose σ_x or σ_y to be imaginary. Obviously, at least we can demonstrate the matrices in Eqs.(10.52)-(10.54) will do the job. However, I could not easily demonstrate the uniqueness.

However, there is more (www.ocw.mit.edu). Pauli Spin Matrices are derived. On page 7, Physical Chemistry-24 *Pauli Spin Matrices*, the following is written: “...we have made an arbitrary choice of the sign.....”. Let us translate this into our notation, (C.10.E.9),

$x_2^* x_2 = 1$ and $x_2 = 1$. This gives for the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ and } \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

The above-mentioned arbitrary choice is a special arbitrary choice. It produces the simplest matrix.

Since $x_2^* x_2 = 1$ gives us as a general solution:

$x_2 = \cos \beta + i \sin \beta$, where β can be any angle. Obviously, $\beta = \pi/2$, or $\beta = 0$ produces the simplest matrices. With $\beta = \pi/2$, σ_x becomes imaginary instead of σ_y . Does it matter? Well, vector space does not represent the real world. Consequently, it does not matter.

However, $x_2 = \cos \beta + i \sin \beta = e^{i\beta}$ cannot be considered as phase ambiguity. For σ_x we have:

$$\sigma_x = \begin{pmatrix} 0 & e^{i\beta} \\ e^{-i\beta} & 0 \end{pmatrix}. \text{ In exercise 2 we will pay some attention to this “ambiguity”}.$$

10.6 Spin Precession

In Eq. (10.57) Fp presented the relation of the electron’s orbital momentum \mathbf{L} and the magnetic moment $\boldsymbol{\mu}$ (See Feynman et al, Vol. II).

Then it is assumed a similar relation between the magnetic moment and spin angular momentum.

The spin angular momenta, $\langle S_x \rangle$ and $\langle S_y \rangle$, depend on the precession angle α and the precession frequency Ω .

The constant α is the angle of the spin angular momentum vector with the z-axis. The angle is chosen as initial condition and does not depend on the precession frequency. We further learn Ω changes sign with the direction of the magnetic field. α does not depend on this direction.

Exercises

Exercise 10.1 The Pauli representations of S_x , S_y and S_z for spin-1 particle

Find the Pauli representations of S_x , S_y and S_z for a **spin-1** particle.

With a spin-1 particle we have three states: $m_s = 1, 0, -1$. Similar to the representation given on pages 134 and 135, we have three eigenstate vectors:

$$\chi_{1,1} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \chi_{1,0} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } \chi_{1,-1} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (\text{C.10.E.10})$$

The first matrix to deal with is S_z . Using Eq.(10.16), the eigenstates and eigenvalues of S_z , and a general 3×3 matrix for S_z we find:

$$S_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

To obtain S_x and S_y let's use the raising and lowering operators. Then,

$$S_+ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, S_+ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = a_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \text{ and } S_+ \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = a_2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}. \quad (\text{C.10.E.11})$$

For S_+ we start with a general 3×3 matrix. With (C.10.E.11) we find for S_+ :

$$S_+ = \begin{pmatrix} 0 & a_1 & 0 \\ 0 & 0 & a_2 \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{C.10.E.12})$$

For the lowering operator we have with Eq.(10.7);

$$S_- = \begin{pmatrix} 0 & 0 & 0 \\ a_1^* & 0 & 0 \\ 0 & a_2^* & 0 \end{pmatrix}. \quad (\text{C.10.E.13})$$

So, with Eq.(10.6):

$$S_x = \frac{1}{2}(S_+ + S_-) = \frac{1}{2} \begin{pmatrix} 0 & a_1 & 0 \\ a_1^* & 0 & a_2 \\ 0 & a_2^* & 0 \end{pmatrix}, \quad (\text{C.10.E.14})$$

and

$$S_y = \frac{1}{2i}(S_+ - S_-) = \frac{i}{2} \begin{pmatrix} 0 & -a_1 & 0 \\ a_1^* & 0 & -a_2 \\ 0 & a_2^* & 0 \end{pmatrix}. \quad (\text{C.10.E.15})$$

Now applying Eq.(10.2) and equating the elements of the matrices we find:

$$a_1 = a_1^* \text{ and } a_2 = a_2^*.$$

Hence, a_1 and a_2 are real numbers.

Again with the commutation relation Eq.(10.1) and equating elements the result is:

$$a_1^2 = a_2^2 \text{ and } a_1^2 = 2\hbar^2.$$

I choose the positive values. Then:

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \text{ and } S_y = \frac{i\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}. \quad (\text{C.10.E.16})$$

Exercise 10.2 Pauli representation of normalized states S_x and S_y for a spin-1/2 particle

Find the Pauli representation of the normalized eigenstates of S_x and S_y for a spin-1/2 particle.

Her I will use the analysis of section 10.5.

For convenience the Eqs. (10.52)-(10.54) has been used. The eigenvalues of the three matrices represented by these equations are : ± 1 . The spin eigenstates of σ_z are presented on page 135 (Fp).

Let us start with σ_x .

For the eigenvalue +1 we have

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

Then the eigen vector is $\begin{pmatrix} a \\ a \end{pmatrix}$. Normalization results into $|a| = \frac{1}{\sqrt{2}}$.

Hence, for the normalized eigenstate the following expression is obtained:

$$e^{i\gamma} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix},$$

where γ represent phase ambiguity (Susskind, page 42). In this case $\gamma = \pi$.

However, keeping in mind the discussion on page 84 of this document, the eigenstate(vector) is:

$$e^{i\gamma} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{e^{-i\beta}}{\sqrt{2}} \end{pmatrix}.$$

For the eigenvalue -1 we find

$$e^{i\gamma} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix} \text{ or } e^{i\gamma} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-e^{-i\beta}}{\sqrt{2}} \end{pmatrix}.$$

Now σ_y , neglect phase ambiguity and in addition set $\beta = 0$:

For the eigenvalue $+1$ we have

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}.$$

The eigenvector is $\begin{pmatrix} a \\ ia \end{pmatrix}$. Normalization gives $|a| = \frac{1}{\sqrt{2}}$.

Set all the phase angles to zero. This results into the following eigenvector:

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}.$$

For the eigenvalue -1 , the eigenvector is:

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}.$$

Exercise 10.3 A spin-1/2 particle and the probabilities of a measurement of S_z

Suppose that a spin-1/2 particle has a spin vector which lies in the $x - z$ plane, making an angle θ with the z - axis. Demonstrate that a measurement of S_z yields $\hbar/2$ with a probability $\cos^2(\frac{\theta}{2})$, and $-\hbar/2$ with probability $\sin^2(\frac{\theta}{2})$.

The spinor makes an angle θ with the z - axis.

I use the notation of section 10.5 and Eqs.(10.38), (10.45) and (10.46):

$$\chi = c_+ \chi_+ + c_- \chi_- ,$$

and

$$\chi = c_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_- \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}. \quad (\text{C.10.E.17})$$

Section 10.3: "A measurement of χ will then yield the result $+$ with probability c_+^2 ."

We have furthermore Eq.(10.55).

Bottom of page 135:

"In this case we can interpret $|c_+|^2$ as the probability that an observation of S_z will yield the result $+\hbar/2$ and $|c_-|^2$ as the probability that an observation of S_z will yield the result $-\hbar/2$."

Now we need to demonstrate $|c_+|^2 = \cos^2(\frac{\theta}{2})$ and consequently $|c_-|^2 = \sin^2(\frac{\theta}{2})$, Eq.(10.56).

So, with (C.10.E.17),

$$\chi = \cos\left(\frac{\theta}{2}\right) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sin\left(\frac{\theta}{2}\right) \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

With Eq. (10.16)

$$S_z \chi = \frac{\hbar}{2} \begin{pmatrix} \cos(\frac{\theta}{2}) \\ 0 \end{pmatrix} - \frac{\hbar}{2} \begin{pmatrix} 0 \\ \sin(\frac{\theta}{2}) \end{pmatrix}.$$

Hence a measurement of S_z gives $+\frac{\hbar}{2}$ with a probability of $\cos^2(\frac{\theta}{2})$ and $-\frac{\hbar}{2}$ with a probability of $\sin^2(\frac{\theta}{2})$.

Exercise 10.4 An electron spin-state: normalizing, values of S_z , S_x and S_y . Probabilities.

An electron is in the spin-state

$$\chi = A \begin{pmatrix} 1 - 2i \\ 2 \end{pmatrix} = A \begin{pmatrix} \sqrt{5}e^{-i\vartheta} \\ 2 \end{pmatrix},$$

in the Pauli representation, where $\tan \vartheta = 2$.

Determine the constant A by normalizing χ . If a measurement of S_z is made, what values will be obtained, and with what probabilities? What is the expectation value of S_z ? Repeat the calculations for S_x and S_y .

Normalization:

$$A^* A (1 + 2i \cdot 2) \begin{pmatrix} 1 - 2i \\ 2 \end{pmatrix} = 1.$$

Then

$$|A|^2 = \frac{1}{9}, \text{ and } |A| = \frac{1}{3}.$$

I choose arbitrarily the positive sign and neglect phase ambiguity.

A measurement of S_z :

$$\chi = \frac{1}{3} \begin{pmatrix} 1 - 2i \\ 2 \end{pmatrix} = c_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_- \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

We express χ in the normalized eigenstates of S_z , Eqs.(10.45) and (10.46),:

$$\chi = \frac{1}{3} \begin{pmatrix} 1 - 2i \\ 2 \end{pmatrix} = c_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_- \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Equate the elements of the column vectors:

$$c_+ = \frac{1}{3} (1 - 2i), \tag{C.10.E.18}$$

and

$$c_- = \frac{2}{3}. \tag{C.10.E.19}$$

Bottom of page 135:

"In this case we can interpret $|c_+|^2$ as the probability that an observation of S_z will yield the result $+\hbar/2$ and $|c_-|^2$ as the probability that an observation of S_z will yield the result $-\hbar/2$."

With (C.10.E.18):

$$|c_+|^2 = \frac{5}{9}, \text{ and}$$

$$|c_-|^2 = \frac{4}{9}.$$

The expectation value of S_z :

$$\langle S_z \rangle = \chi^\dagger S_z \chi.$$

For this expression we have all the ingredients derived:

$$\langle S_z \rangle = \frac{\hbar}{18} (1 + 2i \ 2) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 - 2i \\ 2 \end{pmatrix} = \frac{\hbar}{18}.$$

Next a measurement of S_x :

We express χ in the normalized eigenstates of S_x , see exercise 2,:

$$\chi = \frac{1}{3} \begin{pmatrix} 1 - 2i \\ 2 \end{pmatrix} = c_{x+} \chi_{x+} + c_{x-} \chi_{x-} = c_{x+} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} + c_{x-} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}. \quad (\text{C.10.E.20})$$

Now equate the elements of the column vectors:

$$c_{x+} = \frac{1}{3\sqrt{2}} (3 - 2i), \quad (\text{C.10.E.21})$$

and

$$c_{x-} = -\frac{1}{3\sqrt{2}} (1 + 2i). \quad (\text{C.10.E.22})$$

Bottom of page 135:

"In this case we can interpret $|c_{x+}|^2$ as the probability that an observation of S_x will yield the result $+\hbar/2$ and $|c_{x-}|^2$ as the probability that an observation of S_x will yield the result $-\hbar/2$."

Then with (C.10.E.21):

$$|c_{x+}|^2 = \frac{13}{18},$$

and with (C.10.E.22):

$$|c_{x-}|^2 = \frac{5}{18}.$$

Now something a little bit different. In section 10.5 and exercise 2, we also found, neglecting phase ambiguity, for the eigenstates of S_x :

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{e^{-i\beta}}{\sqrt{2}} \end{pmatrix} \text{ and } \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-e^{-i\beta}}{\sqrt{2}} \end{pmatrix}. \quad (\text{C.10.E.23})$$

Leaving out the detailed calculations, I obtain for the probabilities:

$$|c_{x+}|^2 = \frac{13}{18} - \frac{1}{9} \sin \beta, \quad (\text{C.10.E.24})$$

and

$$|c_{x-}|^2 = \frac{5}{18} + \frac{1}{9} \sin \beta. \quad (\text{C.10.E.25})$$

Do we need to conclude β to be zero?

The expectation value of S_x and $\beta = 0$:

$$\langle S_x \rangle = \chi^\dagger S_x \chi = \frac{\hbar}{18} (1 + 2i \ 2) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 - 2i \\ 2 \end{pmatrix} = \frac{2\hbar}{9}.$$

Next a measurement of S_y :

We express χ in the normalized eigenstates of S_y , see exercise 2,:

$$\chi = \frac{1}{3} \begin{pmatrix} 1 - 2i \\ 2 \end{pmatrix} = c_{y+} \chi_{y+} + c_{y-} \chi_{y-} = c_{y+} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} + c_{y-} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix}. \quad (\text{C.10.E.26})$$

Now equate the elements of the column vectors:

$$c_{y+} = \frac{1}{3\sqrt{2}}(1 - 4i), \quad (\text{C.10.E.27})$$

and

$$c_{y-} = \frac{\sqrt{2}}{6}. \quad (\text{C.10.E.28})$$

Bottom of page 135:

"In this case we can interpret $|c_{y+}|^2$ as the probability that an observation of S_y will yield the result $+\hbar/2$ and $|c_{y-}|^2$ as the probability that an observation of S_y will yield the result $-\hbar/2$."

Then with (C.10.E.27):

$$|c_{y+}|^2 = \frac{17}{18},$$

and with (C.10.E.28):

$$|c_{y-}|^2 = \frac{1}{18}.$$

The expectation value of S_y and $\beta = 0$:

$$\langle S_y \rangle = \chi^\dagger S_y \chi = \frac{\hbar}{18} (1 + 2i \ 2) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 - 2i \\ 2 \end{pmatrix} = \frac{4\hbar}{9}.$$

Now something a little bit different. In section 10.5 and exercise 2, we also found, neglecting phase ambiguity, for the eigenstates of S_y :

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{ie^{-i\beta}}{\sqrt{2}} \end{pmatrix} \text{ and } \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-ie^{-i\beta}}{\sqrt{2}} \end{pmatrix}.$$

Leaving out the detailed calculations, I obtain for the probabilities:

$$|c_{y+}|^2 = \frac{1}{18} (9 + 8 \cos \beta + 4 \sin \beta),$$

and

$$|c_{y-}|^2 = \frac{1}{18} (9 - 8 \cos \beta - 4 \sin \beta).$$

Do we need to conclude β to be zero? Well, for $\beta = 0$ we obtain $|c_{y+}|^2 = \frac{17}{18}$ and $|c_{y-}|^2 = \frac{1}{18}$.

Another question to be raised here is: $8 \cos \beta + 4 \sin \beta \geq 9$?

The maximum value of β is obtained by: $\frac{d}{d\beta} (8 \cos \beta + 4 \sin \beta) = 0$.

Then, $\sin \beta = \frac{1}{\sqrt{5}}$, and $\cos \beta = \frac{2}{\sqrt{5}}$. These values leads to:

$$8 < (8 \cos \beta + 4 \sin \beta) = 4\sqrt{5} < 9.$$

Just curious: is there a matrix operator of which $\begin{pmatrix} 1 - 2i \\ 2 \end{pmatrix}$ is an eigenvector?

Obviously, the unit matrix is one. Alas, a trivial one.

Exercise 10.5 a spin-1/2 system represented by a normalized spinor. Probability of S_y

Consider a spin-1/2 system represented by the normalized spinor

$$\chi = \begin{pmatrix} \cos \alpha \\ \sin \alpha \exp(i\delta) \end{pmatrix},$$

in the Pauli representation where α and δ are real. For reasons I will show below δ instead of β has been used.

What is the probability that a measurement of S_y yields $-\hbar/2$?

We express χ in the normalized eigenstates of S_y , see exercise 2,:

$$\chi = \begin{pmatrix} \cos \alpha \\ \sin \alpha \exp(i\delta) \end{pmatrix} = c_{y+}\chi_{y+} + c_{y-}\chi_{y-} = c_{y+} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} + c_{y-} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix}. \quad (\text{C.10.E.29})$$

Now equate the elements of the column vectors:

$$c_{y+} = \frac{1}{\sqrt{2}} (\cos \alpha - \sin \alpha e^{i(\delta+\frac{\pi}{2})}), \quad (\text{C.10E.30})$$

and

$$c_{y-} = \frac{1}{\sqrt{2}} (\cos \alpha + \sin \alpha e^{i(\delta+\frac{\pi}{2})}). \quad (\text{C.10.E.31})$$

Bottom of page 135:

"In this case we can interpret $|c_{y+}|^2$ as the probability that an observation of S_y will yield the result $+\hbar/2$ and $|c_{y-}|^2$ as the probability that an observation of S_y will yield the result $-\hbar/2$."

With (C.10.E.31):

$$|c_{y-}|^2 = 1 - \sin 2\alpha \sin \delta. \quad (\text{C.10.E.32})$$

Now I like to remind the discussion of exercise 4 and imply the eigenstates presented in (C.10.E.24). Leaving out the detailed calculations we find for $|c_{y-}|^2$:

$$|c_{y-}|^2 = 1 - \sin 2\alpha \sin(\delta + \beta).$$

The question remains: does it matter setting $\beta = 0$?

Exercise 10.6 An electron at rest in an oscillating magnetic field.

An electron is at rest in an oscillating magnetic field

$$\mathbf{B} = B_0 \cos(\omega t) \mathbf{e}_z,$$

where B_0 and ω are real positive constants.

I present here the results of the exercise 5.7 of Chapter 5 on Spin Angular Momentum of *The Graduate Course*, Fitzpatrick. The numbers for the expressions and equations are from my notes on *The Graduate Course*.

(a) Find the Hamiltonian of the system.

The Hamiltonian is given by Eqs.(10.61) and (10.62), *The Undergraduate Course* Ch. 10,

$$H = \Omega S_z, \quad (10.61),$$

and

$$\Omega = \frac{geB_0 \cos(\omega t)}{2m_e} = \Omega_0 \cos(\omega t). \quad (\text{C.5.E.43})$$

Note: Section 5.6 on Spin Precession is about a static magnetic field: $\omega = 0$ in (C.5.E.43).

The same applies for section 10.6 on Spin Precession, *The Undergraduate Course*, Fp.

(b) If the electron starts in the spin-up state with respect to the x -axis, determine the spinor $\chi(t)$ that represents the state of the system in the Pauli representation at all subsequent times." the electron starts in the spin-up state with respect to the x -axis". I suppose the spin state to be: χ_{x+} at $t = 0$.

$$\chi_{x+} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix},$$

Exercise 2, above or Exercise 5.3 (C.5.E.16) of *The Graduate Course*.

I left out the phase ambiguity.

Schrödinger's equation

$$i\hbar \frac{\partial \chi}{\partial t} = H\chi \quad (\text{C.5.E.44})$$

The state vector in Pauli representation

$$\chi = \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix}. \quad (\text{C.5.E.45}).$$

Plug this state vector in to (C.5.E.44), (10.65) *The Under Graduate Course*:

$$\frac{dc_{\pm}}{dt} = \mp i \frac{\Omega}{2} c_{\pm}, \quad (\text{C.5.E.46})$$

where Ω is given in (C.5.E.43), a function of time.

The solutions for both differential equations, (C.5.E.46), are

$$c_+(t) = c_+(0) \exp[-i \frac{\Omega_0}{2\omega} \sin(\omega t)], \quad (\text{C.5.E.47})$$

and

$$c_-(t) = c_-(0) \exp[i \frac{\Omega_0}{2\omega} \sin(\omega t)]. \quad (\text{C.5.E.48})$$

For $t = 0$, the electron starts in the spin-up state with respect to the x -axis.

The state vector at $t = 0$, (C.5.E.16) and (C.5.E.45)

$$\chi(t=0) = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} c_+(0) \\ c_-(0) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (\text{C.5.E.49})$$

Then,

$$c_+(t) = \frac{1}{\sqrt{2}} \exp[-i \frac{\Omega_0}{2\omega} \sin(\omega t)], \quad (\text{C.5.E.50})$$

and

$$c_-(t) = \frac{1}{\sqrt{2}} \exp[i \frac{\Omega_0}{2\omega} \sin(\omega t)]. \quad (\text{C.5.E.51})$$

- Find the probability that a measurement of S_x yields the result $-\hbar/2$.

To this end I express the state vector $\chi(t)$

$$\chi(t) = \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix} = c_{x+} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} + c_{x-} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}. \quad (\text{C.5.E.52})$$

Hence, with (C.5.E.50) and (C.5.E.51),

$$c_{x+} = \cos[\frac{\Omega_0}{2\omega} \sin(\omega t)], \quad (\text{C.5.E.53})$$

and

$$c_{x-} = -i \sin[\frac{\Omega_0}{2\omega} \sin(\omega t)]. \quad (\text{C.5.E.54})$$

The probability

$$|c_{x-}|^2 = \sin^2[\frac{\Omega_0}{2\omega} \sin(\omega t)]. \quad (\text{C.5.E.55})$$

- What is the minimum value of B_0 to force a complete flip in S_x .

“...a complete flip in S_x ”, meaning?

Let's find out about the expectation value of S_x .

$$\langle S_x \rangle = ((c_+(t))^*, (c_-(t))^*) \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix}. \quad (\text{C.5.E.56})$$

With (C.5.E.50) and (C.5.E.51):

$$\langle S_x \rangle = \frac{\hbar}{2} \cos\left[\frac{\Omega_0}{\omega} \sin(\omega t)\right]. \quad (\text{C.5.E.57})$$

Then, rewrite (C.5.E.55) with (C.5.E.57)

$$|c_{x-}|^2 = \frac{1}{2} \left(1 - \frac{2}{\hbar} \langle S_x \rangle\right). \quad (\text{C.5.E.58})$$

Let's analyse $|c_{x-}|^2$ given by ((C.5.E.55)).

I suppose a complete flip to mean a probability of 1 to be in the spin-down state with respect to the x -axis. So,

$$|c_{x-}|^2 = 1.$$

Since,

$$-1 \leq \sin(\omega t) \leq 1,$$

I find for the minimum value of

$$\frac{\Omega_0}{2\omega} \geq \frac{\pi}{2}.$$

With (C.5.E.43):

$$\frac{geB_0}{2m_e} = \Omega_0 \rightarrow B_0 = \frac{2m_e\Omega_0}{ge},$$

it follows from $\frac{\Omega_0}{2\omega} \geq \frac{\pi}{2}$

$$B_0 \geq \frac{2m_e\pi\omega}{ge}.$$

11 Addition of Angular Momentum

11.1 Introduction

The question to be answered in this chapter is: what is the total angular momentum of an electron possesses both orbital and spin angular momentum?

11.2 General principles

The three orbital and spin angular momentum operators are presented.

In Eq.(11.4) the electron's total angular momentum vector is presented. In Chapter 8 we learned the orbital angular momentum operator to be represented by differential quotients. So, what possibly could the orbital angular momentum operator could look like? In Chapter 10 we learned about the spin angular momentum operator to be a 2×2 matrix. What possibly the vector \mathbf{S} could be? Something like;

$$\mathbf{S} = S_x \mathbf{n}_x + S_y \mathbf{n}_y + S_z \mathbf{n}_z \text{ ?(Susskind). What about } \mathbf{L} \text{ ?}$$

Eq.(11.5) is found using Eq.(11.3) :

$$\mathbf{L} \times \mathbf{S} = 0.$$

Eq.(11.12) is found using the definitions of the raising and lowering operators and Eq.(11.3).

Then:

$$L_+ S_- + L_- S_+ = 2L_x S_x + 2L_y S_y ,$$

and

$$2\mathbf{L} \cdot \mathbf{S} = 2L_x S_x + 2L_y S_y + 2L_z S_z \rightarrow 2L_z S_z + L_+ S_- + L_- S_+.$$

Page 142, just below Eq.(11.12):

“.....(and, hence with the raising and lowering operators L_{\pm}),....”.

With $[L^2, L_i] = 0$:

$$[L^2, L_x] + i[L^2, L_y] = 0.$$

Then,

$$L^2(L_x + iL_y) - (L_x + iL_y)L^2 = 0,$$

hence $[L^2, L_+] = 0$, QED, etc.

Electron's orbital angular momentum and the spin angular momentum are unrelated.

Consequently, L^2 commute with all the spin angular momentum operators. So, Eq.(11.13) is obtained. An example:

$$[L_z S_z, L^2] = 0 ?$$

Since $[L_z, S_z] = 0$: $L_z S_z = S_z L_z$,

and $[L^2, L_z] = 0$: $L^2 L_z = L_z L^2$.

With this result we can write for $[L_z S_z, L^2]$:

$$[L_z S_z, L^2] = L_z S_z L^2 - L^2 L_z S_z = L_z S_z L^2 - L_z L^2 S_z = L_z [S_z, L^2] = 0, \text{etc.}$$

Eq.(11.15) follows from Eqs.(8.18) and (8.19).

Eq.(11.16) follows from Eqs.(10.10) and (10.11).

On top of page 143 Fp summarizes the physical quantities which can be simultaneously measured. These are represented in the Eqs.(11.18)-(11.27).

11.3 Angular momentum in the Hydrogen Atom.

The eigenstate of the hydrogen atom can be written in a separable form: Eq.(11.28).

The eigenstates for the angular momentum are represented by Eq.(11.29). The subscripts of Eq.(11.29) indicate, with Eq.(11.23):

$m_j = m + \frac{1}{2}$. This can be obtained in two ways for given values of m_j, m and the two values of m_s :

$$m_j = m + m_s = m + \frac{1}{2},$$

and

$$m_j = m + 1 + m_s = m + 1 - \frac{1}{2} = m + \frac{1}{2}.$$

This explained just below Eq.(11.29).

The general formulation for $\psi^{(2)} : \psi_{l,s;j,m_j}^{(2)}$.

The superscripts in (11.28) and (11.29) indicates the two sets of operators in (11.18)-(11.21) and (11.24)-(11.27). These two sets have two operators in common and consequently the eigenfunction of the first two operators of the second set can be expressed into the eigenfunctions of the first set.

Furthermore, my preferred alternative for (11.29) is :

$$\psi_{l,s;j,m_j}^{(2)} = \alpha \psi_{l,s;m_l,m_s}^{(1)} + \beta \psi_{l,s;m_j+m_s,-m_s}^{(1)} \quad (\text{C.11.E.0})$$

Caveat: for $m + 1$ we have for m : $-l \leq m < l$.

Eqs.(11.42) and (11.43) are found by equating the coefficients of $Y_{l,m}\chi_+$ and $Y_{l,m+1}\chi_-$ respectively.

Without subscripts for ψ , using Eqs.(11.28) and (11.29),:

$$J^2\psi = J^2(\alpha Y_{l,m}\chi_+ + \beta Y_{l,m+1}\chi_-).$$

Then, with Eq.(11.9),:

$$J^2\psi = j(j+1)\hbar^2\alpha Y_{l,m}\chi_+ + j(j+1)\hbar^2\beta Y_{l,m+1}\chi_- \quad (\text{C.11.E.1})$$

With Eqs.(11.40) and (11.41):

$$J^2\psi = \alpha \left[l(l+1) + \frac{3}{4} + m \right] \hbar^2 Y_{l,m}\chi_+ + \alpha [l(l+1) - m(m+1)]^{1/2} \hbar^2 Y_{l,m+1}\chi_- + \beta \left[l(l+1) + \frac{3}{4} - m - 1 \right] \hbar^2 Y_{l,m+1}\chi_- + \beta [l(l+1) - m(m+1)]^{1/2} \hbar^2 Y_{l,m}\chi_+ \quad (\text{C.11.E.2})$$

Now, equating the coefficients of $Y_{l,m}\chi_+$ and $Y_{l,m+1}\chi_-$ of (C.11.E.1) and (C.11.E.2) we obtain Eqs.(11.42) and (11.43).

In Eqs.(11.42) and (11.43):

$$[l(l+1) - m(m+1)]^{1/2} = [(l-m)(l+m+1)]^{1/2}.$$

From Eq.(11.42), Eq.(11.46) has been derived and Eq.(11.43) can be written as:

$$[(l-m)(l+m+1)]^{1/2} \frac{\alpha}{\beta} = x + m + 1 \quad (\text{C.11.E.3})$$

Then with Eq.(11.46)

$$[(l-m)(l+m+1)]^{1/2} \frac{\alpha}{\beta} = \frac{(l-m)(l+m+1)}{x-m} \quad (\text{C.11.E.4})$$

Equating the right hand side of (C.11.E.3) and (C.11.E.4) respectively, we have Eq.(11.45):

$$x(x+1) = l(l+1).$$

Then x ;

$x = -\frac{1}{2} \pm (l + \frac{1}{2})$. Plug this result into Eq.(11.44) and two values for j are found, as given at the bottom of page 145: $j = l + 1/2$ or $j = l - 1/2$.

In Eq.(11.47) α and β are chosen to be positive. The negative values could have been chosen.

The difference is phase ambiguity: $e^{i\pi}$.

In Eq.(11.48) α and β are of the opposite sign, α positive and β negative. We could have chosen it to be the other way around. The difference is again phase ambiguity: $e^{i\pi}$.

The coefficients α and β are presented in Table 11.1 for the various quantum numbers.

On page 146, Fp considered the states of an hydrogen atom for $l = 1$.

Let's start with Eq.(11.51).

$j = l + \frac{1}{2} = \frac{3}{2}$, and $m_j = m + m_s = \frac{3}{2}$. Now there are two possibilities: $m_s = \frac{1}{2}$ and $m_s = -\frac{1}{2}$.

What is the correct value? With $m_s = \frac{1}{2}$, we have $m = 1$. This result gives us with Eq.(11.47) :

$$\alpha = 1 \text{ and } \beta = 0.$$

The other value $m_s = -\frac{1}{2}$, leads to $m = 2$. We learned this to be impossible since $-l \leq m \leq l$.

Next

$j = l + \frac{1}{2} = \frac{3}{2}$, and $m_j = m + m_s = -\frac{3}{2}$. There are two possibilities: $m_s = \frac{1}{2}$ and $m_s = -\frac{1}{2}$.

With $m_s = \frac{1}{2}$, we have $m = -2$. Again, this is impossible. For $m_s = -\frac{1}{2}$, $m = -1$. Plug these values into the scheme presented in Table 11.1 and we have:

$\alpha = \sqrt{\frac{1}{3}}$ and $\beta = \sqrt{\frac{2}{3}}$. As you notice, this differs from the result presented in Table 11.2. Now

what to do? Let's investigate the amplitudes for the values of m making the amplitudes 1 or 0.

So,

$\sqrt{\frac{l+m+1}{2l+1}} = 1$: with $l = 1$, $m = 1$. This represent the state $j = l + \frac{1}{2} = \frac{3}{2}$, and $m_j = \frac{3}{2}$. The

state bottom right in Table 11.2 with amplitude 1.

$\sqrt{\frac{l+m+1}{2l+1}} = 0$: with $l = 1$, $m = -2$. This represent the (impossible?) state $j = \frac{3}{2}$, and $m_j = -\frac{3}{2}$.

This m is out of the range $-l \leq m \leq l$.

$\sqrt{\frac{l-m}{2l+1}} = 1$: with $l = 1$, $m = -2$. This represent the (impossible?) state $j = \frac{3}{2}$, and $m_j = -\frac{3}{2}$.

Well, now $m + 1 = -1$ is in the range $-l \leq -1 \leq l$. The state with amplitude 1 top left in Table 11.2.

$\sqrt{\frac{l-m}{2l+1}} = 0$: with $l = 1$, $m = 1$. This represent the state $j = l + \frac{1}{2} = \frac{3}{2}$, and $m_j = \frac{3}{2}$. The state

bottom right in Table 11.2.

With Eq.(11.52).

$j = l + \frac{1}{2} = \frac{3}{2}$, and $m_j = m + m_s = \frac{1}{2}$. There are two possibilities: $m_s = \frac{1}{2}$ and $m_s = -\frac{1}{2}$.

This results into $m = 0$ and $m + 1 = 1$ respectively. Giving the amplitudes:

$\alpha = \sqrt{\frac{2}{3}}$ and $\beta = \sqrt{\frac{1}{3}}$.

And so on.

In Table 11.2 Fp collected all the possible amplitude.

I prefer the following correction for this table, trading places of the states $3/2, 1/2$ and $1/2, 1/2$.

As presented in the table below.

1					
	$\sqrt{1/3}$	$\sqrt{2/3}$			

	$\sqrt{2/3}$	$-\sqrt{1/3}$			
			$\sqrt{1/3}$	$-\sqrt{2/3}$	
			$\sqrt{2/3}$	$\sqrt{1/3}$	
					1

Table 11.2 Revised.

There remains the problem of the impossible state $m = -2$. Unless the state is basically $m + 1$. However, this looks like a trick.

Remark :

We have for $m : -l \leq m \leq l$.

Consequently, in Eq.(11.29) $\psi_{l, \frac{1}{2}; m+1, -\frac{1}{2}}^{(1)}$ does not exist for $l = 0$.

Now, just above Eq.(11.29) Fp writes : “For instance ..”.

So, we could have chosen:

$$\psi_{l, \frac{1}{2}; j, m-\frac{1}{2}}^{(2)} = \alpha \psi_{l, \frac{1}{2}; m, -\frac{1}{2}}^{(1)} + \beta \psi_{l, \frac{1}{2}; m-1, \frac{1}{2}}^{(1)} = \alpha Y_{l,m} \chi_- + \beta Y_{l,m-1} \chi_+ .$$

Consequently in the wavefunction $\psi_{l, \frac{1}{2}; m-1, \frac{1}{2}}^{(1)}$ does not exist for $l = 0$.

We can do the analysis of section 11.3 for $\psi_{l, \frac{1}{2}; j, m-\frac{1}{2}}^{(2)}$. I will show some results:

$$J^2 Y_{l,m} \chi_- = \left[l(l+1) + \frac{3}{4} - m \right] \hbar^2 Y_{l,m} \chi_- + [l(l+1) - m(m-1)]^{1/2} \hbar^2 Y_{l,m-1} \chi_+ .$$

$$J^2 Y_{l,m-1} \chi_+ = \left[l(l+1) + \frac{3}{4} + m - 1 \right] \hbar^2 Y_{l,m-1} \chi_+ + [l(l+1) - m(m-1)]^{1/2} \hbar^2 Y_{l,m} \chi_- .$$

$$J^2 \psi_{l, \frac{1}{2}; j, m-\frac{1}{2}}^{(2)} = j(j+1) \hbar^2 (\alpha Y_{l,m} \chi_- + \beta Y_{l,m-1} \chi_+) .$$

Collecting the coefficients of $Y_{l,m} \chi_-$ and $Y_{l,m-1} \chi_+$, using Eq.(11.44), we obtain

$$x(x+1) = l(l+1) , \text{ Eq.(11.45),}$$

and

$$\frac{\alpha}{\beta} = \frac{(l+m)^{1/2}(l-m+1)^{1/2}}{x+m} .$$

$$\text{Again } x = l \rightarrow j = l + \frac{1}{2},$$

$$\text{or } x = -l - 1 \rightarrow j = l - \frac{1}{2} .$$

Now we can calculate α and β .

$$\text{For } x = l \rightarrow j = l + \frac{1}{2} :$$

$$\alpha = \left(\frac{l-m+1}{2l+1} \right)^{1/2} \text{ and } \beta = \left(\frac{l+m}{2l+1} \right)^{1/2} .$$

$$\text{For } x = -l - 1 \rightarrow j = l - \frac{1}{2} :$$

$$\alpha = \left(\frac{l+m}{2l+1} \right)^{1/2} \text{ and } \beta = - \left(\frac{l-m+1}{2l+1} \right)^{1/2} .$$

These results differ from the results in Eqs.(11.47) and (11.48). Does it matter? Yes, it does. We

analysed a different state: $\psi_{l, \frac{1}{2}, j, m-\frac{1}{2}}^{(2)}$. Fp did not mention this state. This state is one of the two for spin $\frac{1}{2}$: $\psi_{l, s; j, m_j}^{(2)}$. Or does this state not exist? Well, it does:

$$-l \leq m \leq l,$$

so, there is not really a difference except for the minus sign of $\beta = -(\frac{l-m+1}{2l+1})^{1/2}$. This indicates phase ambiguity. I come to this later in Section 12.8.

The French saying came to my mind: “Reculer pour mieux Sauter.”

11.4 Two Spin One-Half Particles

Now we will analyse two spin one-half particles without orbital momentum. Here the analogy with section 11.3 is used.

For the top left amplitude in Table 11.3, page 149 (Fp):

$$m_{s_1} + 1 = -\frac{3}{2} + 1 = -\frac{1}{2}, \text{ see Table 11.1, page 146 (Fp).}$$

Then, with $s = \frac{1}{2}$:

$$\sqrt{\frac{s - (-\frac{3}{2})}{2s+1}} = 1 \text{ and } \sqrt{\frac{s - (\frac{3}{2}) + 1}{2s+1}} = 0.$$

The analogy: $l \rightarrow s$ and $m \rightarrow m_{s_1}$.

In this section the triplet and singlet states are introduced. Susskind presented these states in his Lecture on Entanglement.

Here I will present the states as can be found in Fitzpatrick section 11.4 and in Susskind's Lecture 6.7. I will use the Pauli representation:

Table of singlet state and triplet states:

States	Susskind	Fitzpatrick	number
Singlet	$\frac{1}{\sqrt{2}} [\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}]$	$\frac{1}{\sqrt{2}} [\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}]$	1
Triplet	$\frac{1}{\sqrt{2}} [\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}]$	$\frac{1}{\sqrt{2}} [\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}]$	2
Triplet	$\frac{1}{\sqrt{2}} [\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}]$	$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$	3
Triplet	$\frac{1}{\sqrt{2}} [\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}]$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$	4

In the Table above, numbers 3 and 4, as given by Fitzpatrick, can be constructed by adding and subtracting respectively 3 and 4 given by Susskind. Fp gives the simplest set of eigenstates. Clebsch-Gordon coefficients are not mentioned by Susskind. Well, it is about the theoretical minimum.

In Mahan, Chapter 4 the results of Fp are derived using the Dirac notation with bra's and kets.

Exercises.

Exercise 11.1 . An electron in a hydrogen atom occupies the combined spin(angular and spin) and position state.

The wave function:

$$\psi = R_{2,1} \left(\sqrt{\frac{1}{3}} Y_{1,0} \chi_+ + \sqrt{\frac{2}{3}} Y_{1,1} \chi_- \right). \quad (\text{C.11.E.5})$$

$n = 2, l = 1$ and $m = 0, 1$.

$n > l \geq m_j$, and $m_j = m + m_s$

(a) What values would a measurement of L^2 yield, and with what probabilities?

With Eq.(8.32), $m = 0$:

$$L^2 Y_{1,0} = l(l+1) \hbar^2 Y_{1,0} = 2 \hbar^2 Y_{1,0} ,$$

and

$$L^2 Y_{1,m+1} = l(l+1) \hbar^2 Y_{1,1} = 2 \hbar^2 Y_{1,1} .$$

A measurement of L^2 yield $2 \hbar^2$ with probability 1/3 and $2 \hbar^2$ with probability 2/3.

So $2 \hbar^2$ is measured with a probability 1.

(b) What values would a measurement of L_z yield, and with what probabilities?

With Eq.(8.31) :

$$L_z Y_{1,0} = m \hbar Y_{1,0} = 0 \text{ with probability } 1/3,$$

$$L_z Y_{1,1} = (m+1) \hbar Y_{1,1} = \hbar .$$

And a measurement of L_z yields \hbar with probability 2/3.

(c) What values would a measurement of S^2 yield, and with what probabilities?

With Eqs.(10.17) and (10.35):

$$S^2 \chi_{\pm} = s(s+1) \hbar^2 \chi_{\pm} = \frac{3}{4} \hbar^2 \chi_{\pm} .$$

A measurement of S^2 yield $\frac{3}{4} \hbar^2$ with probability 1/3 and $\frac{3}{4} \hbar^2$ with probability 2/3.

So $\frac{3}{4} \hbar^2$ is measured with a probability 1.

(d) What values would a measurement of S_z yield, and with what probabilities?

With Eqs.(10.16) and (10.35):

$$S_z \chi_{\pm} = \pm \frac{1}{2} \hbar \chi_{\pm} .$$

A measurement of S_z yield $\frac{1}{2} \hbar$ with probability 1/3 and $-\frac{1}{2} \hbar$ with probability 2/3.

(e) What values would a measurement of J^2 yield, and with what probabilities?

With Eq.(11.26):

$$J^2 \psi = j(j+1) \hbar^2 \psi .$$

For the hydrogen atom we have $j = l + s$.

$$|l - s| \leq j \leq l + s$$

So, with $j = \frac{3}{2}$

$$J^2 \psi = j(j+1) \hbar^2 \psi = \frac{15}{4} \hbar^2 \psi ,$$

or, with $j = \frac{1}{2}$

$$J^2 \psi = j(j+1)\hbar^2 \psi = \frac{3}{4}\hbar^2 \psi$$

A measurement of J^2 yields $\frac{15}{4}\hbar^2$ with probability 2/3 and $\frac{3}{4}\hbar^2$ with probability 1/3.

(f) What values would a measurement of J_z yield, and with what probabilities?

With Eq.(11.8):

$$J_z \psi = m_j \hbar \psi ,$$

and

$$m_j = m + m_s$$

$$m_j = \frac{1}{2} \text{ and } m_j = 1$$

Then : $m = 0$, $m_s = \frac{1}{2}$, and $m = 1$, $m_s = -\frac{1}{2}$.

A measurement of J_z yield $\frac{1}{2}\hbar$ with probability 1/3 and $\frac{1}{2}\hbar$ with probability 2/3.

So, $\frac{1}{2}\hbar$ is measured with a probability 1.

(g) What is the probability density for finding the electron at r, θ, ϕ ?

The probability density : $|\psi|^2$.

With (C.11.E.6) :

$$|\psi|^2 = |R_{2,1}|^2 \left(\frac{1}{3} |Y_{1,0}|^2 |\chi_+|^2 + \frac{2}{3} |Y_{1,1}|^2 |\chi_-|^2 - \frac{2}{3} Y_{1,0}^* Y_{1,1} \chi_+^* \chi_- - \frac{2}{3} Y_{1,1}^* Y_{1,0} \chi_-^* \chi_+ \right) . \quad (\text{C.11.E.7})$$

Using normalization and orthogonalization (C.11.E.7) becomes:

$$|\psi|^2 = |R_{2,1}|^2 \left(\frac{1}{3} |Y_{1,0}|^2 + \frac{2}{3} |Y_{1,1}|^2 \right) . \quad (\text{C.11.E.8})$$

Now plug the expression for the spherical harmonics, Eqs. (8.92) and (8.91), into (C.11.E.8), then we have:

$|\psi|^2 = |R_{2,1}|^2$. Finally, this expression can be written with Eq.(9.67) as:

$$|\psi|^2 = \frac{1}{96\pi a_0^3} \left(\frac{r}{a_0} \right)^2 e^{-r/a_0} . \quad (\text{C.11.E.9})$$

As we see, the probability density does not depend on θ, ϕ . Explanation?

(h) What is the probability density for finding the electron in the spin up state (with respect to the z-axis) at radius r ?

Well, how to understand with respect the z-axis : $\theta = 0$.

In that case we have to evaluate: $|R_{2,1}|^2 \left(\frac{1}{3} |Y_{1,0}|^2 |\chi_+|^2 \right)$ given $Y_{1,0} = \sqrt{\frac{3}{4\pi}}$.

This results into the expression given in (C.11.E.9). A surprise?

Exercise 11.2 The Potential Energy of a Proton-Neutron System

In a low energy neutron-proton system (with zero orbital angular momentum) the potential energy is given by:

$$V(r) = V_1(r) + V_2(r) \left(3 \frac{(\sigma_1 \cdot r)(\sigma_1 \cdot r)}{r^2} - \sigma_1 \cdot \sigma_2 \right) + V_3(r) \sigma_1 \cdot \sigma_2 , \quad (\text{C.11.E.10})$$

where σ_1 denotes the vector of the Pauli matrices of the neutron, and σ_2 denotes the vector of the Pauli matrices of the proton.

Calculate the potential energy for the neutron-proton system:

(a) in the spin singlet state.

(b) in the spin triplet state.

(C.11.E.10) represents a special potential energy. I have not seen such one before. Well, section 12.10 on the hyperfine structure shows an example, partially, of such a potential energy.

I need to obtain: $\langle V(r) \rangle$

The vector of the Pauli matrices reads:

$$\sigma = (\sigma_x, \sigma_y, \sigma_z).$$

Consequently, the inner product of the matrices is:

$$\sigma_1 \cdot \sigma_2 = \sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}. \quad (\text{C.11.E.11})$$

When we operate $\sigma_1 \cdot \sigma_2$ on the singlet state and the triplet state respectively, what will be the result?

ad (a), let us start with the singlet state:

$$\frac{1}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right].$$

With (C.11.E.11), the eigenvalues of the product operator $\sigma_1 \cdot \sigma_2$:

$$(\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}) \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right].$$

σ_{1x} operates on the first column vector between square brackets. σ_{2x} on the second of the product of the two column vectors, etc. With the Eqs. (10.52)-(10.54), the result is:

$$(\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}) \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] = -\frac{3}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right].$$

Hence, the singlet state is an eigenvector of $\sigma_1 \cdot \sigma_2$. The eigenvalue is -3 .

Now with the triplet state. I choose one, number 2 in the Table above on page 104 (my notes):

$$(\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}) \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right].$$

With the Eqs. (10.52)-(10.54), the result is:

$$(\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}) \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] = (1 + 1 - 1) \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right].$$

Hence, the triplet state is an eigenvector of $\sigma_1 \cdot \sigma_2$. The eigenvalue is 1.

What about $\langle \frac{(\sigma_1 \cdot r)(\sigma_1 \cdot r)}{r^2} \rangle$?

$$\sigma_1 \cdot r = \sigma_{1x}x + \sigma_{1y}y + \sigma_{1z}z. \quad (\text{C.11.E.12})$$

So,

$$(\sigma_1 \cdot r)(\sigma_2 \cdot r) = (\sigma_{1x}x + \sigma_{1y}y + \sigma_{1z}z)(\sigma_{2x}x + \sigma_{2y}y + \sigma_{2z}z). \quad (\text{C.11.E.13})$$

Now calculate $\langle V(r) \rangle$.

ad (a) The spin singlet state as given by Eq.(11.75).

Hence, in general we have to find out about, with Eq.(10.15),:

$$\chi^\dagger V(r) \chi.$$

Now:

$$\chi = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right], \chi^\dagger = \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right]^\dagger,$$

and $V(r)$ is given by (C.11.E.10).

We already calculated:

$$(\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}) \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] = -\frac{3}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right].$$

So, the easy part of the job:

$$\langle V_1 \rangle = \chi^\dagger V_1 \chi = V_1,$$

and,

$$(-V_2 + V_3) \sigma_1 \cdot \sigma_2 \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] = -(-V_2 + V_3) \frac{3}{\sqrt{2}} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right].$$

For the expectation value of the easy part we find:

$$-3(-V_2 + V_3) + V_1. \quad (\text{C.11.E.14})$$

To obtain:

$$\langle V_2(r) \left(3 \frac{(\sigma_1 \cdot r)(\sigma_1 \cdot r)}{r^2} \right) \rangle,$$

we must operate (C.11.E.13) on the singlet state. Instead of 3, we have to find the result of 9 operators given in (C.11.E.13) in order to calculate the additional part of the expectation value.

We start, neglecting for the time being $\frac{3V_2}{\sqrt{2}\sqrt{2}r^2}$, with:

$$\left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right]^\dagger (\sigma_{1x}x + \sigma_{1y}y + \sigma_{1z}z)(\sigma_{2x}x + \sigma_{2y}y + \sigma_{2z}z) \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right]. \quad (\text{C.11.E.15})$$

It's not difficult, but asks for carefully bookkeeping. The above expression results into,

$$-2(x^2 + y^2 + z^2).$$

Combining this result with (C.11.E.14) gives us for the expectation value, including the factor

$$\frac{3V_2}{\sqrt{2}\sqrt{2}r^2}, \text{ with (C.11.E.15), } -3V_2:$$

$$\langle V(r) \rangle = V_1 - 3V_3.$$

Hence V_2 does not contribute.

ad(b) I choose the spin triplet state as given by Eq.(11.74), number 3 in the Table given above(The Pauli representation):

$$\chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \chi^\dagger = \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right]^\dagger.$$

Again we have to calculate

$$\chi^\dagger V(r) \chi.$$

I start with, what I called the easy part of the job:

$$\langle V_1 \rangle = V_1,$$

and

$$(-V_2 + V_3) \chi^\dagger \sigma_1 \cdot \sigma_2 \chi.$$

Then

$$(-V_2 + V_3) \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right]^\dagger (\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = (-V_2 + V_3). \quad (\text{C.11.E.16})$$

So for the easy part of the job we find:

$$V_1 - V_2 + V_3 . \quad (\text{C.11.E.17})$$

In addition we have to calculate:

$$[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}]^\dagger (\sigma_{1x}x + \sigma_{1y}y + \sigma_{1z}z)(\sigma_{2x}x + \sigma_{2y}y + \sigma_{2z}z) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad (\text{C.11.E.18})$$

where I neglected $\frac{3V_2}{r^2}$ in (C.11.E.18).

The result of (C.11.E.18) is, $\frac{3V_2}{r^2}$ included,

$$3V_2 \frac{z^2}{r^2} . \quad (\text{C.11.E.19})$$

The expectation value of the potential energy for the triplet $\chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is, combining (C.11.E.17) and (C.11.E.19):

$$\langle V(r) \rangle = V_1 - V_2(1 - \frac{3z^2}{r^2}) + V_3 .$$

Exercise 11.3 Two Electrons in a Spin Singlet State

- If a measurement of the spin of one of the electrons shows that it is in the state with $S_z = \hbar/2$, what is the probability that a measurement of the z -component of the spin of the other electron yields $S_z = \hbar/2$?
- If a measurement of the spin of one of the electrons shows that it is in the state with $S_y = \hbar/2$, what is the probability that a measurement of the x -component of the spin of the other electron yields $S_x = -\hbar/2$?

Finally, if electron 1 is in a spin state described by $\psi_1 = \cos \alpha_1 \chi_+ + \sin \alpha_1 e^{i\beta_1} \chi_-$, and electron 2 is in a spin state described by $\psi_2 = \cos \alpha_2 \chi_+ + \sin \alpha_2 e^{i\beta_2} \chi_-$, what is the probability that the two-electron spin state is a triplet state?

The states are normalized. The normalization produces no additional information on α_i and β_i . What about orthogonality?

We have $\psi_1^* \psi_2 = 0$ or $\psi_2^* \psi_1 = 0$. This gives us two expressions resulting into:

$$\beta_1 = \beta_2 + n\pi, \text{ where } n \in \mathbb{N} .$$

The singlet state:

$$\psi = \frac{1}{\sqrt{2}}(\chi_- \chi_+ - \chi_+ \chi_-) . \quad (\text{C.11.E.20})$$

ad.a) Remark: Here I think with S_z , Fp meant S_{1z} or S_{2z} .

Intermezzo singlet state.

Susskind: a singlet state is a maximally entangled state (page 167).

- An entangle state is a complete description of the combined system. No more can be known about it.

- In a maximally entangled state, nothing is known about the individual subsystem.

End of intermezzo.

Conclusion? Can we perform a measurement on one electron?

Well, I suppose we can. The other electron can, in general be, in a state + or – . However, when one of the electrons is in state + leads to the conclusion, intuitively, for the other electron to be in the state – . It is about Pauli's exclusion principle. Consequently, the probability of $S_z = \hbar/2$ is 0. However, is there more to be said?

First we calculate the expectation value $\langle S_{1z} \rangle$ and with Eqs.(10.45)-(10.47) and (10.54) we have:

$$S_{1z} \frac{1}{\sqrt{2}} (\chi_- \chi_+ - \chi_+ \chi_-) = -\frac{\hbar}{2\sqrt{2}} (\chi_- \chi_+ + \chi_+ \chi_-), \text{ a triplet.}$$

Then

$$\langle S_{1z} \rangle = \psi^* S_{1z} \psi = -\left[\frac{1}{\sqrt{2}} (\chi_- \chi_+ - \chi_+ \chi_-) \right]^* \frac{\hbar}{2\sqrt{2}} (\chi_- \chi_+ + \chi_+ \chi_-) = 0 .$$

Similarly for the expectation value $\langle S_{2z} \rangle$

$$S_{2z} \frac{1}{\sqrt{2}} (\chi_- \chi_+ - \chi_+ \chi_-) = \frac{\hbar}{2\sqrt{2}} (\chi_- \chi_+ + \chi_+ \chi_-) .$$

and

$$\langle S_{2z} \rangle = 0 .$$

Susskind on page 174 and 175: *"If the expectation value of a component of S is zero, it means that the experimental outcome is equally likely to be +1 or –1 . In other words, the outcome is completely uncertain , we know nothing at all about the outcome of any measurement of any component of either spin."*

The expectation value is 0. So, anything goes, meaning the measurement of S_{2z} produces $\hbar/2$ or $-\hbar/2$. Then, instead of a probability to be 0, the probability is 1/2.

Fp teaches, page 148, S_{1z} and S_{2z} can be measured simultaneously. How? Well, that does not matter. Here we measure in a 'mathematical' way. Susskind showed this for the singlet on page 176-177 .

ad b) From the analysis of ad a) we learned:

$$\langle S_{1y} \rangle = 0 \text{ and } \langle S_{2x} \rangle = 0 , \text{ nothing new here.}$$

Again we operate the separate operators on the singlet state:

$$S_{1y} \frac{1}{\sqrt{2}} (\chi_- \chi_+ - \chi_+ \chi_-) = -\frac{i\hbar}{2\sqrt{2}} (\chi_+ \chi_+ + \chi_- \chi_-) ,$$

and

$$S_{2x} \frac{1}{\sqrt{2}} (\chi_- \chi_+ - \chi_+ \chi_-) = \frac{\hbar}{2\sqrt{2}} (\chi_- \chi_- - \chi_+ \chi_+) .$$

Conclusion: the probability that a measurement of the x -component of the spin of the other electron yields $S_x = -\hbar/2$ is 1/2.

Now electron 1 is in the state $\psi_1 = \cos \alpha_1 \chi_+ + \sin \alpha_1 e^{i\beta_1} \chi_-$ and electron 2 is in the state $\psi_2 = \cos \alpha_2 \chi_+ + \sin \alpha_2 e^{i\beta_2} \chi_-$.

Can these two electrons be in a triplet state and with what probability?

Let us return to chapter 6 , section 5. On page 91, Eq.(6.42) the stationary wave function of the whole system for two identical non-interacting fermions is presented.

I denote the first wave function of fermion by ψ_1 and the second fermion by ψ_2 . Then:

$$\psi = \frac{1}{\sqrt{2}}(\psi_1\psi_2 - \psi_2\psi_1) . \quad (\text{C.11.E.21})$$

This resembles the singlet state (C.11.E.20).

Now I rephrase the question to be answered: what is the probability for a singlet to represent a triplet? Intuitively: the probability is 0.

With

$$\psi_1 = \cos \alpha_1 \chi_+ + \sin \alpha_1 e^{i\beta_1} \chi_- \equiv a_1 \chi_+ + b_1 \chi_- ,$$

and

$$\psi_2 = \cos \alpha_2 \chi_+ + \sin \alpha_2 e^{i\beta_2} \chi_- \equiv a_2 \chi_+ + b_2 \chi_- .$$

With (C.11.E.21) and the short hand expressions for ψ_1 and ψ_2 :

$$\psi = \frac{(a_2 b_1 - a_1 b_2)}{\sqrt{2}} [\chi_- \chi_+ - \chi_+ \chi_-] .$$

Normalization of ψ gives us $|a_2 b_1 - a_1 b_2| = 1$.

The above expression for ψ is clearly a singlet. So, the answer to the question about a triplet representation is no.

12 Time-Independent Perturbation Theory

12.1 Introduction

The Hamiltonian

$$H = H_0 + H_1 ,$$

will be discussed where $H_1 \ll H_0$, "in some sense" , Fp.

12.2 Improved Notation

At the bottom of page 151 the notation

$$\langle \psi_i | \psi_j \rangle \equiv \langle i | j \rangle = \delta_{ij} ,$$

is introduced. I expected the name Dirac would pop up.

On page 152, Fp presents the expectation value of the general operator A . Reference is made to Sect. 4.9 and the expectation value is:

$$\langle A \rangle = \sum_{i,j} c_i^* c_j A_{ij} , \text{ Eq.(12.14) .}$$

In section 4.9 we find:

$$A\psi_i = a_i \psi_i , \text{ Eq.(4.126).}$$

With the expansion for the one-dimensional case and Eq.(12.7);

$$\langle A \rangle = \int_{-\infty}^{\infty} \sum_i c_i^* \psi_i^* \sum_j a_j \psi_j dx . \quad (\text{C.12.E.1})$$

Then we use the general expression $\langle \psi_i | \psi_j \rangle \equiv \langle i | j \rangle = \delta_{ij}$ and (C.12.E.1) reduces into:

$$\langle A \rangle = \sum_i |c_i|^2 A_{ii} , \text{ and } A_{ii} \text{ the diagonal matrix elements. This differs a bit from Eq.(12.14).}$$

Lecture 1.9 of Susskind is of some help to appreciate this section.

12.3 Two-State system.

In this section Fp analysed the simplest non-trivial mechanical system.

Just as a reminder, Eq.(12.25) and Eq.(12.12):

$$\psi_a = \langle \psi_1 | \psi_a \rangle \psi_1 + \langle \psi_2 | \psi_a \rangle \psi_2 = \langle 1 | a \rangle \psi_1 + \langle 2 | a \rangle \psi_2 .$$

Then Eq.(12.25) is obtained.

Sandwiching $H_0 + H_1$ between ψ_i and ψ_E , Eq.(12.26) is found, since the eigenvalue E is a number.

To obtain Eq.(12.28), see Mahan page 158:

Multiply Eq.(12.24) with $\psi_1 \equiv |1\rangle$ and for the right-hand side of Eq.(12.24), expand ψ_E using Eq.(12.25):

$$\langle 1|H_0 + H_1|E\rangle = \langle 1|E\rangle\langle 1|(H_0 + H_1)|1\rangle + \langle 2|E\rangle\langle 1|(H_0 + H_1)|2\rangle. \quad (\text{C.12.E.2})$$

With Eqs.(12.22), (12.27), (12.29) and (12.31), (C.12.E.2) becomes:

$$\langle 1|H_0 + H_1|E\rangle = \langle 1|E\rangle(E_1 + e_{11}) + \langle 2|E\rangle e_{12}. \quad (\text{C.12.E.3})$$

Multiply Eq.(12.24) with $\psi_1 \equiv |1\rangle$:

$$\langle 1|H_0 + H_1|E\rangle = \langle 1|E\rangle E. \quad (\text{C.12.E.4})$$

Subtract (C12.E.4) from (C12.E.3):

$$\langle 1|E\rangle(E_1 - E + e_{11}) + \langle 2|E\rangle e_{12} = 0. \quad (\text{C.12.E.5})$$

Completely similar you will find:

$$\langle 2|E\rangle(E_2 - E + e_{22}) + \langle 1|E\rangle e_{21} = 0. \quad (\text{C.12.E.6})$$

A set of two equations which can be written as Eq.(12.28), where $e_{21} = e_{12}^*$.

This two-state system is also presented by Mahan page 160.

At the bottom of page 154 Fp writes: "*It is easily demonstrated....*". It took me some time to find out how easily. For this I returned to Mahan section 6.2 : Matrix Methods. It is about to find the eigenvectors of the matrix(which one?) for each eigenvalue E'_1 and E'_2 , Eqs. (12.36) and (12.37) respectively. The coefficients are $\langle 1|E\rangle$ and $\langle 2|E\rangle$, where the eigenvalue $E = E'_1$ or $E = E'_2$. For ψ_E we need to find $\psi_{E'_1}$ and $\psi_{E'_2}$, denoted ψ'_1 and ψ'_2 respectively by Fp. I find the notation of Fp confusing.

What about the matrix? For the matrix we have Eqs.(12.28) and (12.32), I think.

So,

$$\begin{pmatrix} E_1 & e_{12} \\ e_{12}^* & E_2 \end{pmatrix} \begin{pmatrix} \langle 1|E'_i\rangle \\ \langle 2|E'_i\rangle \end{pmatrix} = E'_i \begin{pmatrix} \langle 1|E'_i\rangle \\ \langle 2|E'_i\rangle \end{pmatrix}, \quad (\text{C.12.E.7})$$

where $i = 1, 2$ and E'_i are given by Eqs. (12.36) and (12.37).

For $i = 1$, there are two solution. However, neglecting $O(\epsilon^2)$ one solution is:

$$\langle 1|E'_1\rangle = -\frac{e_{12}}{E_1 - E'_1} \langle 2|E'_1\rangle \rightarrow -\infty, \text{ see Eq.(12.36).}$$

Remark: The question I left unanswered is: does the term with ϵ^2 comes into play? Well, it does. However, this term will grow to infinity for $\epsilon \rightarrow 0$.

The other solution is:

$$\langle 2|E'_1\rangle = \frac{e_{12}^*}{E'_1 - E_2} \langle 1|E'_1\rangle \approx \frac{e_{12}^*}{E_1 - E_2} \langle 1|E'_1\rangle$$

Then we find for $\begin{pmatrix} \langle 1|E'_i\rangle \\ \langle 2|E'_i\rangle \end{pmatrix}$, (12.C.E.7),:

$$\langle 1|E'_1\rangle \left(\frac{1}{e_{12}^*} \right). \quad (\text{C.12.E.8})$$

Now what about $\langle 1|E'_1\rangle$ in this expression? With Eq. (12.25) and (C.12.E.8)

$$\psi_{E'_1} = \langle 1|E'_1\rangle \psi_1 + \langle 1|E'_1\rangle \frac{e_{12}^*}{E_1 - E_2} \psi_2. \quad (\text{C.12.E.9})$$

Then, set $H_1 = 0$, and the left-hand side of (C.12.E.9) equals the right-hand side:

$$\psi_{E'_1} = \psi_1.$$

Consequently $\langle 1|E'_1\rangle = 1$.

On the other hand, using normalization and (C.12.E.8), neglecting $O(\epsilon^2)$ we find again

$$\langle 1|E'_1\rangle = 1.$$

For $i = 2$, we find totally similar:

$$\psi_{E'_2} = -\frac{e_{12}}{E_1 - E_2} \psi_1 + \psi_2. \quad (\text{C.12.E.10})$$

Since for $H_1 = 0$,

$$\psi_{E'_2} = \psi_2.$$

Remark: “easily” got a meaning.

12.4 Non-Degenerate Perturbation Theory

In this section Fp analyses systems with more than two eigen states.

Eqs.(12.41)-(12.45) are the basic equations.

In order to arrive at Eq.(12.46) I present here a few equations.

Combine Eqs.(12.44) and (12.45):

$$\langle m|H_0 + H_1|E\rangle = \sum_k \langle k|E\rangle \langle m|H_0 + H_1|k\rangle. \quad (\text{C.12.E.11})$$

Select the m -th term of (C.12.E.11), and use Eqs.(12.41), (12.42) and (12.47):

$$\langle m|H_0 + H_1|E\rangle = \langle m|E\rangle E_m + \langle m|E\rangle e_{mm} + \sum_{k \neq m} e_{mk} \langle k|E\rangle. \quad (\text{C.12.E.12})$$

Subtract Eq.(12.44) from (C.12.E.12) and you obtain Eq.(12.46).

Page 156, derivation of Eq.(12.53):

Substitute Eq.(12.50) into Eq.(12.46). Use Eq.(12.49), we obtain:

$$[E_m - E_n + O(\epsilon) + E_m O(\epsilon)] \langle m|E\rangle + \sum_{k \neq m} e_{mk} \langle k|E\rangle = 0. \quad (\text{C.12.E.13})$$

Neglecting terms which are $O(\epsilon^2)$, use Eqs.(12.48), (12.49) and (12.52), you arrive at Eq.(12.53).

The latter equation results into Eq.(12.54).

Fp substituted $\langle m|E\rangle$ given by Eq.(12.54) into Eq.(12.46). Then evaluated the resulting expression for $m = n$, giving Eq.(12.55) where terms of $O(\epsilon^3)$ are neglected.

Caveat: e_{nn} , given by Eq.(12.49), remains $O(\epsilon)$ in Eq.(12.55). Eq. (12.48) could make you think otherwise.

With Eq.(12.55) we find $E = E'_n$, the modified n th energy eigenstate.

What about the modified eigenstate $\psi_{E'_n} \equiv \psi'_n$?

We started with Eq.(12.45):

$$\psi_E = \sum_k \langle k|E\rangle \psi_k.$$

For the n -th term we have, with Eq.(12.54),:

$$\psi'_n \equiv \psi_{E'_n} = \psi_n + \sum_{k \neq n} \frac{e_{kn}}{E_n - E_k} \psi_k + O(\epsilon^2),$$

and for $\epsilon \rightarrow 0 : \psi'_n \equiv \psi_{E'_n} = \psi_n$.

Remark: for a two-state system $n = 2$, Eqs.(12.56) and (12.57), the Eqs.(12.36)-(12.37) are obtained.

Fp mentioned the modified eigenstates remain orthonormal to $O(\epsilon^2)$.

Demonstrate by calculating :

$$\left(\psi_n + \sum_{k \neq n} \frac{e_{kn}}{E_n - E_k} \psi_k \right)^* \left(\psi_m + \sum_{k \neq m} \frac{e_{km}}{E_m - E_k} \psi_k \right),$$

we find:

$$\psi_n^* \psi_m = \delta_{nm}, \left(\sum_{k \neq n} \frac{e_{kn}}{E_n - E_k} \psi_k \right)^* \psi_m + \left(\sum_{k \neq m} \frac{e_{km}}{E_m - E_k} \psi_k \right) (\psi_n)^* = 0 + O(\epsilon^2) \text{ and}$$

$$\left(\sum_{k \neq n} \frac{e_{kn}}{E_n - E_k} \psi_k \right)^* \left(\sum_{k \neq m} \frac{e_{km}}{E_m - E_k} \psi_k \right) = 0 + O(\epsilon^2).$$

12.5 Quadratic Stark Effect

This section is about a hydrogen atom in a uniform external electric field. The unperturbed and perturbed Hamiltonian are presented in Eqs.(12.58) and (12.59) respectively.

On page 157 Fp presented:

$$[L_z, z] = 0, \text{ Eq.(12.62) .}$$

With Eq.(12.61) we find:

$$[L_z, z] = x p_y z - y p_x z - z x p_y + z y p_x. \quad (\text{C.12.E.14})$$

Eqs.(7.15) and (7.17) :

$$xz = zx, yz = zy \text{ and } [p_i, x_j] = i\hbar \delta_{ij}. \text{ Plugging these results into (C.12E.14):}$$

$$x[p_y, z] + y[z, p_x] = 0.$$

At the bottom of page 157, use has been made of:

$$[L_z^2, z] = 0.$$

Eq.(12.65) is found by using a.o. $L_x[L_x, z] = -i\hbar L_x y$.

Furthermore, by plugging into the last line of Eq.(12.65) the expressions for L_x and L_y , you will obtain the equality.

In the first line of Eq.(12.66) the square brackets should replace ().

Above Eq.(12.67) Fp writes: “which reduces to”. However, before the reduction you need to plug in $\{L_z z L_z - L_z^2 z (= 0)\}$.

From Eq.(12.60) it is clear $l = l'$ and both are 0.

Top page 160: $E_{n10} = E_{n00}$, since the energies just depend on n .

Eq.(12.84) is clearly the expectation value. In Eq.(12.83) we are dealing with the matrix elements. Hence, the matrix elements are about expectation values?

Remark: Mahan page 166, you will find “The $n = 1$ state of atomic hydrogen does not have a Stark effect.” Probably Mahan indicates the linear Stark effect. Since later Mahan shows the lowest energy level, $n = 1$, has a nonlinear quadratic correction. This is discussed in section 6.5, Mahan, on polarizability.

12.6 Degenerate Perturbation Theory

In this section Fp starts with analysing degenerate states of the hydrogen atom, $n > 1$, with non-degenerate perturbation theory.

Remark: On page 161 Fp introduced the expression: coupled states. Definition? Reading the text, it appears to me to be a different wording for degenerate states: states with the same eigenvalue.

It becomes more complicated when Fp denote $n = 1$ one coupled state. I suppose there is just one state with one eigenvalue E_1 .

Below Eq.(12.91) Fp mentioned : “Unfortunately, the above equation is not satisfied.” Not satisfied in what sense? Since for $n > 1$, $l' \neq l$. Consequently, $\delta_{ll'} = 0$.

However, for $n \geq 2$ we can have $l' = l \pm 1$ and the matrix element can be non-zero. See top of page 159 on selection rules. This selection rule implicates “Unfortunately....”? I suppose so.

Page 162: Eq. (12.95) is obtained by multiplying Eq.(12.93) with $\psi_{nl'm}^{(1)}$ and using Eq.(12.94).

To arrive at Eq.(12.97) start with Eq.(12.93):

$$H_1 \psi_{nlm}^{(1)} = \lambda_{nl} \psi_{nlm}^{(1)} .$$

Then

$$H_1 |n, l^{(1)}, m\rangle = \lambda_{nl} |n, l^{(1)}, m\rangle .$$

Multiply this expression with $\langle n, l', m|$:

$$\langle n, l', m| H_1 |n, l^{(1)}, m\rangle = \lambda_{nl} \langle n, l', m| n, l^{(1)}, m\rangle .$$

Plug into this expression the identity operator Eq.(12.96), where the dummy index l has been replaced by l'' , and you obtain Eq.(12.97).

12.7 Linear Stark Effect.

In section 12.5 the quadratic Stark effect is presented.

Fp started to introduce a new notation for the various states of a hydrogen atom. The states are indicated with a number, referring to n , and a character referring to l . For this character Fp uses capitals. Mahan uses lower case characters.

The core of this section is to solve the matrix eigenvalue equation Eq.(12.98). In this case we have a 2×2 matrix, $n = 2$. The elements U_{jk} are given in Eq.(12.99).

j presents the rows and k the columns. So, these quantum numbers are the suffices for the matrix elements. That can be confusing.

$$U_{jk} = \langle n, j, m| H_1 |n, k, m\rangle .$$

The matrix is:

$$\begin{pmatrix} \langle n, 1, m| H_1 |n, 1, m\rangle & \langle n, 1, m| H_1 |n, 2, m\rangle \\ \langle n, 2, m| H_1 |n, 1, m\rangle & \langle n, 2, m| H_1 |n, 2, m\rangle \end{pmatrix} . \quad (C.12.E.15)$$

We know $n = 2$ and the selection rules $l' = l \pm 1$ and $m' = m$.

$m' = m$ has been plugged into (C.12.E.15).

Now, how to deal with the numbers for j and k in (C.12.E.15)?

When $j = k = 1$, the matrix element is 0. For $j = k = 2$, no matrix element exists.

So we are left with the off-diagonal elements. What to do? I think that what usually is expected with matrix mathematics $j = k = 1$, has to be replaced by $j = k = 0$.

Then (C.12.E.15) becomes:

$\begin{pmatrix} \langle 2,0,0|H_1|2,0,0\rangle & \langle 2,0,0|H_1|2,1,0\rangle \\ \langle 2,1,0|H_1|2,0,0\rangle & \langle 2,1,0|H_1|2,1,0\rangle \end{pmatrix}$, and this results into:

$$\begin{pmatrix} 0 & \langle 2,0,0|H_1|2,1,0\rangle \\ \langle 2,1,0|H_1|2,0,0\rangle & 0 \end{pmatrix}, \text{ Eq.(12.105).}$$

Eq.(12.106) is obtained with help of Eqs.(8.91), (8.92), (9.66), (9.77), $z = r \cos \theta$, $H_1 = e|\mathbf{E}|z$ and evaluating the integral:

$$\int_0^{2\pi} \int_0^\pi \int_0^\infty \psi_{200} r \cos \theta \psi_{210} r^2 \sin \theta dr d\theta d\phi.$$

The eigenvalues of the matrix in Eq.(12.105) are found with Eq.(12.106) and:

$$\begin{vmatrix} -\lambda & 3a_0 \\ 3a_0 & -\lambda \end{vmatrix} = 0, \rightarrow \lambda = \pm 3a_0.$$

The eigenvectors, Eqs.(12.107) and (12.108), are found from:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathbf{x} = \pm \mathbf{x}.$$

Now we have to find out about Eq.(12.109) and (12.110). There the simultaneous eigenstates of H_0 and H_1 are given.

In Eq.(12.92) these eigenstates are defined:

$$\psi_{nlm}^{(1)} = \sum_{k=1, N_n} \langle n, k, m | n, l^{(1)}, m \rangle \psi_{nkm}.$$

For this expression we write:

$$\psi = \sum_{k=1, N_2} \langle 2, k, 0 | 2, l^{(1)}, 0 \rangle \psi_{2k0}. \quad (\text{C.12.E.16})$$

Now I have a problem:

$k = 1, N_2$, where $N_2 = 2$. I think this should be: $k = 0, 1$.

Then with the expression for \mathbf{x} defined in Eqs. (12.97) and (12.98) presented in Eqs.(12.107) and (12.108), the resulting simultaneous eigenstates are:

$$\psi = \frac{1}{\sqrt{2}} \psi_{200} + \frac{1}{\sqrt{2}} \psi_{210},$$

and

$$\psi = \frac{1}{\sqrt{2}} \psi_{200} - \frac{1}{\sqrt{2}} \psi_{210}.$$

12.8 Fine Structure of Hydrogen

In this section the lowest order relativistic correction to the energy is presented, Eq.(12.115).

Use is made of the Hamiltonian given in Eq.(7.20):

$$H = \frac{p^2}{2m} + V, \text{ where } p^2 = p_x^2 + p_y^2 + p_z^2.$$

On page 165 just below Eq.(12.122): "Note ...assumes..... p^4 is an Hermitian operator. It turns out.....this is not the case for $l = 0$."

The $l = 0$ state gives a wavefunction dependent on r , $\psi(r)$ say.

The definition, for $l = 0$, of an Hermitian operator, page 46, Eq.(4.57):

$$\int_0^{2\pi} \int_0^\pi \int_0^\infty \psi(r)^* p^4 \psi(r) r^2 \sin \theta d\theta d\phi = \int_0^{2\pi} \int_0^\pi \int_0^\infty [p^4 \psi(r)]^* \psi(r) r^2 \sin \theta d\theta d\phi, (C.12.E.17)$$

with $p^4 \propto \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right]$.

So (C.12.E.17) is not correct for $l = 0$.

Still, Fp mentioned, the calculations on page 165 give the correct answer for $l = 0$.

Furthermore the perturbing Hamiltonian commutes with both L^2 and L_z .

For example $[L_z, p^4] = 0$, in Cartesian coordinates,

$$(xp_y - yp_x)p^4 - p^4(xp_y - yp_x) = 0.$$

Hence, the non-degenerate perturbation theory can be used. The Hamiltonian H_0 , the perturbing Hamiltonian H_1 , L^2 and L_z commute and have the same eigenstates.

Next, Fp discussed the spin-orbit coupling.

At the bottom of page 166 Fp presented the general notation for the eigenstates $\psi_{l,s;j,m_j}^{(2)}$. In

section 11.3 $m_j = m + \frac{1}{2}$ has been analysed. Below $m_j = m - \frac{1}{2}$ is taken into account

To obtain Eq.(12.138), $j = l + \frac{1}{2}$ can be used or $j = l - \frac{1}{2}$.

At the bottom of page 167 the fine structure induced energy-shifts for the hydrogen atom

Keep in mind: Page 142 Fp: “..j can take positive integer, or half integer, values.....”.

(Note: We learned on page 145: $j = l \pm \frac{1}{2}$. This $\frac{1}{2}$ represents s instead of m_s , see page 146.)

For $n = 1, 2$ and 3 the fine structure energy- shift is presented in Figure 12.1.

Here I will analyse the three quantum numbers in more detail.

Let us summarize some formulas in the following tables.

Throughout the analysis I left the radial wave function out.

Remark: In the table below, I presented the wave function:

$$\psi_{l,s;j,m-1/2}^{(2)}.$$

Fp did not present this wave function. See Section 11.3. This wave function is basically the same wave function as $\psi_{l,s;j,m+1/2}^{(2)}$.

	$\psi_{l,s;j,m_j}^{(2)}$
$j = l + \frac{1}{2}$ $m_j = m + \frac{1}{2}$ (12.143)	$\left(\frac{l+m+1}{2l+1}\right)^{1/2} Y_{l,m} \chi_+ + \left(\frac{l-m}{2l+1}\right)^{1/2} Y_{l,m+1} \chi_-$ or $\left(\frac{j+m_j}{2l+1}\right)^{1/2} Y_{l,m_j-\frac{1}{2}} \chi_+ + \left(\frac{j-m_j}{2l+1}\right)^{1/2} Y_{l,m_j+\frac{1}{2}} \chi_-$
$j = l - \frac{1}{2}$ $m_j = m + \frac{1}{2}$ (12.144)	$\left(\frac{l-m}{2l+1}\right)^{1/2} Y_{l,m} \chi_+ - \left(\frac{l+m+1}{2l+1}\right)^{1/2} Y_{l,m+1} \chi_-$ or $\left(\frac{j-m_j+1}{2l+1}\right)^{1/2} Y_{l,m_j-\frac{1}{2}} \chi_+ - \left(\frac{j+m_j+1}{2l+1}\right)^{1/2} Y_{l,m_j+\frac{1}{2}} \chi_-$

--	--

	$\psi_{l,s;j,m-1/2}^{(2)}$
$j = l + \frac{1}{2}$ $m_j = m - \frac{1}{2}$	$\left(\frac{l-m+1}{2l+1}\right)^{1/2} Y_{l,m} \chi_- + \left(\frac{l+m}{2l+1}\right)^{1/2} Y_{l,m-1} \chi_+$ or $\left(\frac{j-m_j}{2l+1}\right)^{1/2} Y_{l,m_j-\frac{1}{2}} \chi_- + \left(\frac{j+m_j}{2l+1}\right)^{1/2} Y_{l,m_j+\frac{1}{2}} \chi_+$
$j = l - \frac{1}{2}$ $m_j = m - \frac{1}{2}$	$\left(\frac{l+m}{2l+1}\right)^{1/2} Y_{l,m} \chi_- - \left(\frac{l-m+1}{2l+1}\right)^{1/2} Y_{l,m-1} \chi_+$ or $\left(\frac{j+m_j+1}{2l+1}\right)^{1/2} Y_{l,m_j-\frac{1}{2}} \chi_- - \left(\frac{j-m_j+1}{2l+1}\right)^{1/2} Y_{l,m_j+\frac{1}{2}} \chi_+$

Note: in the tables above: substitute for m in the first table $m - 1 \rightarrow$ the second table is obtained, except for the minus sign of the second row of the second table \rightarrow phase ambiguity. I shall use (12.143) and/or (12.144) in the analyses of states.

$1S_{1/2}$:

The two states for $n = 1$.

The subscript of $S_{1/2} \rightarrow j = l + \frac{1}{2} \rightarrow j = \frac{1}{2}$.

$j = l - \frac{1}{2} \rightarrow j = -\frac{1}{2}$ does not contribute.

Unless, it is about $|l - \frac{1}{2}|$. Fp did not mention such a possibility.

The constraint: $m_j = m_l (\equiv m) + m_s$.

$-l - \frac{1}{2} \leq m_j \leq l + \frac{1}{2} \rightarrow$ with $l = 0 \rightarrow -\frac{1}{2} \leq m_j \leq \frac{1}{2}$, $m = 0$.

So, there are 2 values of m_j giving two wave functions(12.143)

$m_j = \frac{1}{2}$: $\psi_{l,s;1/2,1/2}^{(2)} = Y_{0,0} \chi_+$,

and

$m_j = -\frac{1}{2}$: $\psi_{l,s;1/2,-1/2}^{(2)} = Y_{0,0} \chi_-$.

The two states are presented in the table below.

$\Delta E_{0,\frac{1}{2},\frac{1}{2},m_j} = \frac{1}{4} E_1 \alpha^2$, Eq.(12.138).

	m_j	$\psi_{l,s;j,1/2}^{(2)}$	m_j	$\psi_{l,s;j,-1/2}^{(2)}$
$n = 1, l = 0$ $j = l + \frac{1}{2}, nS_{1/2}$	$1/2$	$Y_{0,0}\chi_+$	$-1/2$	$Y_{0,0}\chi_-$
$\Delta E_{0,\frac{1}{2},\frac{1}{2},m_j} = \frac{1}{4}E_n\alpha^2$				

$2S_{1/2}$:

Start with $n = 2, l = 0$ and $j = \frac{1}{2}$.

Again we find two $2S_{1/2}$ states: $m_j = \pm \frac{1}{2} \rightarrow Y_{0,0}\chi_+$ and $Y_{0,0}\chi_-$.

$$\Delta E_{0,\frac{1}{2},\frac{1}{2},m_j} = \frac{5}{16}E_2\alpha^2.$$

	m_j	$\psi_{l,s;j,1/2}^{(2)}$	m_j	$\psi_{l,s;j,-1/2}^{(2)}$
$n = 2, l = 0$ $j = l + \frac{1}{2}, nS_{1/2}$	$1/2$	$Y_{0,0}\chi_+$	$-1/2$	$Y_{0,0}\chi_-$
$\Delta E_{0,\frac{1}{2},\frac{1}{2},m_j} = \frac{5}{16}E_n\alpha^2$				

$2P_{1/2}$:

For $n = 2, l = 1$ and $j = \frac{1}{2} \rightarrow j = l - \frac{1}{2} \rightarrow (12.144)$.

$-l + \frac{1}{2} \leq m_j \leq l - \frac{1}{2} \rightarrow -\frac{1}{2} \leq m_j \leq \frac{1}{2} \rightarrow$ two wave functions.

$m_j = +\frac{1}{2}$:

$$\psi_{1,\frac{1}{2},\frac{1}{2},+\frac{1}{2}}^{(2)} = \sqrt{\frac{1}{3}}Y_{1,0}\chi_+ - \sqrt{\frac{2}{3}}Y_{1,1}\chi_- \quad (\text{C.E.12.18})$$

$m_j = -\frac{1}{2}$:

$$\psi_{1,\frac{1}{2},\frac{1}{2},-\frac{1}{2}}^{(2)} = \sqrt{\frac{2}{3}}Y_{1,-1}\chi_+ - \sqrt{\frac{1}{3}}Y_{1,0}\chi_- \quad (\text{C.E.12.19})$$

$$\Delta E_{1,\frac{1}{2},\frac{1}{2},m_j} = \frac{5}{16}E_2\alpha^2.$$

	m_j	$\psi_{l,s;j,+1/2}^{(2)}$	m_j	$\psi_{l,s;j,-1/2}^{(2)}$
$n = 2, l = 1$ $j = l - \frac{1}{2}, nP_{1/2}$	$\frac{1}{2}$	$\sqrt{\frac{1}{3}}Y_{1,0}\chi_+ - \sqrt{\frac{2}{3}}Y_{1,1}\chi_-$	$-\frac{1}{2}$	$-\sqrt{\frac{1}{3}}Y_{1,0}\chi_- + \sqrt{\frac{2}{3}}Y_{1,-1}\chi_+$
$\Delta E_{1,\frac{1}{2},\frac{1}{2},m_j} = \frac{5}{16}E_2\alpha^2$				

Two wave functions indeed.

For $2P_{3/2}$:

$$n = 2, l = 1 \text{ and } j = \frac{3}{2} \rightarrow -\frac{3}{2} \leq m_j \leq \frac{3}{2}.$$

Hence, there are 4 values of m_j : $-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$, and $j = l + \frac{1}{2}$.

$$m_j = \frac{3}{2}:$$

$$\psi_{1, \frac{1}{2}, \frac{3}{2}}^{(2)} = Y_{1,1}\chi_+.$$

$$m_j = \frac{1}{2}:$$

$$\psi_{1, \frac{1}{2}, \frac{3}{2}}^{(2)} = \sqrt{\frac{2}{3}}Y_{1,0}\chi_+ + \sqrt{\frac{1}{3}}Y_{1,1}\chi_-.$$

$$m_j = -\frac{1}{2}:$$

$$\psi_{1, \frac{1}{2}, -\frac{1}{2}}^{(2)} = \sqrt{\frac{1}{3}}Y_{1,-1}\chi_+ + \sqrt{\frac{2}{3}}Y_{1,0}\chi_-.$$

$$m_j = -\frac{3}{2}:$$

$$\psi_{1, \frac{1}{2}, -\frac{3}{2}}^{(2)} = Y_{1,-1}\chi_-$$

$$\Delta E_{1, \frac{1}{2}, \frac{1}{2}, m_j} = \frac{1}{16}E_2\alpha^2.$$

	m_j	$\psi_{l,s;j,m+1/2}^{(2)}$	m_j	$\psi_{l,s;j,m-1/2}^{(2)}$
$n = 2, l = 1$ $j = l + \frac{1}{2}, nP_{3/2}$	$3/2$	$Y_{1,1}\chi_+$	$-3/2$	$Y_{1,-1}\chi_-$
	$\frac{1}{2}$	$\sqrt{\frac{2}{3}}Y_{1,0}\chi_+ + \sqrt{\frac{1}{3}}Y_{1,1}\chi_-$	$-\frac{1}{2}$	$\sqrt{\frac{2}{3}}Y_{1,0}\chi_- + \sqrt{\frac{1}{3}}Y_{1,-1}\chi_+$
$\Delta E_{1, \frac{1}{2}, \frac{1}{2}, m_j} = \frac{1}{16}E_n\alpha^2$				

So, as mentioned by Fp, four $2P_{3/2}$ states.

$3S_{1/2}$:

$$l = 0 \text{ and } j = \frac{1}{2}, (\rightarrow j = l + \frac{1}{2} \rightarrow j = \frac{1}{2}), \text{ and } m_j = \pm \frac{1}{2}.$$

again we find two $3S_{1/2}$ states: $Y_{0,0}\chi_+$ and $Y_{0,0}\chi_-$.

$$\Delta E_{0, \frac{1}{2}, \frac{1}{2}, m_j} = \frac{1}{4}E_3\alpha^2.$$

	m_j	$\psi_{l,s;j,+1/2}^{(2)}$	m_j	$\psi_{l,s;j,-1/2}^{(2)}$
$n = 3, l = 0$ $j = l + \frac{1}{2}, nS_{1/2}$	$1/2$	$Y_{0,0}\chi_+$	$-1/2$	$Y_{0,0}\chi_-$

$\Delta E_{0,\frac{1}{2},\frac{1}{2},m_j} = \frac{1}{4}E_n\alpha^2$				
---	--	--	--	--

$3P_{1/2}$:

For $n = 3, l = 1$ and $j = \frac{1}{2} \rightarrow j = l - \frac{1}{2} \rightarrow (12.144)$.

$$-l + \frac{1}{2} \leq m_j \leq l - \frac{1}{2} \rightarrow -\frac{1}{2} \leq m_j \leq \frac{1}{2},$$

The constraint: $m_j = m_l (\equiv m = 0, \pm 1) + m_s (= \pm \frac{1}{2})$.

$$m_j = +\frac{1}{2}$$

$$\psi_{1,\frac{1}{2},\frac{1}{2},+\frac{1}{2}}^{(2)} = \sqrt{\frac{1}{3}}Y_{1,0}\chi_+ - \sqrt{\frac{2}{3}}Y_{1,1}\chi_-.$$

$$m_j = -\frac{1}{2}$$

$$\psi_{1,\frac{1}{2},\frac{1}{2},-\frac{1}{2}}^{(2)} = \sqrt{\frac{1}{3}}Y_{1,0}\chi_- - \sqrt{\frac{2}{3}}Y_{1,-1}\chi_+.$$

$$\Delta E_{1,\frac{1}{2},\frac{1}{2},m_j} = \frac{1}{4}E_3\alpha^2.$$

	m_j	$\psi_{l,s;j,+\frac{1}{2}}^{(2)}$	m_j	$\psi_{l,s;j,-\frac{1}{2}}^{(2)}$
$n = 3, l = 1$ $j = l - \frac{1}{2}, nP_{1/2}$	$1/2$	$\sqrt{\frac{1}{3}}Y_{1,0}\chi_+ - \sqrt{\frac{2}{3}}Y_{1,1}\chi_-$	$-1/2$	$\sqrt{\frac{1}{3}}Y_{1,0}\chi_- - \sqrt{\frac{2}{3}}Y_{1,-1}\chi_+$
$\Delta E_{1,\frac{1}{2},\frac{1}{2},m_j} = \frac{1}{4}E_n\alpha^2$				

$3P_{3/2}$:

$$l = 1 \text{ and } j = \frac{3}{2} \rightarrow -\frac{3}{2} \leq m_j \leq \frac{3}{2}$$

Hence, there are 4 values of m_j : $-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$, and $j = l + \frac{1}{2}$.

The results are the same as for $n = 2, l = 1$: $2P_{3/2}$

The energy shift:

$$\Delta E_{1,\frac{1}{2},\frac{3}{2},m_j} = \frac{1}{12}E_3\alpha^2.$$

	m_j	$\psi_{l,s;j,m_j}^{(2)}$	m_j	$\psi_{l,s;j,m_j}^{(2)}$
$n = 3, l = 1$ $j = l + \frac{1}{2}, nP_{3/2}$	$3/2$	$Y_{1,1}\chi_+$	$-3/2$	$Y_{1,-1}\chi_-$
	$1/2$	$\sqrt{\frac{2}{3}}Y_{1,0}\chi_+ + \sqrt{\frac{1}{3}}Y_{1,1}\chi_-$	$-1/2$	$\sqrt{\frac{2}{3}}Y_{1,0}\chi_- + \sqrt{\frac{1}{3}}Y_{1,-1}\chi_+$
$\Delta E_{1,\frac{1}{2},\frac{3}{2},m_j} = \frac{1}{12}E_n\alpha^2$				

$3D_{\frac{3}{2}}$:

$l = 2$ and $j = \frac{3}{2} \rightarrow j = l - \frac{1}{2} \rightarrow -\frac{3}{2} \leq m_j \leq \frac{3}{2}$: 4 values of m_j : $-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$.

The same result as found for $2P_{\frac{3}{2}}$ and $3P_{\frac{3}{2}}$:

	m_j	$\psi_{l,s;j,m_j}^{(2)}$	m_j	$\psi_{l,s;j,m_j}^{(2)}$
$n = 3, l = 2$ $j = l + \frac{1}{2}, nD_{3/2}$	$3/2$	$Y_{1,1}\chi_+$	$-3/2$	$Y_{1,-1}\chi_-$
	$1/2$	$\sqrt{\frac{2}{3}}Y_{1,0}\chi_+ + \sqrt{\frac{1}{3}}Y_{1,1}\chi_-$	$-1/2$	$\sqrt{\frac{2}{3}}Y_{1,0}\chi_- + \sqrt{\frac{1}{3}}Y_{1,-1}\chi_+$
$\Delta E_{1,\frac{1}{2},\frac{3}{2},m_j} = \frac{1}{12}E_n\alpha^2$				

$3D_{\frac{5}{2}}$:

$l = 2$ and $j = \frac{5}{2} \rightarrow j = l + \frac{1}{2} \rightarrow -\frac{5}{2} \leq m_j \leq \frac{5}{2}$: 6 values of m_j : $-\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$.

$$\Delta E_{2,\frac{1}{2},\frac{5}{2},m_j} = \frac{1}{36}E_3\alpha^2.$$

In the following table, I will summarize the results of $3D_{5/2}$ states:

	m_j	$\psi_{l,s;j,m_j}^{(2)}$	m_j	$\psi_{l,s;j,m_j}^{(2)}$
$n = 3, l = 2$ $j = l + \frac{1}{2}, nD_{5/2}$	$5/2$	$Y_{2,2}\chi_+$	$-5/2$	$Y_{2,-2}\chi_-$
	$3/2$	$\sqrt{\frac{4}{5}}Y_{2,1}\chi_+ + \sqrt{\frac{1}{5}}Y_{2,2}\chi_-$	$-3/2$	$\sqrt{\frac{2}{5}}Y_{2,1}\chi_- + \sqrt{\frac{3}{5}}Y_{2,0}\chi_+$
	$1/2$	$\sqrt{\frac{3}{5}}Y_{2,0}\chi_+ + \sqrt{\frac{2}{5}}Y_{2,1}\chi_-$	$-1/2$	$\sqrt{\frac{3}{5}}Y_{2,0}\chi_- + \sqrt{\frac{2}{5}}Y_{2,-1}\chi_+$
$\Delta E_{2,\frac{1}{2},\frac{5}{2},m_j} = \frac{1}{36}E_n\alpha^2$				

12.9 Zeeman Effect

A hydrogen atom placed in a uniform magnetic field.

Deriving Eq.(12.142), keep in mind:

$$H_1 = \frac{eB}{2m_e} (L_z + 2S_z) = \frac{eB}{2m_e} (J_z + S_z) .$$

Then with Eq.(12.134) , Eq.(12.142) is found.

Eqs.(12.143) and (12.144) compare, e.g., with details on pages 113-118 of my notes.

Take a look at Eqs.(12.143) and (11.47) use $j = l + 1/2$ and $m_j = m + 1/2$, then:

$$\frac{j+m_j}{2l+1} = \frac{l+\frac{1}{2}+m+\frac{1}{2}}{2l+1} = \frac{l+m+1}{2l+1} ,$$

$$\psi_{m_j-\frac{1}{2}}^{(1)} = \psi_{m,1/2}^{(1)} = Y_{l,m}\chi_+ ,$$

$$\frac{j-m_j}{2l+1} = \frac{l+\frac{1}{2}-m-\frac{1}{2}}{2l+1} = \frac{l-m}{2l+1} ,$$

and

$$\psi_{m_j+\frac{1}{2}}^{(1)} = \psi_{m+1,-1/2}^{(1)} = Y_{l,m+1}\chi_- .$$

Now with $j = l - 1/2$ and $m_j = m + 1/2$ you will obtain Eq.(11.48).

In the discussion of section 11.3 and 12.8, Fp did not mention $m_j = m - 1/2$. Well, plug into

Eq.(12.143) $m_j = m - \frac{1}{2}$:

$$\frac{j+m_j}{2l+1} = \frac{l+\frac{1}{2}+m-\frac{1}{2}}{2l+1} = \frac{l+m}{2l+1} ,$$

$$\psi_{m_j-\frac{1}{2}}^{(1)} = \psi_{m-1,1/2}^{(1)} = Y_{l,m-1}\chi_+ ,$$

$$\frac{j-m_j}{2l+1} = \frac{l+\frac{1}{2}-m+\frac{1}{2}}{2l+1} = \frac{l-m+1}{2l+1} ,$$

and

$$\psi_{m_j+\frac{1}{2}}^{(1)} = \psi_{m,-1/2}^{(1)} = Y_{l,m}\chi_- .$$

So, Eqs.(12.143) and (12.144) elegantly summarizes all the states.

Keep in mind:

S_z in Eq.(12.146) operates on χ_{\pm} and the \pm sign in Eq.(12.146) is about $j = l \pm \frac{1}{2}$.

Eq.(12.147) can be written as:

$$\Delta E_{l,\frac{1}{2};j,m_j} = \mu_B B m_j \frac{2l+1\pm 1}{2l+1} . \quad (C.12.E.34)$$

Remark: In Eqs.(12.149) and (12.150): where did m_j go? Well, it is about the energy split between two next states. Consequently this difference is $\Delta m_j = 1$.

Just below Eq.(12.150), Fp discussed the energy split due to a weak external magnetic field for a couple of states.

$1S_{1/2}$: there are two states $Y_{0,0}\chi_+$ and $Y_{0,0}\chi_-$.

We know $l = 0, m = 0$ and $m_j = \pm 1/2$.

Then the energy split for $1S_{1/2}$ becomes with (C.12.E.34):

$$\mu_B B \Delta m_j \frac{2l+1+1}{2l+1} = \mu_B B \left[\frac{1}{2} - \left(-\frac{1}{2} \right) \right] 2 = 2\mu_B B .$$

$2S_{1/2}$: there are two states $Y_{0,0}\chi_+$ and $Y_{0,0}\chi_-$.

$$l = 0, m = 0, j = l + 1/2, m_j = \pm 1/2.$$

The energy split for $2S_{1/2}$ becomes with (C.12.E.34):

$$\mu_B B \Delta m_j \frac{2l+1+1}{2l+1} = \frac{\mu_B B \left[\frac{1}{2} - \left(-\frac{1}{2} \right) \right]^2}{3} = \frac{2}{3} \mu_B B.$$

$2P_{1/2}$: the two states are $\sqrt{\frac{1}{3}} Y_{1,0} \chi_+ - \sqrt{\frac{2}{3}} Y_{1,1} \chi_-$ ($m = 0$) and

$$\sqrt{\frac{2}{3}} Y_{1,-1} \chi_+ - \sqrt{\frac{1}{3}} Y_{1,0} \chi_-$$
 ($m = -1$).

$$l = 1, m = 0, -1, j = l - \frac{1}{2}, \text{ and } m_j = \pm \frac{1}{2}.$$

The energy split for $2P_{1/2}$ becomes with (C.12.E.34):

$$\mu_B B \Delta m_j \frac{2l}{2l+1} = \mu_B B \left[\frac{1}{2} - \left(-\frac{1}{2} \right) \right] \frac{2}{3} = \frac{2}{3} \mu_B B.$$

$2P_{3/2}$: the states are, presented in the table at the top of page 116.

$$l = 1, m = 1, 0, -1, j = l + \frac{1}{2}, \text{ and } m_j = m \pm \frac{1}{2}.$$

So we have 3 values of m and four values m_j . I expect 4 states and three energy split numbers.

The four states are derived from Eq.(12.143):

$$m = 1, m_j = m + \frac{1}{2} = \frac{3}{2} \rightarrow \psi_{1,1/2}^{(1)} = Y_{1,1} \chi_+.$$

$$m = 0, m_j = \frac{1}{2} \rightarrow \sqrt{\frac{2}{3}} \psi_{0,1/2}^{(1)} + \sqrt{\frac{1}{3}} \psi_{1,-1/2}^{(1)} = \sqrt{\frac{2}{3}} Y_{1,0} \chi_+ + \sqrt{\frac{1}{3}} Y_{1,1} \chi_-.$$

The energy split between these two states becomes with (C.12.E.34):

$$\mu_B B \Delta m_j \frac{2l+2}{2l+1} = \mu_B B \left[\frac{3}{2} - \frac{1}{2} \right] \frac{4}{3} = \frac{4}{3} \mu_B B.$$

$$m = -1, m_j = -\frac{1}{2} \rightarrow \sqrt{\frac{1}{3}} \psi_{-1,1/2}^{(1)} + \sqrt{\frac{2}{3}} \psi_{0,-1/2}^{(1)} = \sqrt{\frac{1}{3}} Y_{1,-1} \chi_+ + \sqrt{\frac{2}{3}} Y_{1,0} \chi_-.$$

The energy split between these two states $m = 0$ and $m = -1$ becomes with (C.12.E.34):

$$\mu_B B \Delta m_j \frac{2l+2}{2l+1} = \mu_B B \left[\frac{1}{2} - \left(-\frac{1}{2} \right) \right] \frac{4}{3} = \frac{4}{3} \mu_B B.$$

To obtain the fourth state I need

$$m = -1, m_j = m - \frac{1}{2} = -\frac{3}{2} \rightarrow \psi_{-1,-1/2}^{(1)} = Y_{1,-1} \chi_-.$$

The energy split is again $\frac{4}{3} \mu_B B$.

For given j, l and in this case a spin $\frac{1}{2}$ particle, I summarize the steps to be taken in the following table:

m	$m + 1/2$	$m - 1/2$
1	3/2	1/2
0	1/2	-1/2
-1	-1/2	-3/2

To find the four states, start at the top left(3/2) move to the right(1/2) and end with the bottom right(-3/2). Or again start at the top left(3/2) move downwards to (-1/2) then move to the

right($-3/2$).

12.10 Hyperfine Structure

This section is about the proton of a hydrogen atom.

Eqs.(12.125) and (12.151) give:

$$\frac{\mu_p}{\mu_e} \propto \frac{m_e}{m_p}.$$

Eq.(12.156): the expectation value of the perturbation Hamiltonian H_1 given by Eq.(12.153), with (12.60) the e_{nn} diagonal element:

$$\Delta E = \langle 0,0,0 | H_1 | 0,0,0 \rangle. \quad (\text{C.12.E.35})$$

The three zeros' in (C.12.E.35) represents: ψ_{000} .

$$n = 1, l = 0, m = 0.$$

Then, with (8.91) and (9.65):

$$|0,0,0\rangle = \psi_{000} = R_{1,0} Y_{0,0} = \frac{2}{\sqrt{4\pi}} \frac{1}{a_0^{3/2}} e^{-\frac{r}{a_0}}. \quad (\text{C.12.E.36})$$

In Eq.(12.156) the first term vanishes by symmetry. I appreciate that. However, I did not see it. So, I calculated the expectation value by making use of (Exercise 11.2: C.11.E.19). There you can find that I need to evaluate:

$$\left(\frac{3z^2}{r^2} - 1\right) \frac{1}{r^3}.$$

Then with $z = r \cos \theta$, the integral of the expectation value is:

$$\int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{1}{r} (3 \cos^2 \theta - 1) \sin \theta e^{-\frac{2r}{a_0}} dr d\theta d\phi = 0. \quad (\text{C.12.E.37})$$

With (C.12.E.36):

$$|\psi_{000}(0)|^2 = \frac{1}{\pi a_0^3}. \quad (\text{C.12.E.38})$$

Plug (C.12.E.37) and (C.12.E.38) into (12.150)→(12.157).

The results of addition of angular momentum and spin angular momentum, see Chapter 11.4 about *Two Spin One-Half Particles*:

Eq.(12.158) and Eq.(12.159) are obtained.

furthermore, just below (11.71):

$$s = \frac{1}{2} \pm \frac{1}{2},$$

so there are two states one with $s = 1$ and $m_s = -1, 0, 1$,

the other with $s = 0$ and $m_s = 0$.

For S_e^2 and S_p^2 the eigenvalues are $(3/4)\hbar^2$. See Eq. (10.35)→ $S^2 \chi_\pm = \frac{3}{4}\hbar^2 \chi_\pm$, and $s = \frac{1}{2}$.

The eigenvalue of S_{trip}^2 with $s = 1$:

with $S_{trip}^2 \chi_{trip} = s(s+1)\hbar^2 \chi_{trip}$, equals $2\hbar^2$.

The eigenvalue of S_{sing}^2 with $s = 0$, equals 0.

To determine ΔE in Eq.(12.157), I need to evaluate $\langle \mathbf{S}_p \cdot \mathbf{S}_e \rangle$.

With (12.159):

$$\langle \mathbf{S}_p \cdot \mathbf{S}_e \rangle = \frac{1}{2} (\langle S^2 \rangle - \langle S_e^2 \rangle - \langle S_p^2 \rangle). \quad (\text{C.12.E.39})$$

For the singlet state:

$$\langle \mathbf{S}_p \cdot \mathbf{S}_e \rangle = \frac{1}{2} \left(0 - \frac{3}{4} \hbar^2 - \frac{3}{4} \hbar^2 \right) = -\frac{3}{4} \hbar^2, \quad (12.160).$$

For the triplet states:

$$\langle \mathbf{S}_p \cdot \mathbf{S}_e \rangle = \frac{1}{2} \left(2\hbar^2 - \frac{3}{4} \hbar^2 - \frac{3}{4} \hbar^2 \right) = \frac{1}{4} \hbar^2, \quad (12.161).$$

For completeness I present the table of Glebsch-Gordon coefficients, see Table 11.3 page 149: see the next page

		1	2	3	4
m_{sp}	m_{se}	<i>trip</i>	<i>trip</i>	<i>trip</i>	<i>sing</i>
1/2	1/2	1	0	0	0
1/2	-1/2	0	$1/\sqrt{2}$	0	$1/\sqrt{2}$
-1/2	1/2	0	$1/\sqrt{2}$	0	$-1/\sqrt{2}$
-1/2	-1/2	0	0	1	0
$s_p = 1/2$ $s_e = 1/2$	s	1	1	1	0
	m_s	1	0	-1	0

No Exercises.

13 Time-dependent Perturbation Theory

13.1 Introduction

Now the perturbation Hamiltonian H_1 is time dependent.

Fp: "... a time-dependent perturbation can cause the system to make transitions between its unperturbed energy eigenstates."

13.2 Preliminary Analysis

Eq.(13.4) is based on Eq.(4.158).

Eq.(13.5), with (13.4) and (13.6):

$$P_n(t) = |\langle \psi_n | \psi \rangle|^2 = |\langle c_n^* e^{iE_n t/\hbar} \psi_n | \sum_m c_m e^{-iE_m t/\hbar} \psi_m \rangle|^2 = |c_n|^2 = P_n(0).$$

Just below (13.7) on page 176 Fp writes : "Here we have separated". There Fp has assumed on beforehand the phase oscillations to vary fast and the perturbation varies slowly.

Below (13.11) Fp used the expression "Projecting out". Well, this means multiplying (13.11) to the left on both sides with $\langle \psi_n |$.

So, projecting out with the inner product. Rather prosaic.

Note: in (13.13):

$$\psi_m = |\psi_m\rangle \equiv |m\rangle.$$

13.3 Two-State System

As mentioned by Fp, of Eqs. (13.12) in general exact solutions cannot be found. For a two-state system (13.12) can be solved exactly.

In Eqs. (13.22) and (13.23) the solutions for the two states are given.

The solutions are derived from the second order linear differential equation given in (13.21).

By plugging (13.22) into (13.21) it is demonstrated (13.22) to be an appropriate solution. Using (13.20), (13.22) and $c_1(t = 0) = 1$, the coefficient $\frac{-i\gamma}{\Omega}$ is obtained.

On the other hand from a textbook on differential equations or with WolframAlpha, with $c_2(t = 0) = 0$, the general solution is:

$c_2 = d \exp\left[\frac{-i(\omega - \omega_{21})t}{2}\right] \sin(\Omega t)$, is found. Plugging this expression into (13.20) and set $c_1(t = 0) = 1$, results into $d = \frac{-i\gamma}{\Omega}$.

13.4 Spin Magnetic Resonance

A spin $\frac{1}{2}$ particle with no orbital angular momentum is placed in a magnetic field and is subjected to a small time-dependent magnetic field rotating in the x-y plane.

Eqs.(13.31) and (13.32) are derived from, Eq.(10.58),:

$$\bar{\mu} \propto \bar{S},$$

where,

$$\bar{S} = (S_x, S_y, S_z).$$

For a $\frac{1}{2}$ spinor we have:

$$\chi = c_+ \chi_+ + c_- \chi_- . \quad (\text{C.13.E.1})$$

All the results of a two-state system presented in section 13.3 can be used.

The time evolution with perturbation reads:

$$\chi(t) = c_+(t) e^{-iE_+ t/\hbar} \chi_+ + c_-(t) e^{-iE_- t/\hbar} \chi_- . \quad (\text{C.13.E.2})$$

Now, with Eqs.(13.29) and (13.31),:

$$H_0 \chi_{\pm} = E_{\pm} \chi_{\pm} = -\frac{geB_0}{2m} S_z \chi_{\pm} = \mp \frac{geB_0}{4m} \chi_{\pm} . \quad (\text{C.13.E.3})$$

Hence,

$$E_{\pm} = \mp \frac{geB_0}{4m}, \text{ see (13.33).}$$

With (C.13.E.2), the differential equation for $\chi(t)$ is found (see (13.10)).

Returning to the spinor, using the “language” of Fp, the differential equations for χ_{\pm} result. In these two equations we have to deal with

$$c_+(t) \chi_+^{\dagger} H_1 \chi_+ \text{ and } c_-(t) \chi_-^{\dagger} H_1 \chi_- .$$

To find out about these two expressions (13.32) comes into play. To this end the term in square brackets in (13.32) is written as:

$$\frac{e^{i\omega t}}{2} (S_x - iS_y) + \frac{e^{-i\omega t}}{2} (S_x + iS_y) = \frac{e^{i\omega t}}{2} S_- + \frac{e^{-i\omega t}}{2} S_+ .$$

With this expression (13.34) is found.

Then according to the action of the raising and lowering operators, we finally have:

$$c_+(t) \chi_+^{\dagger} H_1 \chi_+ = 0 \text{ and } c_-(t) \chi_-^{\dagger} H_1 \chi_- = 0, \text{ see (13.35).}$$

As a reminder: $S_+ \chi_+ = 0$ and $S_- \chi_- = 0$,
and

$\chi_-^\dagger S_- \chi_+ = 1$ and $\chi_+^\dagger S_+ \chi_- = 1$. These latter expressions are needed in the two linear differential first order linear differential equations:

$$i\hbar \frac{dc_+}{dt} = c_+ \chi_+^\dagger H_1 \chi_- e^{i(E_+ - E_-)t/\hbar}, \quad (\text{C.13.E.4})$$

and

$$i\hbar \frac{dc_-}{dt} = c_- \chi_-^\dagger H_1 \chi_+ e^{-i(E_+ - E_-)t/\hbar}. \quad (\text{C.13.E.5})$$

With Eqs. (13.18), (13.32) and (13.34) we obtain, using the expressions just above (C.13.E.4), (13.36).

At the bottom of page 179 and the following page 180, Fp presented with the indentifications (13.37)-(13.40) the analysis of spin magnetic resonance.

Remark, with (C.13.E.3) and Eq.(13.14),:

$$\text{Since } \omega_{+-} = \omega_{-+} = \frac{(E_+ - E_-)}{\hbar} = \frac{geB_0}{2m}.$$

13.5 Perturbation Expansion

Fp summarizes the results of section 13.2.

Eq.(13.44), with Eq.(13.41):

$$\psi(0) = c_i(0)\psi_i \rightarrow (13.44).$$

Bottom page 180, Fp: "... (or H_{nm} to $\hbar\omega_{nm}$, to be more exact) ...". To be more exact? Is it about the matrix elements?

To arrive at (31.49), $\delta_{fi} = 0$.

13.6 Harmonic Perturbations

A Hermitian perturbation which oscillates sinusoidally in time is considered.

To obtain (13.55), use has been made of:

$$\frac{e^{i\alpha} - 1}{2i} = e^{i\alpha/2} \frac{e^{i\alpha/2} - e^{-i\alpha/2}}{2i} = e^{i\alpha/2} \sin \frac{\alpha}{2}.$$

As mentioned at the bottom of page 182, for large $t \gg 2\pi/|\omega_{fi}|$, (13.59) is found. Use has been made of

$$\omega + \omega_{fi} \approx 0,$$

or

$$\omega - \omega_{fi} \approx 0.$$

Then expressions like

$$\text{sinc}[(\omega - \omega_{fi}) t/2] \text{sinc}[(\omega + \omega_{fi}) t/2],$$

which are obtained from (13.55) and $|c_f|^2$, vanish.

Keep in mind $\text{sinc } 0 = 1$.

The width of the resonance can be defined as;

$$(\omega \pm \omega_{fi})t/2 = \pi \text{ or } \text{sinc}\left[\frac{(\omega \pm \omega_{fi})t}{2}\right] = 0.$$

Fp indicates this with: "... the widths of these resonances decrease linearly as time increases".

(13.60) and (13.61) are obtained with (13.14):

$$\omega_{fi} = \frac{E_f - E_i}{\hbar}.$$

Note: a typo above Eq.(13.60): $\sinh 0 \rightarrow \text{sinc } 0 = 1$.

Fp introduced stimulated emission and absorption.

13.7 Electromagnetic Radiation

In this section Fp used the results of the foregoing section to investigate the interaction of an atomic electron with classical electromagnetic radiation. Another application of time-dependent perturbation theory.

In Eq.(13.69), Fp presented the related Hamiltonian.

For the vector potential \mathbf{A} , Fp adopted the gauge $\nabla \cdot \mathbf{A} = 0$.

The perturbing Hamiltonian is presented in Eq.(13.78).

In (13.85)

$$\int_{-\infty}^{\infty} \text{sinc}^2 x dx = \pi,$$

is presented. This result can be found using

$$\int_{-\infty}^{\infty} \text{sinc } x dx = \pi.$$

The latter result is obtained applying Fourier transform of the “hat” function centred at the origin. This “hat” function is : $f(y) = 1$ for $|y| < 1$ and $f(y) = 0$ for $|y| \geq 1$.

Then $\int_{-\infty}^{\infty} \text{sinc}^2 x dx = \pi$, applying integration by parts and $2 \sin x \cos x = \sin 2x$, is finally obtained.

Just for the sake of curiosity, applying twice integration by parts and

$$4 \sin^3 x = 3 \sin x - \sin 3x,$$

we have

$$\int_{-\infty}^{\infty} \text{sinc}^3 x dx = 3\pi/4.$$

Furthermore, again using basic goniometrical expressions like $\sin x \cos x = \frac{1}{2} \sin 2x$, we obtain:

$$\int_{-\infty}^{\infty} \text{sinc}^4 x dx = 2\pi/3.$$

By doing this one, it is helpful to realize:

$$\int_{-\infty}^{\infty} \frac{\sin^2 2x}{x^4} dx = 8 \int_{-\infty}^{\infty} \frac{\sin^2 2x}{(2x)^4} d2x = 8 \int_{-\infty}^{\infty} \text{sinc}^2 y dy.$$

Another one:

$$\int_{-\infty}^{\infty} \text{sinc}^8 x dx = 38\pi/63.$$

Take a close look to (13.84) and (13.86), it appears the sinc function operates similar to the Dirac-delta function $\delta(x)$. So,

$$\int_{-\infty}^{\infty} \delta(x) dx \approx \frac{1}{\pi} \int_{-\infty}^{\infty} \text{sinc}^2 x dx.$$

Now we could ask ourselves:

$$\int_{-\infty}^{\infty} \delta(x) dx = \lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} \text{sinc}^n x dx ? \text{ Alas, with help of the WolframAlpha app,}$$

$$\int_{-\infty}^{\infty} \text{sinc}^{18} x dx > 1 \text{ and } \int_{-\infty}^{\infty} \text{sinc}^{19} x dx < 1. \text{ A demonstration, not a proof.}$$

Intuitively I think (13.86) to be correct. To prove it, $\rho(\omega)/\omega^2$ should be a reasonable smooth function.

From (13.87) we learn $\frac{dP_{i \rightarrow f}^{abs}}{dt}$ is constant in time. Now look at (13.90). Differentiate this

expression with respect to time and I found $\frac{dP_{i \rightarrow f}^{abs}}{dt}$ not to be a constant.

There is more. Take (13.88) and plug into this expression the identity

$$w_{i \rightarrow f}^{abs} \equiv \frac{dP_{i \rightarrow f}^{abs}}{dt}.$$

I find $\frac{d}{dt} (P_{i \rightarrow f}^{abs})^2 = 0$.

Well, let's spend a few thoughts on this.

On page 186 below (13.87) Fp writes: ".....Given thatwe can write (see Cha.2)....". Then (13.88) is presented. I suppose Fp refers to section 2.5 and (2.23) since we are working with Continuous Probability Distributions. In exercise 3 of chapter 2, Fp deals with a subject like the one in Section 13.7.

In the Exercise 3, w represents a uniform(constant) decay probability per unit time. I will pay some attention to this exercise (page 7 of my notes).

In this exercise $P(t)$ is the probability of the atom not having decayed at time t m. At time t the atom has been created.

Given:

$$P(t) = e^{-wt}.$$

The probability of having decayed is denoted by $P_d(t)$. So

$$P_d = 1 - P = 1 - e^{-wt}. \quad (\text{C.13.E.6})$$

Then

$$\frac{dP_d}{dt} = we^{-wt} = Pw,$$

or

$$P_d(t + dt) - P_d(t) = (1 - P_d)w dt. \quad (\text{C.13.E.7})$$

Now (C.13.E.7) is like (13.88) and (C.13.E.6) like (13.91).

Is this of some help?

Just below (13.90) Fp writes: " $w_{i \rightarrow f}^{abs} \ll 1$ ".

Plug this into (13.90) and expand:

$$P_{i \rightarrow f}^{abs} = w_{i \rightarrow f}^{abs} \cdot t + O(w_{i \rightarrow f}^{abs} \cdot t)^2.$$

This we already know \rightarrow (13.86).

Hence, why doing all the work on (13.88)-(13.91) and referring to Ch.2? I have no idea.

A few things in this section are not clear to me.

I leave this section.

13.8 Electric Dipole Approximation

In this section an example of electromagnetic radiation is presented.

On page 187 Fp writes below (13.94):

"Now it is readily demonstrated that..." \rightarrow (13.95).

I demonstrate this for the one-dimensional case:

$$\chi \frac{p^2}{2m_e} - \frac{p^2}{2m_e} \chi.$$

We know: $p = -i\hbar \frac{\partial}{\partial x}$. Then

$$\left(x \frac{p^2}{2m_e} - \frac{p^2}{2m_e} x\right) \psi = -x \frac{\hbar^2}{2m_e} \frac{\partial^2 \psi}{\partial x^2} + x \frac{\hbar^2}{2m_e} \frac{\partial^2 \psi}{\partial x^2} - \frac{\hbar^2}{m_e} \frac{\partial \psi}{\partial x} = \frac{i\hbar}{m_e} p \cdot$$

Next I derive (13.96) with (13.95):

$$\langle f | \mathbf{p} | i \rangle = -i \frac{m_e}{\hbar} \langle f | [\mathbf{r}, H_0] | i \rangle = -i \frac{m_e}{\hbar} \langle f | \mathbf{r} H_0 - H_0 \mathbf{r} | i \rangle.$$

Operate $\mathbf{r} H_0$ on f and $H_0 \mathbf{r}$ on i .

Then

$$-i \frac{m_e}{\hbar} \langle f | \mathbf{r} H_0 - H_0 \mathbf{r} | i \rangle = -i \frac{m_e}{\hbar} \langle f | \mathbf{r} E_f - \mathbf{r} E_i | i \rangle = -i \frac{m_e}{\hbar} \langle f | \mathbf{r} (E_f - E_i) | i \rangle.$$

Finally with (13.60) and $\omega = -\omega_{fi}$:

$$-i \frac{m_e}{\hbar} \langle f | \mathbf{r} (E_f - E_i) | i \rangle \rightarrow (13.96).$$

(13.104) is evaluated for the unit sphere.

Straightforward applying the goniometrical building blocks:

$$\int_0^{2\pi} \int_0^\pi \sin^3 \theta \cos^2 \phi d\theta d\phi = \frac{4\pi}{3}.$$

13.9 Spontaneous Emission

It is about emission without external radiation.

In (13.109) the expression for the energy spectrum of black body radiation is presented.

In (13.84) -(13.86) I assumed $\rho(\omega)/\omega^2$ to be a “reasonable smooth” function. Well, in (13.109) we see:

$$\rho(\omega)/\omega^2 \propto \omega / [\exp(\frac{\hbar\omega}{k_B T}) - 1].$$

Keep in mind (13.97) and (13.98).

Then with (13.109), (13.116) and (13.117) are obtained.

To conclude this section Fp estimated the typical value of the spontaneous emission for a hydrogen atom.

13.10 Radiation from a Harmonic Oscillator.

An electron in a one-dimensional harmonic oscillator is analysed.

To obtain (13.120) look at the three Dimensional expression (13.99).

When the probability of spontaneous emission is zero, (13.115), the electric dipole is zero.

In (13.121), for $n > n' \rightarrow \delta(n, n' + 1) = 1$ and $\delta(n, n' - 1) = 0$.

Top of page 191 “...whose quantum numbers differ by unity.” This is just a statement about the harmonic oscillator?

The mean radiated power: in each “unity step” $\hbar\omega_0$ is radiated. Consequently, the mean radiated power is $\hbar\omega_0$ times the transition probability per unit time.

In (13.126) use has been made of:

$$E_n - \frac{1}{2} \hbar\omega_0 = n \hbar\omega_0.$$

13.11 Selection Rules

In this section Fp dealt with the spontaneous transition between the different energy levels of a hydrogen atom.

Here we have to consider the radial – and orbital quantum numbers.

Keep in mind: when the dipole moment is zero , the transition probability is zero.

I suppose (13.129) should read:

$$x_{\pm} = x \pm iy , \text{ a typo.}$$

To obtain (13.130), plug (13.129) into the commutator:

$$[L_z, x_{\pm}] = L_z(x \pm iy) - (x \pm iy)L_z .$$

In the subsequent analysis remember the commutator operates on the wave function

$$\begin{aligned} L_z(x \pm iy)\psi - (x \pm iy)L_z\psi &= L_z(x \pm iy)\psi + (x \pm iy)L_z\psi - (x \pm iy)L_z\psi = \\ &= L_z(x \pm iy)\psi . \end{aligned} \quad (\text{C.13.E.8})$$

Furthermore, I use

$$L_z = xp_y - yp_x .$$

Then, with (C.13.E.8):

$$\begin{aligned} L_z(x \pm iy) &= (xp_y - yp_x)(x \pm iy) = x^2p_y + \hbar x + ixyp_y + i\hbar y - yxp_x - iy^2p_x = \\ &= \hbar x_{\pm} + x_{\pm}L_z . \end{aligned}$$

So,

$$[L_z, x_{\pm}] = \hbar x_{\pm} ,$$

and,

$$[L_z, x_{\pm}] = \pm \hbar x_{\pm} , \text{ (13.130).}$$

This is the result of the operation of the commutator on the wave function.

In (13.131), $L_z x_{\pm}$ operates on m resulting into $\hbar m x_{\pm}$ and $x_{\pm} L_z$ operates on m' giving $\hbar m' x_{\pm}$.

(13.132) is found in a similar way. See for example (12.63).

The results for x and y are obtained with:

$$x = (x_{+} + x_{-})/2 ,$$

and

$$y = -i(x_{+} - x_{-})/2 .$$

In this way the selection rules for electric dipole transitions are obtained.

13.12 2P→1S Transitions in Hydrogen

In this section Fp calculates the rate of spontaneous emission between the first excited state and the ground-state of a hydrogen atom.

Keep in mind: P and S are explained at the bottom of page 167 of the Undergraduate Course.

In (13.135), $R_{n,l}$ and $Y_{l,m}$ are given by (9.65), (9.66), (8.91) and (8.92) respectively.

For example, with $z = r \cos \theta$, to find (13.138) the following integral need to be evaluated:

$$\int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} R_{1,0} Y_{0,0} r \cos \theta R_{2,1} Y_{1,0} r^2 \sin \theta dr d\theta d\phi .$$

With all the ingredients available (13.138) results.

The dipole moment for $m = 0$ is found with:

$$|\langle 1,0,0 | ez | 2,1,0 \rangle|^2 \text{ and (13.138).}$$

The dipole moment for $m = \pm 1$ is found with:

$$|\langle 1,0,0 | ex | 2,1, \pm 1 \rangle|^2 + |\langle 1,0,0 | ey | 2,1, \pm 1 \rangle|^2 , \text{ (13.136) and (13.137).}$$

(13.140) is found with (13.123).

So,

$$\hbar\omega_0 = E_2 - E_1 = \frac{E_0}{2^2} - \frac{E_0}{1^2} = -\frac{3}{4}E_0.$$

α in (13.142) is defined on page 190, just below (13.118).

In (13.143) the mean life time of a first excited state of 2P of the hydrogen atom is presented. (See (13.90) and exercise 3 page 6 of my notes).

The spectral line-width is calculated and given in (13.145).

This is based on

$$\lambda = \frac{2\pi c}{\omega}.$$

Then

$$\frac{\Delta\lambda}{\lambda} \sim \frac{2\pi c}{\omega^2 \lambda} \Delta\omega = \frac{\hbar\Delta\omega}{\hbar\omega} = \frac{\Delta E_{2P}}{\hbar\omega}.$$

Remarks with respect to (13.136)-(13.138):

$$-\langle 1,0,0|ex|2,1,0\rangle = 0,$$

$$-\langle 1,0,0|ey|2,1,0\rangle = 0.$$

Is $m = 0$ just for z ?

What do I find for $\langle 1,0,0|ez|2,1,\pm 1\rangle$? The first relevant integral to evaluate is:

$$\int_0^{2\pi} e^{i\phi} d\phi = 0, \quad (8.93).$$

Hence, $\langle 1,0,0|ez|2,1,\pm 1\rangle$ does not exist.

What about a transition between the second excited state and the ground-state?

Due to the selection rules, the only transition is $3P \rightarrow 1S$.

Consequently, I have to evaluate:

$$\langle 1,0,0|ex|3,1,\pm 1\rangle,$$

$$\langle 1,0,0|ey|3,1,\pm 1\rangle$$

and

$$\langle 1,0,0|ez|3,1,0\rangle.$$

13.13 Intensity Rules

In this section Fp discussed the effect of spin for the hydrogen atom.

To derive (13.146), I use (12.138):

$$n = 2, j = \frac{3}{2} \rightarrow \Delta E_{1,\frac{1}{2},\frac{3}{2},m_j} = \frac{E_2\alpha^2}{4} \left(1 - \frac{3}{4}\right) = \frac{\alpha^2}{64} E_0,$$

$$n = 2, j = \frac{1}{2} \rightarrow \Delta E_{1,\frac{1}{2},\frac{1}{2},m_j} = \frac{E_2\alpha^2}{4} \left(2 - \frac{3}{4}\right) = \frac{5\alpha^2}{64} E_0.$$

Hence,

$$\Delta E_{1,\frac{1}{2},\frac{3}{2},m_j} - \Delta E_{1,\frac{1}{2},\frac{1}{2},m_j} = \Delta E = -\frac{\alpha^2}{16} E_0, \quad (13.146).$$

On the middle of page 194: "Well, we have seen the transition rate is independent of spin.....".

In (13.77) H_1 does not contain spin operators. On page 193, below (13.139), the transition rate is also independent of m . Consequently, the transition rate is independent on m_j . Hereafter Fp writes: "However, if this is the case, then the transition rate is plainly also independent of j ." What about l ? Well, for any transition into the ground state $l = 1$. However, for $n = 3 \rightarrow n = 2$ we have $l = 2$ and $l' = 1$.

13.14 Forbidden Transitions.

To analyse forbidden transitions Fp used the second term in the expansion (13.93).

The forbidden transition is estimated to be by a factor $(kr)^2$ smaller than the dipole transition.

With the estimations of Fp:

$$(kr)^2 \sim \left(\frac{a_0}{\lambda}\right)^2.$$

With the expressions for a_0 , α , an approximation of the wave length $\lambda \sim \frac{\hbar c}{|E_0|} = |R|$, (9.79) and

$|E_0| = \frac{\alpha^2}{2} m_e c^2$ (see page 123) I obtained:

$$(kr)^2 \sim \alpha^2.$$

No Exercises

14 Variational Methods

14.1 Introduction

In this chapter a common method for finding approximate solutions of Schrödinger's equation is a method based on the variational principle.

14.2 Variational principle

The time-independent Schrödinger equation is solved by the variational principle.

With a good approximation for the ground-state wave, $\widetilde{\psi}_0$, Fp mentioned:

$\langle \psi | H | \psi \rangle \geq E_1$, (14.13), is easily demonstrated.

Well, I use $\langle \psi | \widetilde{\psi}_0 \rangle = 0$, given by Fp, then with (14.6),

$$\langle \psi | \widetilde{\psi}_0 \rangle = \langle c_0 \widetilde{\psi}_0 + c_1 \psi_1 + c_2 \psi_2 \dots \dots | \widetilde{\psi}_0 \rangle = 0 \rightarrow c_0 = 0.$$

Given this result, (14.10) leads to:

$$|c_1|^2 = 1 - \sum_{n>1} |c_n|^2,$$

and (14.9) – (14.11) :

$$\langle \psi | H | \psi \rangle = E_1 + \sum_{n>1} |c_n|^2 (E_n - E_1) \rightarrow (14.13).$$

This cannot continue for reasons mentioned by Fp. Additionally, it cannot give (14.3) and (14.6), since in that case ψ_n constitutes no complete set. Note: Fp did not write $\langle \psi | \widetilde{\psi}_0 \rangle \approx 0$.

14.3 Helium atom

In this section Fp calculates the ground-state with the variational principle.

In (14.30) the cosine rule is used.

The approximation for the ground-state energy $\langle H \rangle$ is obtained by minimizing the Hamiltonian with respect to the charge number Z . In this way an effective charge number is found.

14.4 Hydrogen Molecule Ion

In this section Fp investigated the possibility of a bound state.

In (14.63) use has been made of the cosine rule. Furthermore, obviously $x = \frac{r}{a_0}$.

In (14.69), the first term on the right hand side should read: $E_0 \psi_{\pm}$

To obtain (14.70) $\frac{e^2}{4\pi\epsilon_0}$ is replaced by $-2E_0a_0$, (9.57) and (9.58).

Keep in mind the symmetry by calculating $\langle \psi_{\pm}^* | H | \psi_{\pm} \rangle$.

So:

$$\left\langle \psi_0(\mathbf{r}_1) \left| \frac{a_0}{r_2} \right| \psi_0(\mathbf{r}_1) \right\rangle = \left\langle \psi_0(\mathbf{r}_2) \left| \frac{a_0}{r_1} \right| \psi_0(\mathbf{r}_2) \right\rangle,$$

and

$$\left\langle \psi_0(\mathbf{r}_2) \left| \frac{a_0}{r_2} \right| \psi_0(\mathbf{r}_1) \right\rangle = \left\langle \psi_0(\mathbf{r}_1) \left| \frac{a_0}{r_1} \right| \psi_0(\mathbf{r}_2) \right\rangle.$$

Fp established the bound state for H_2^+ ion.

No Exercises

15 Scattering Theory.

15.1 Introduction.

In this chapter the quantum theory of scattering is examined.

15.2 Fundamentals

The Hamiltonian of a free particle with scattering potential is presented.

It is about energy conserving scattering → Elastic scattering.

Scattering means the existence of an incident beam of particles.

The Helmholtz equation is introduced: (15.7) with solution (15.8).

(15.10) is obtained with the cosine rule:

$$\lim_{r \gg r'} |\mathbf{r} - \mathbf{r}'| = \lim_{r \gg r'} \sqrt{r^2 + (r')^2 - 2\mathbf{r} \cdot \mathbf{r}'} = r - \hat{\mathbf{r}} \cdot \mathbf{r}' + O\left(\frac{(r')^2}{r}\right). \quad (\text{C.15.E.1})$$

In (C.15.E.1) $\hat{\mathbf{r}}$ is the unit vector and I used the notation of Mahan page 181 or 322. Mahan illustrated the scattering in Figure 7.8, page 232.

Remark: Fp denotes $\hat{\mathbf{r}}/r$ to be the unit vector.

Then in (15.13) Fp introduced the probability flux (i.e., particle flux) as given in Section 7.2.

There, in 3-D, the probability flux reads:

$$\mathbf{j} = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi).$$

In (15.13):

$\mathbf{j} = \frac{\hbar}{m} \text{Im}(\psi^* \nabla \psi)$. This can be considered as a concise notation. It took me a moment to draw that conclusion.

(15.3) represents the incident beam of particles. The incident particle flux is given by (15.14).

The scattered wave function gives the flux of the scattered particles, with (15.3) and (15.13),:

$$\mathbf{j}' = \frac{\hbar}{m} \text{Im}[(\psi - \psi_0)^* \nabla (\psi - \psi_0)].$$

Then I obtained (15.15), except for \mathbf{v}' I found \mathbf{v} . Since after differentiating I obtained the quotient $\frac{\hbar k}{m} = \mathbf{v}$ in (15.15). Well, is that a problem? I do not think so. At the end of section 15.2

Fp mentioned the scattering conserves energy. However, there is still a difference, since Fp mentioned $|\mathbf{v}'|$ to be equal to $|\mathbf{v}|$. I cannot explain the difference obsolete.

15.3 Born Approximation

In this section Fp assumed the total wave function not differ substantially from the incident wave function as given in section 15.2 .

(15.21) results from the isosceles triangle with $|k| = |k'|$, as explained by Fp.

As an example of the scattering potential Fp considered the Yukawa potential presented in (15.22):

$$V(r) = \frac{V_0 e^{-\mu r}}{\mu r} ,$$

$$r \rightarrow 0 : V(r) \rightarrow \infty \text{ and } r \rightarrow \infty : V(r) \rightarrow 0 .$$

(15.24) is found by integration by parts twice.

Just above (15.27) Fp writes: “..provided $\frac{V_0}{\mu} \rightarrow \frac{ZZ' e^2}{4\pi\epsilon_0}$.” ZZ' ? I could not find ZZ' .

$$\text{In (15.28), } E = \frac{(\hbar k)^2}{2m} .$$

Intermezzo: Yukawa Potential and Bound States

In Mahan, section 2.5.1, a similar example of an exponential potential is presented. Solutions are presented in terms of Bessel functions (one-dimensional case).

The potential is:

$$V = -|V_0| e^{\frac{2x}{a}} .$$

Then we can set $a = \frac{2}{\mu}$.

The threshold for bound states is:

$$\left(\frac{8m|V_0|}{\hbar^2 \mu^2} \right)^{\frac{1}{2}} = 2.4 ,$$

or

$$\frac{2m|V_0|}{\hbar^2 \mu^2} = 1.44$$

This number, 1.44, is pretty close to the threshold as calculated by Fp: 2.7.

There is more. In *Bound States and Critical Behaviour of the Yukawa Potential*, Luo et al took the Yukawa potential to be

$$V(r) = -\frac{\lambda e^{-\alpha r}}{r} .$$

Compare this potential with the one presented by Fp, then

$$\mu = \alpha \text{ and } |V_0| = \lambda \alpha .$$

In the paper by Luo et al, the Schrödinger equation is solved numerically and with the Monte Carlo Hamiltonian approach.

The critical value for bound states is:

$$\alpha_c = 1.19\lambda .$$

For the threshold I obtained, using the notation of Fp,:

$$\frac{|V_0|}{\mu^2} \geq 1.19 .$$

In (15.31) the threshold for bounds states reads:

$$\frac{2m}{\hbar^2} \frac{|V_0|}{\mu^2} \geq 2.7 .$$

We know $\frac{2m}{\hbar^2}$ to be about 16×10^{37} .

The two critical values obtained for the Yukawa potential differ a bit more than an order of magnitude. May be Luo at al included the factor $\frac{2m}{\hbar^2}$ into a new λ .

End of intermezzo.

Just below (15.31) Fp writes V_0 to be a negative number. Hence the Yukawa potential is an attractive potential for the case discussed in this section.

Furthermore Fp concludes, when the Yukawa potential is strong enough, then the Born approximation breaks down. The Born approximation is about continuous states.

I interpret “strong enough” to be: $\frac{2m}{\hbar^2} \frac{|V_0|}{\mu^2} < 2.7$.

15.4 Partial Waves

Partial waves are about spherical scattering potential.

In this section θ is the angle subtended between the incoming wavevector \mathbf{k} and the scattered wave factor \mathbf{k}' . \mathbf{k} is aligned with the z-axis. Now, according to Fp, θ is also the angle between \mathbf{r} and \mathbf{k} .

The incoming wave is a plane wave:

$$\psi_0 = \sqrt{n} e^{i\mathbf{k} \cdot \mathbf{r}}.$$

Outside the scattering range the differential equation for the radial part of the wave function is given in equation (15.39). See also (9.25) with $V(r) = 0$ and $E = \frac{k^2 \hbar^2}{2m}$, (9.29).

(15.42) and (15.43) can be found in, i.e., Whittaker and Watson.

(15.44) is the generating function for spherical Bessel functions (Mahan, page 111). With a_l given in (15.48). I suppose (15.44) is just a given expression. May be, it could have been the subject matter of a mathematics undergraduate course.

(15.45) is obtained by integrating the spherical harmonics over the solid angle. No dependence on φ .

Multiply (15.44) with $P_l \cos \theta$. Then (15.46) is found.

The term “Partial Waves” follows from the decomposition of the plane wave into a series of spherical waves, Fp.

Just below (15.56), Fp presented C_l as introduced in (15.52). The implication of the statement on the coefficients of the incoming waves gives:

$$-C_l e^{-i\delta_l} = -i^l (2l + 1).$$

Consequently,

$$C_l = (2l + 1) \exp\left[i\left(\frac{l\pi}{2} + \delta_l\right)\right] \rightarrow (15.56).$$

15.5 Determination of Phase-Shifts

In this section δ_l , derived in section 15.4, is evaluated.

With (15.50), the definitions of A_l and B_l on top of page 215 and

$$C_l = (2l + 1) i^l e^{i\delta_l}, (15.56), (15.60) \text{ and } (15.61) \text{ are obtained.}$$

Below (15.61) Fp introduced the logarithmic derivative as defined in (15.68), and calculated the logarithmic of the radial wave function $R_l(r)$ just outside the range of the potential $V(r)$ at $r = a$.

The result is presented in (15.62). I do not understand the factor ka in front of the square brackets. I can imagine a factor k .

Fp also indicates the solution for the wave function within the range of the potential. For this solution Fp calculates the logarithmic derivative for $r = a$. By matching the derivatives as presented in (15.69) the phase-shift δ_l is obtained.

15.6 Hard Sphere Scattering

The scheme derived in section 15.5 is tested for a simple example in this section.

(15.71) has been obtained from (15.63). On the other hand, the potential is infinite inside the sphere. So, $R_l = 0$ for $r \leq a$. Consequently, with (15.61), (15.71) is found.

As a reminder: the incident plane wave has been decomposed into a series of spherical waves. Then (15.75) is obtained for $l = 0$.

The differential scattering cross-section, (15.17), using (15.57) and $l = 0$, becomes:

$$\frac{d\rho}{d\Omega} = \frac{\sin^2 \delta_0}{k^2},$$

where use has been made of $P_0(\cos \theta) = \sqrt{4\pi} Y_0 = 1$.

Then, with (15.73), (15.79) is found.

(15.81) follows from (15.59) with an upper bound in the summation: l_{\max} .

Now, in (15.81) l_{\max} has been replaced by ka ($\gg 1$). This approximation means l_{\max} to be the integer closest to ka .

The summation of the arithmetic series in (15.82) gives, with $ka \gg 1$:

$$\frac{2\pi}{k^2} (1 + 2ka + 1) \frac{ka}{2} \cong 2\pi a^2.$$

15.7 Low Energy Scattering.

With this type of scattering only S-wave ($l = 0$) scattering is important.

The outside wave function defines the wave function outside the range of the potential ($r > a$).

Consequently, the inside wave function: $r < a$.

The radial wave functions, inside and outside, and their derivatives are matched at $r = a$.

At $r = a$ and $E > V_0$:

the wave functions as given in (15.83) and (15.85) are matched,

the derivatives of the same wave functions are matched.

Then divide the left hand side and the right hand side of both expressions, resulting into:

$$k \cot(ka + \delta_0) - 1 = k' \cot(k'a) - 1 \rightarrow (15.88).$$

Likewise (15.89) is found for $r = a$ and $E < V_0$.

(15.93) has been derived from (15.87).

At the end of this section I suppose for a perfect transmission the scattering cross-section to be zero.

15.8 Resonances

This section is about the exception to the independence of the cross-section on energy.

With (15.96) and $k'a = \frac{\pi}{2} \rightarrow ka \cong 0$. From this result Fp concludes the bound energy for a potential well to be zero. To me it appears to be a continuum state with about zero energy.

Below (15.96) Fp writes: "... the energy of the scattering system ($\frac{k'^2 \hbar^2}{2m}$?) is the same as the energy of the bound state."? The energy of the bound state is about zero. Well, I think this is all about stability and resonance.

No exercises

End of the under-graduate course.

Literature

Abramowitz, M. and I.A. Stegun, *Handbook of Mathematical Functions*, Dover Publications, 1964.

Chisholm, J.S.R., and R.M. Morris, *Mathematical Methods in Physics, Vol II*, North-Holland Publishing Company-Amsterdam, 1964.

Dirac, P. A. M., *The Principles of Quantum Mechanics*, Oxford University Press, fourth edition, 1958.

Feynman, R. P., Leighton, R. B., and M. Sands, *The Feynman Lectures on Physics*, Pearson Addison Wesley, edition 2006.

Fitzpatrick, R., *Quantum Mechanics Lectures*, <http://farside.ph.utexas.edu> .

Luo, X. Q. ,Li, Y. Y. and H. Kröger, *Bound States and Critical Behaviour of the Yukawa Potential*, 2008, www.arxiv.org July 2005.

Mahan, G. D., *Quantum Mechanics in a Nutshell*, Princeton University Press, 2009.

Noordzij, L., *Quantum Mechanics and Theoretical Minimum*, www.leennoordzij.me ,2015.

Noordzij, L., *Quantum Mechanics in Texas Part 3*, www.leennoordzij.me, 2019.

Susskind, L. and Art Friedman, *Quantum Mechanics, The Theoretical Minimum*, Basic Books 2014.

Whittaker, E.T. and G.N. Watson, *A course of Modern Analysis*, Cambridge at The University Press, 1950.

