Quantum Mechanics in Texas, The Graduate Course

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dr.l.noordzij@leennoordzij.nl
www.leennoordzij.me

Remarks, Questions and Exercises.
Based on the *Graduate Course* by Fitzpatrick, Professor of Physics

http://farside.ph.utexas.edu
Quantum Mechanics Homepage for Richard Fitzpatrick
I shall also refer several times to *The Undergraduate Course of Fitzpatrick*(Fp).
The equations in my notes are presented by: (C.x.xx) .
The equations of The (Under)Graduate Course by: (x.xx) .

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1 Fundamental Concepts

1.1 Breakdown of Classical Physics

In this section Fp demonstrates the need for the departure of classical physics.

1.2 Photon Polarization

In this section Fp illustrates the role of quantum mechanics for the polarization of photons.

1.3 fundamental Principles of Quantum Mechanics

In this section Fp presented three fundamental principles.

1.4 Ket Space

In this section Fp introduced Dirac's quantum algebra.

1.5 Bra Space

Here Dirac's Algebra is further completed.
The principal of dual correspondence is defined.
Most of the time I shall refer to equations without prefix: Eq.
Fp: (1.20) "*is easily demonstrated*":
- (1.19) → $\langle B|A\rangle = \sum_i^N \beta_i^* \alpha_i$.
- (1.16) and (1.8)→ $\langle A|B\rangle = \sum_{i,j}^N \alpha_i^* \beta_j \langle i|j\rangle = \sum_{i,j}^N \alpha_i^* \beta_j \delta_{ij} = \sum_i^N \alpha_i^* \beta_i$.

The complex conjugate of $\langle A|B\rangle \rightarrow \langle A|B\rangle^* = \sum_i^N \alpha_i \beta_i^*$.
Then (1.19) and $\langle A|B\rangle^* = \sum_i^N \alpha_i \beta_i^* \rightarrow \langle B|A\rangle = \langle A|B\rangle^* \rightarrow (1.20)$.
In deriving (1.24), keep in mind $\sqrt{\langle A|A\rangle}$ is a number and $\langle A|A\rangle$ is a real number.

1.6 Operators

In this section operators are introduced. From a historical point of view, it is nice to know why Fp called an operator a machine. Well, as indicated by Susskind(page 52), Wheeler *"liked to call such objects machines".*
Just below (1.37), Fp mentioned the adjoint of the adjoint operator is equivalent to the original operator:
$(X^\dagger)^\dagger = X$.
Proof: with (1.35)
$X|A\rangle \leftrightarrow \langle A|X^\dagger \leftrightarrow (X^\dagger)^\dagger|A\rangle \longrightarrow (X^\dagger)^\dagger = X.$ (C.1.1)
To prove (1.37), use is made of (C.1.1) and the assumption $(XY)^\dagger = Y^\dagger X^\dagger$ to be correct.
Proof:
Take the adjoint of $(XY)^\dagger = Y^\dagger X^\dagger$:
$[(XY)^\dagger]^\dagger = [Y^\dagger X^\dagger]^\dagger.$ (C.1.2)
Apply (C.1.1) to the left hand side of (C.1.2)
$[(XY)^\dagger]^\dagger = XY.$
Use $(XY)^\dagger = Y^\dagger X^\dagger$ to be correct, then for the right hand side of (C.1.2)
$(Y^\dagger X^\dagger)^\dagger = (X^\dagger)^\dagger (Y^\dagger)^\dagger = XY.$
No contradiction has been found.
Consequently, the above "assumption to be correct" is correct.
Furthermore, Fp indicated $\langle B|X^\dagger|A\rangle = (\langle A|X|B\rangle)^*$, (1.36), to be easily demonstrated.
Already demonstrated
$\langle B|A\rangle = \langle A|B\rangle^*$, (1.20).
Plug into the left hand side of (1.20)
$|A\rangle = \chi^\dagger|C\rangle.$
The right hand side of (1.20) becomes:
$\langle C|\chi|B\rangle^*,$
where use has been made of (1.35) and (C.1.1).
Hence,

$\langle B|\chi^{\dagger}|C\rangle = (\langle C|\chi|B\rangle)^{*}$,
for any $|C\rangle$.

1.7 Outer Product

In this section the product $|B\rangle\langle A|$, (1.39), is evaluated.
Fp indicates:
$(|B\rangle\langle A|)^{\dagger} = |A\rangle\langle B|$, (1.41), *is easily demonstrated.*
Well, since $|B\rangle\langle A|$ is an operator, I assume (1.41) to be correct.
So, take the adjoint of the left hand side and the right hand side of (1.41):
$[(|B\rangle\langle A|)^{\dagger}]^{\dagger} = (|A\rangle\langle B|)^{\dagger}$. (C.1.3)
With (C.1.2), $[(|B\rangle\langle A|)^{\dagger}]^{\dagger}$ in (C.1.3) becomes:
$[(|B\rangle\langle A|)^{\dagger}]^{\dagger} = |B\rangle\langle A|$.
Consequently, with (C.1.3):
$|B\rangle\langle A| = (|A\rangle\langle B|)^{\dagger}$, or $|A\rangle\langle B| = (|B\rangle\langle A|)^{\dagger}$.
So, the assumption of (1.41) to be correct is not contradicted.

1.8 Eigenvalues and Eigenvectors

The eigenkets and their eigenvalues are discussed.
Reminder: a Hermitian operator is its own adjoint:
$\xi = \xi^{\dagger}$.
Fp proved eigenvalues to be real numbers.
Here I present the case for one ket. The eigenket and eigen value of the operator ξ are:
$\xi|\xi'\rangle = \xi'|\xi'\rangle$, (1.44),
and the dual bra
$\langle\xi'| = \xi'^{*}\langle\xi'|$. (C.1.4)
Multiply (1.44) with $\langle\xi'|$ and (C.1.4) with $|\xi'\rangle$.
Comparing both expressions and with normalization $\langle\xi'|\xi'\rangle = 1$ leads to
$\xi' = \xi'^{*}$, and consequently, ξ' is real.
Now with $|\xi'\rangle$ and $|\xi''\rangle$ to be different states and with different eigenvalues as presented in (1.46), (1.48)
$\langle\xi''|\xi'\rangle = 0$,
is obtained with the conclusion the eigenkets to be orthogonal.

1.9 Observables

This section is about the results of a measurement. A measurement can considered to be represented by an operator. The operator works on a ket. The result of this measurement, i.e., the operator is the observable or eigenvalue of the ket or state.

1.10 Measurements

The result of a measurement is the eigenvalue, a real number.
On page 16, Fp writes: (1.51)-(1.53) are easily demonstrated.
Instead of ξ' I shall use i.
$|A\rangle = \sum_i \alpha_i |i\rangle$, (1.11),
where $|i\rangle$ represents a complete set of independent eigenstates.
Multiply into (1.11) a bra of a particular eigenstate, $|j\rangle$ say.
Then,
$\langle j|A\rangle = \sum_i \alpha_i \langle j|i\rangle$, (C.1.5)

and
$\langle j|i\rangle = \delta_{ij}$, (1.13).
Consequently, in (C.1.5)
$\langle j|A\rangle = \alpha_j$. Plug this result into (1.11), with (1.13)
$|A\rangle = \sum_i \langle i|A\rangle\, |i\rangle = \sum_i |i\rangle\, \langle i|A\rangle$, (1.51).
Simarlily, (1.52) is obtained.
Below (1.53) Fp writes: *"Note all the above results follow from the extremely useful (and easily proved result*
$\sum_i |i\rangle\langle i| = 1$, *(1.54)."*
Well, I did not use (1.54) to find (1.51) and (1.52). I just presented the results of Susskind page 34
$|A\rangle = \sum_i |i\rangle\, \langle i|A\rangle$, (1.51).
$|A\rangle = (\sum_i |i\rangle\, \langle i|A\rangle \rightarrow \ \sum_i |i\rangle\langle i| = 1.$

Remark: The proof of this outer product is presented by Dirac, pages 62 and 63 for the basic vectors given in Eq.(22).

To find (1.53), multiply (1.51) by the bra $\langle A|$ and use (1.20).
Then Fp discussed the transition probability. Just above (1.51), on page 16, Fp guessed the probability. In Lecture 3, Susskind defined this as Principle 4.

1.11 Expectation value

In this section Fp answered the question about the mean value of the measurement.
The mean value or expectation value of the operator $\langle \xi \rangle$ is given in (1,58). See also *The Undergraduate Course*, section 4.4, Fp.
All states are eigenstates of the unity operator $U = \begin{pmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix}$:

$$\begin{pmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix} \begin{pmatrix} \ \end{pmatrix} = \begin{pmatrix} \ \end{pmatrix}.$$

So,
$U|A\rangle = |A\rangle$,
for any $|A\rangle$.

1.12 Degeneracy

In this section Fp shows how to construct orthogonal degenerate eigenstates.
The result is shown in (1.61) and (1.62).
The assumption is the two eigenstates $|\xi'_a\rangle$ and $|\xi'_b\rangle$ are not orthogonal. I assume these eigenstates to be normalized. In addition one of the new two states:
$|\xi'_1\rangle = |\xi'_a\rangle$,(1.61).
A slightly different approach to construct two mutually orthogonal degenerate states by expressing $|\xi'_2\rangle$ in $|\xi'_a\rangle$ and $|\xi'_b\rangle$:
$|\xi'_2\rangle = \alpha|\xi'_a\rangle + \beta|\xi'_b\rangle$, (C.1.6)
where α and β are, in general, complex numbers.
Then, with (C.161) and (C.1.6):

$$\langle \xi'_a|\xi'_2\rangle = 0 = \alpha + \beta\langle \xi'_a|\xi'_b\rangle \rightarrow \beta = -\frac{\alpha}{\langle \xi'_a|\xi'_b\rangle}, \tag{C.1.7}$$

and

$\langle \xi'_a|\xi'_b\rangle$ can also be a complex number.
(C.1.6) and (C.1.7):

$$|\xi'_2\rangle = \alpha \frac{\langle \xi'_a|\xi'_b\rangle |\xi'_a\rangle - |\xi'_b\rangle}{\langle \xi'_a|\xi'_b\rangle},$$

so,

$$|\xi'_2\rangle = \alpha[|\xi'_a\rangle - \frac{\langle \xi'_a|\xi'_b\rangle^* |\xi'_b\rangle}{|\langle \xi'_a|\xi'_b\rangle|^2}]. \tag{C.1.8}$$

With $\langle \xi'_2|\xi'_2\rangle = 1$ an expression for α is obtained, using $\langle \xi'_a|\xi'_b\rangle^* = \langle \xi'_b|\xi'_a\rangle$,

$$1 = |\alpha|^2 \left[\langle \xi'_a| - \frac{\langle \xi'_a|\xi'_b\rangle}{|\langle \xi'_a|\xi'_b\rangle|^2}\langle \xi'_b|\right]\left[|\xi'_a\rangle - \frac{\langle \xi'_a|\xi'_b\rangle^*}{|\langle \xi'_a|\xi'_b\rangle|^2}|\xi'_b\rangle\right] \rightarrow$$

$$\rightarrow 1 = |\alpha|^2[1 - \frac{\langle \xi'_a|\xi'_b\rangle^*}{|\langle \xi'_a|\xi'_b\rangle|^2}\langle \xi'_a|\xi'_b\rangle - \frac{\langle \xi'_a|\xi'_b\rangle}{|\langle \xi'_a|\xi'_b\rangle|^2}\langle \xi'_b|\xi'_a\rangle + \frac{1}{|\langle \xi'_a|\xi'_b\rangle|^2}] \rightarrow$$

$$\rightarrow 1 = |\alpha|^2[1 - 1 - 1 + \frac{1}{|\langle \xi'_a|\xi'_b\rangle|^2}]. \tag{C.1.9}$$

$\alpha = |\alpha|e^{i\gamma}$
I choose the positive value of α and neglect the arbitrary phase angle γ, with (C.1.9)

$$\alpha = \sqrt{\frac{|\langle \xi'_a|\xi'_b\rangle|^2}{1-|\langle \xi'_a|\xi'_b\rangle|^2}}. \tag{C.1.10}$$

Again I choose the positive value of $\sqrt{|\langle \xi'_a|\xi'_b\rangle|^2}$, neglecting the arbitrary phase angle, with (C.1.10):

$$\alpha = \frac{\langle \xi'_a|\xi'_b\rangle}{\left[1-|\langle \xi'_a|\xi'_b\rangle|^2\right]^{1/2}}. \tag{C.1.11}$$

Then, with (C.1.8) and (C.1.11):

$$|\xi'_2\rangle = \frac{\langle \xi'_a|\xi'_b\rangle |\xi'_a\rangle - |\xi'_b\rangle}{\left[1-|\langle \xi'_a|\xi'_b\rangle|^2\right]^{1/2}}. \tag{C.1.12}$$

Except for the minus sign, (C.1.12) equals (1.62).
The procedure to derive two new orthogonal states, is the Gram-Schmidt Procedure (Susskind, pages 67-69). A slightly different approach.

1.13 Compatible Observables

This section is about the simultaneously measurement of two observables and commutation. The Stern-Gerlach apparatuses are mentioned (see also Feynman, ea.,).
First Fp introduced compatible observables.
Then, incompatible observables are discussed.
This section ended with commutation when dealing with compatible observables.

Page 18: simultaneous measurable means for the two observables to possess simultaneous eigenstates⇒Eqs.(1.63) and (1.64). Left-multiply (1.63) with η:
$\eta\xi|\xi'\eta'\rangle = \eta\xi'|\xi'\eta'\rangle = \xi'\eta|\xi'\eta'\rangle = \xi'\eta'|\xi'\eta'\rangle$.
Left-multiply (1.64) with ξ:
$\xi\eta|\xi'\eta'\rangle = \xi\eta'|\xi'\eta'\rangle = \eta'\xi|\xi'\eta'\rangle = \eta'\xi'|\xi'\eta'\rangle$.
ξ' and η' are (complex) numbers. Hence, $\xi'\eta' - \eta'\xi' = 0$.
Now, take the difference of $\eta\xi|\xi'\eta'\rangle$ and $\xi\eta|\xi'\eta'\rangle$ ⇒Eq.(1.65), leading to the conclusion at the top of page 19 ⇒eq.(1.67).
A slightly different approach based on : *"Every eigenstate of η should also be an eigenstate of ξ"*.
$\xi|\xi'\rangle = \xi'|\xi'\rangle$,
and
$\eta|\eta'\rangle = \eta'|\eta'\rangle$.
Assume $|\eta'\rangle$ to be an eigenfunction of ξ:
$\xi|\eta'\rangle = \xi'|\eta'\rangle$, left-multiply this expression with η ⇒
⇒ $\eta\xi|\eta'\rangle = \eta\xi'|\eta'\rangle = \xi'\eta|\eta'\rangle = \xi'\eta'|\eta'\rangle$.
Now left-multiply $\eta|\eta'\rangle = \eta'|\eta'\rangle$, with ξ ⇒
⇒ $\xi\eta|\eta'\rangle = \xi\eta'|\eta'\rangle = \eta'\xi|\eta'\rangle = \eta'\xi'|\eta'\rangle$.
Take the difference of $\xi\eta|\eta'\rangle = \eta'\xi'|\eta'\rangle$ and $\eta\xi|\eta'\rangle = \xi'\eta'|\eta'\rangle$ ⇒ $(\xi\eta - \eta\xi)|\eta'\rangle = |0\rangle$, leading to the conclusion at the top of page 19 ⇒eq.(1.67).

Remark: Dirac made, on page 28, a remark on operators which appears to me to be a bit mystical: *"Thus the conjugate complex of the product of two linear operators equals the product of the conjugate complexes of the factors in reverse order. A simple example of the result, it should be noted, if ξ and η are real, in general $\xi\eta$ is not real."*?

1.14 Uncertainty Relation

In this section the uncertainty relation has been derived.
Derivation of (1.69), with (1.68):
$\langle(\Delta\xi)^2\rangle = \langle(\xi - \langle\Delta\xi\rangle)^2\rangle = \langle\xi^2 - 2\xi\langle\Delta\xi\rangle + \langle\xi\rangle^2\rangle = \langle\xi^2\rangle - 2\langle\Delta\xi\rangle\langle\Delta\xi\rangle + \langle\Delta\xi^2\rangle =$
$\langle\xi^2\rangle - \langle\Delta\xi^2\rangle$.
Then Fp introduced the Schwarz inequality.
In (1.72) consider $|A\rangle$ and $|B\rangle$ orthonormal. Hence
$1 + |c|^2 > 0$.
(1.76) has been derived using, i.e., $\Delta\xi$ to be Hermitian,
$\langle A|A\rangle = \langle|\Delta\xi^\dagger\Delta\xi|\rangle$,
where $|\rangle$ is a general ket.
In (1.80) Fp proved the commutator $[\Delta\xi, \Delta\eta]$ to be anti-Hermitian.
In my notes on section 1.8, I proved the eigenvalue of an Hermitian operator to be real. Consequently the expectation value of an Hermitian operator is a real number.
Given
$\langle\xi\rangle = \langle A|\xi|A\rangle$, (1.59),
then
$\langle\xi\rangle = \langle A|\xi|A\rangle = \xi'$, where ξ' is a real number.
The property of the anti-Hermitian operator is:
$\xi = -\xi^\dagger$.

Applying the procedure as presented in my notes on section 1.8, leaving out the details:
$\xi' = -\xi'^*$.
So, the eigenvalue ξ' is an imaginary number.
In (1.81), $\langle\{\Delta\xi, \Delta\eta\}\rangle$ is an imaginary number: the expectation value of the anti-Hermitian commutator. With this information (1.82) is obtained and finally the uncertainty relation (1.83).

1.15 Continuous Spectra

In this section Fp dealt with continuous eigenvalues.
The results obtained for a finite-dimensional ket space with discrete eigenvalues are generalized to ket spaces of nondenumerably infinite dimensions.

Exercises

Exercise 1.1 Calculate the radiated energy of a "classical" electron

According to classical physics, a non-relativistic electron whose instantaneous acceleration is of magnitude a radiates electromagnetic energy at the rate

$$P = \frac{e^2 a^2}{6\pi\epsilon_0 c^3}, \qquad \text{(C.1.E.1)}$$

Larmor's formula, where e is the magnitude of the electron charge and ϵ_0 the permittivity of vacuum. Consider a classical electron in a circular orbit of radius r around the proton. Demonstrate that the radiated energy would cause the orbital radius to decrease in time according to

$$\frac{d}{dt}\left(\frac{r}{a_0}\right)^3 = -\frac{1}{\tau},$$

where $a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$, the Bohr radius and $\tau = \frac{a_0}{4c\alpha^4}$.

Here, c is the velocity of light in vacuum and $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$, the fine structure constant.

With (C.1.E.1), the energy of the electron, E decreases by

$$\frac{dE}{dt} = -\frac{e^2 a^2}{6\pi\epsilon_0 c^3}. \qquad \text{(C.1.E.2)}$$

The classical model of the Hydrogen atom: The electron orbits the nucleus.
The centrifugal force is balanced by the Coulomb force, the equation for the circular orbit:

$$\frac{m_e v^2}{r} - \frac{e^2}{4\pi\epsilon_0 r^2} = 0, \qquad \text{(C.1.E.3)}$$

where the instantaneous acceleration

$$a = \frac{v^2}{r}.$$

The energy of the electron

$$E = \frac{1}{2} m_e v^2 - \frac{e^2}{4\pi\epsilon_0 r}. \qquad \text{(C.1.E.4)}$$

Substitute $m_e v^2 = \frac{e^2}{4\pi\epsilon_0 r}$,(C.1.E.3), into (C.1.E.4):

$$E = \frac{1}{2}\frac{e^2}{4\pi\epsilon_0 r}. \qquad \text{(C.1.E.5)}$$

With (C.1.E.5)

$$\frac{dE}{dt} = \frac{e^2}{8\pi\epsilon_0 r^2}\frac{dr}{dt}. \qquad \text{(C.1.E.6)}$$

(C.1.E.3), with $a = \frac{v^2}{r}$,

$$a^2 = (\frac{e^2}{4\pi\epsilon_0 m_e r^2})^2. \qquad \text{(C.1.E.7)}$$

$\frac{dE}{dt}$ given in (C.1.E.2) and (C.1.E.6) gives:

$$-\frac{e^2a^2}{6\pi\epsilon_0 c^3} = \frac{e^2}{8\pi\epsilon_0 r^2}\frac{dr}{dt}. \qquad \text{(C.1.E.8)}$$

Then, with

$\frac{dr}{dt} = \frac{a_0^3}{3r^2}\frac{d}{dt}(\frac{r}{a_0})^3$,

(C.1.E.8), with (C.1.E.7) and the above definitions of $\tau = \frac{a_0}{4c\alpha^4}$ and $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$, results into

$$\frac{d}{dt}(\frac{r}{a_0})^3 = -\frac{1}{\tau}. \qquad \text{(C.1.E.9)}$$

The classical lifetime of a hydrogen atom, with $a_0 = 5.3 \times 10^{-11}$m and $\alpha = \frac{1}{137}$, becomes $\tau \cong 1.56 \times 10^{-11}$ sec.

Exercise 1.2 The equality of the inner product and its conjugate

Demonstrate that

$\langle B|A\rangle = \langle A|B\rangle^*$

in a finite ket space.

- (1.19) → $\langle B|A\rangle = \sum_i^N \beta_i^* \alpha_i$.
- (1.16) and (1.8)→ $\langle A|B\rangle = \sum_{i,j}^N \alpha_i^* \beta_j \langle i|j\rangle = \sum_{i,j}^N \alpha_i^* \beta_j \delta_{ij} = \sum_i^N \alpha_i^* \beta_i$.

The complex conjugate of $\langle A|B\rangle \rightarrow \langle A|B\rangle^* = \sum_i^N \alpha_i \beta_i^*$.

Then (1.19) and $\langle A|B\rangle^* = \sum_i^N \alpha_i \beta_i^* \rightarrow \langle B|A\rangle = \langle A|B\rangle^* \rightarrow (1.20)$.

Exercise 1.3 Derivation of operator relations in ket space. X and Y are general operators

a Demonstrate: $\langle B|X^\dagger|A\rangle = \langle A|X|B\rangle^*$.

In (1.20) and exercise 1.2: $\langle B|A\rangle = \langle A|B\rangle^*$, (1.20).

Plug into the left hand side of (1.20)

$|A\rangle = X^\dagger|C\rangle$.

The right hand side of (1.20) becomes:

$\langle C|X|B\rangle^*$,

where use has been made of (1.35) and (C.1.1).

Hence,

$\langle B|X^\dagger|C\rangle = (\langle C|X|B\rangle)^*$,

for any $|C\rangle$.

This result is presented by Dirac on page 27 (4).

Dirac denotes $X^\dagger$ the adjoint of X.

b Demonstrate: $(XY)^\dagger = Y^\dagger X^\dagger$

In my notes on section 1.6, Operators, I did prove this equality:

Use is made of (C.1.1) and the assumption $(XY)^\dagger = Y^\dagger X^\dagger$ to be correct.

Proof:

Take the adjoint of $(XY)^\dagger = Y^\dagger X^\dagger$:

$[(XY)^\dagger]^\dagger = [Y^\dagger X^\dagger]^\dagger$, (C.1.2) .

Apply (C.1.1) to the left hand side of (C.1.2)

$[(XY)^\dagger]^\dagger = XY$.

Use $(XY)^\dagger = Y^\dagger X^\dagger$ to be correct, then for the right hand side of (C.1.2)
$(Y^\dagger X^\dagger)^\dagger = (X^\dagger)^\dagger (Y^\dagger)^\dagger = XY.$
No contradiction has been found.
Consequently, the above "assumption to be correct" is correct.
Here I present also Dirac's result bottom page 27, using (1.20), (1.35) and (1.36).
" $\langle A| = \langle P|Y$, *and* $\langle B| = \langle Q|X^\dagger$,
so that
$|A\rangle = Y^\dagger|P\rangle$, *and* $|B\rangle = X|Q\rangle$.
with (1.20)
$\rightarrow \langle B|A\rangle = \langle Q|X^\dagger Y^\dagger|P\rangle = \langle A|B\rangle^* = \langle P|YX|Q\rangle^* = \langle Q|(XY)^\dagger|P\rangle$.
This holds for any $|P\rangle$ *and* $|Q\rangle$, *we can infer that* $(XY)^\dagger = Y^\dagger X^\dagger$*".*

c Demonstrate $(X^\dagger)^\dagger = X$.
First I will demonstrate this with (1.35):
$X|A\rangle \leftrightarrow \langle A|X^\dagger \leftrightarrow (X^\dagger)^\dagger|A\rangle \longrightarrow (X^\dagger)^\dagger = X.$
See also Noordzij, page 20 , on operators.
Another proof is based on
(1.36): $\langle B|X^\dagger|A\rangle = \langle A|X|B\rangle^*$.
Plug into (1.36) $X^\dagger$ for X:
$\langle B|(X^\dagger)^\dagger|A\rangle = \langle A|X^\dagger|B\rangle^* = \langle B|X|A\rangle.$
This holds for any ket and bra.
Consequently,
$(X^\dagger)^\dagger = X$.

d Demonstrate $(|B\rangle\langle A|)^\dagger = |A\rangle\langle B|$, (1.41).
I assume (1,41) to be correct.
Take the adjoint of the left hand side and the right hand side of (1.41):
$[(|B\rangle\langle A|)^\dagger]^\dagger = (|A\rangle\langle B|)^\dagger.$ (C.1.E.10)
With $(X^\dagger)^\dagger = X \longrightarrow [(|B\rangle\langle A|)^\dagger]^\dagger = |B\rangle\langle A|.$
Plug this result into (C.1.E.10):
$|B\rangle\langle A| = (|A\rangle\langle B|)^\dagger \longrightarrow |A\rangle\langle B| = (|B\rangle\langle A|)^\dagger.$
So, the assumption of (1.41) to be correct, is not contradicted.
Proof by Dirac:
"….$|A\rangle\langle B|$ is a linear operator. We may get its conjugate complex by referring directly to the definition of the adjoint. Multiplying $|A\rangle\langle B|$ into a general bra $\langle P|$, we get $\langle P|A\rangle\langle B|$, whose conjugate imaginary ket is
$\langle P|A\rangle^*|B\rangle = \langle A|P\rangle|B\rangle = |B\rangle\langle A|P\rangle.$
Hence
$(|A\rangle\langle B|)^\dagger = |B\rangle\langle A|$."
The definition of the adjoint: (1.35)

Exercise 1.4. Hermitian operators commute.

If A and B are Hermitian operators, then demonstrate AB is only Hermitian provided A and B
commute. In addition, show that $(A+B)^n$ is Hermitian, where n is a positive integer.
$A^\dagger = A$ and $B^\dagger = B$.
- AB Hermitian?

$[A,B]=0$ for $AB-BA=0$ or $AB=BA$.
Then
$(AB)^\dagger=B^\dagger A^\dagger=BA=AB$.
Consequently, AB is Hermitian.
- $(A+B)^n$ is Hermitian?
$A^\dagger=A$ and $B^\dagger=B\rightarrow(A+B)^\dagger=A+B$.
I substitute X for $A+B\rightarrow X=X^\dagger$.
What about X^2?
$(XX)^\dagger=X^\dagger X^\dagger=X^2$.
Now I assume $(A+B)^n=(X)^n$ to be Hermitian. So, $(X^n)^\dagger=X^n$.
What about X^{n+1} ?
$[(A+B)^{n+1}]^\dagger=(X^{n+1})^\dagger=(X^nX)^\dagger=X^\dagger(X^n)^\dagger=XX^n=X^{n+1}=(A+B)^{n+1}$.

Exercise 1.5 Show various operators to be Hermitian

Let A be a general operator.
-Show that $A+A^\dagger$ is Hermitian
For a general operator
$(A^\dagger)^\dagger=A\rightarrow(A+A^\dagger)^\dagger=A^\dagger+A=A+A^\dagger$.
-Show $i(A-A^\dagger)$ is Hermitian.
$[i(A-A^\dagger)]^\dagger=-i\left(A^\dagger-A\right)=i(A-A^\dagger)$.
-Show $AA^\dagger$ is Hermitian.
$(AA^\dagger)^\dagger=(A^\dagger)^\dagger A^\dagger=AA^\dagger$.

Exercise 1.6 H is a Hermitian operator. Show $\exp(iH)=\exp(-iH)$.

Given the results of the above exercise: $H^\dagger=H$ and $(H^n)^\dagger=H^n$.
Then:

$$[\exp(iH)\equiv\sum_{n=0}^{\infty}\frac{(iH)^n}{n!}]^\dagger=\sum_{n=0}^{\infty}\frac{(i^nH^n)^\dagger}{n!}=\sum_{n=0}^{\infty}(-\frac{iH)^n}{n!}=\exp(-iH).$$

Exercise 1.7 The outer product

Let $|\xi'\rangle$ be the eigenkets of the observable ξ, whose corresponding eigenvalues, ξ', are discrete. Demonstrate that:
$\sum_{\xi'}|\xi'\rangle\langle\xi'|=1,$
where the sum is over all eigenvalues, and 1 denotes the unit operator.
In section 1.10 on Measurements, $\sum_{\xi'}|\xi'\rangle\langle\xi'|=1$, (1.54) is presented.
In my notes on this section , $\sum_{\xi'}|\xi'\rangle\langle\xi'|=1$ has been demonstrated.
(1.51), $|i\rangle\equiv|\xi'\rangle$:
$|A\rangle=\sum_i|i\rangle\langle i|A\rangle\rightarrow\sum_i(|i\rangle\langle i|)|A\rangle\rightarrow\sum_i|i\rangle\langle i|=1.$

Exercise 1.8 The construction of a mutually orthogonal, unnormalized degenerate eigenkets.

Let $|\xi_i'\rangle$, where $i=1,N$ and $N>1$, be a set of degenerate eigenkets of some observable ξ. Suppose that the $|\xi_i'\rangle$'s are not mutually orthogonal. Demonstrate a set of mutually orthogonal (but unnormalized) degenerate eigenkets, $|\xi_i''\rangle$, for $i=1,N$, can be constructed as follows

$$|\xi_i''\rangle = |\xi_i'\rangle - \sum_{j=1,i-1} \frac{\langle \xi_j''|\xi_i'\rangle}{\langle \xi_j''|\xi_j''\rangle} |\xi_j''\rangle. \qquad \text{(C.1.E.11)}$$

This process is known as *Gram-Schmidt orthogonalization*(Lipschutz).
The subject is discussed in section 1.12 on Degeneracy.

I suppose the $|\xi_i'\rangle$'s to be normalized.
Start with
$|\xi_1''\rangle = |\xi_1'\rangle$.
Consequently, $|\xi_1''\rangle$ is normalized.
With (C.1.E.11)

$$|\xi_2''\rangle = |\xi_2'\rangle - \frac{\langle \xi_1''|\xi_2'\rangle}{\langle \xi_1''|\xi_1''\rangle} |\xi_1''\rangle \rightarrow \quad |\xi_2''\rangle = |\xi_2'\rangle - \langle \xi_1''|\xi_2'\rangle |\xi_1''\rangle, \qquad \text{(C.1.E.12)}$$

and $\langle \xi_1''|\xi_1''\rangle = 1$.
Multiply the bra $\langle \xi_1''|$ into (C.1.E.12):
$\langle \xi_1''|\xi_2''\rangle = \langle \xi_1''|\xi_2''\rangle - \langle \xi_1''|\xi_2''\rangle \langle \xi_1''|\xi_1''\rangle = 0$,
and $|\xi_2''\rangle$ is orthogonal with $|\xi_1''\rangle$.
The exercise is to demonstrate the orthogonality.

Remark: Normalization (n) of $|\xi_2''\rangle$:

$$|\xi_{2n}''\rangle = \frac{|\xi_2'\rangle - \langle \xi_1''|\xi_2'\rangle |\xi_1''\rangle}{\langle \xi_2''|\xi_2''\rangle},$$

where $\langle \xi_2''|\xi_2''\rangle$ is the "length" of the vector.

The third ket with (C.1.E.11),

$$|\xi_3''\rangle = |\xi_3'\rangle - \frac{\langle \xi_1''|\xi_3'\rangle}{\langle \xi_1''|\xi_1''\rangle} |\xi_1''\rangle - \frac{\langle \xi_2''|\xi_3'\rangle}{\langle \xi_2''|\xi_2''\rangle} |\xi_2''\rangle. \qquad \text{(C.1.E.13)}$$

Multiply the bra $\langle \xi_1''|$ into (C.1.E.13) with the result $\langle \xi_1''|\xi_3''\rangle = 0$, since $\langle \xi_1''|\xi_2''\rangle = 0$.
Multiply the bra $\langle \xi_2''|$ into (C.1.E.13) with the result $\langle \xi_2''|\xi_3''\rangle = 0$.
I demonstrated (C.1.E.11) for three new kets.
Now assume it is demonstrated for $(i-1)$ kets.
Multiply the bra $\langle \xi_1''|$ into (C.1.E.11):

$$\langle \xi_1''|\xi_i''\rangle = \langle \xi_1''|\xi_i'\rangle - \sum_{j=1,i-1} \frac{\langle \xi_j''|\xi_i'\rangle}{\langle \xi_j''|\xi_j''\rangle} \langle \xi_1''|\xi_j''\rangle =$$

$$= \langle \xi_1''|\xi_i'\rangle - \frac{\langle \xi_1''|\xi_i'\rangle}{\langle \xi_1''|\xi_1''\rangle} \langle \xi_1''|\xi_1''\rangle - \sum_{j=2,i-1} \frac{\langle \xi_j''|\xi_i'\rangle}{\langle \xi_j''|\xi_j''\rangle} \langle \xi_1''|\xi_j''\rangle = 0,$$

since, for $2 \le j \le i-1 \rightarrow \langle \xi_1''|\xi_j''\rangle = \delta_{1j} = 0$.

Exercise 1.9 About the expectation value of a Hermitian and an anti-Hermitian operator.

-The Expectation value of a Hermitian operator.
Reminder a Hermitian operator is its own adjoint:
$\xi = \xi^\dagger$, (1.39).
First I will prove the eigenvalues to be real numbers. I present the approach of Susskind.

The eigenket and eigenvalue presented in (1.44) of the operator in (1.39) are:
$\xi|\xi'\rangle = \xi'|\xi'\rangle$, (1.44),
and the dual bra, with (1.39),
$\langle\xi'|\xi^\dagger = (\xi')^*\langle\xi'|$. (C.1.E.14)
Multiply (1.44) with $\langle\xi'|$ and (C.1.E.14) with $|\xi'\rangle$.
Comparing both expressions leads to:
$\xi' = (\xi')^*$.
Consequently, the eigenvalue is real. This is just the definition of being a Hermitian operator.

The expectation value, definition,
$\langle\xi\rangle = \langle\xi'|\xi|\xi'\rangle = \xi'\langle\xi'|\xi'\rangle = \xi'$,
and the eigenvalue is a real number.

The property of the anti-Hermitian operator is:
$\xi = -\xi^\dagger$.
(1.44):
$\xi|\xi'\rangle = \xi'|\xi'\rangle$,
and the dual bra, (C.1.E.14)
$\langle\xi'|\xi^\dagger = -(\xi')^*\langle\xi'|$. (C.1.E.15)
Multiply (1.44) with $\langle\xi'|$ and (C.1.E.15) with $|\xi'\rangle$.
Comparing both expressions:
$\xi' = -(\xi')^*$,
and ξ' is imaginary.
Suppose ξ' to be a complex number: $a + ib$,
then $a + ib = -(a + ib)^* \rightarrow a = 0$.
Simarlily, the expectation value of the anti-Hermitian operator is an imaginary number.

Exercise 1.10 The expectation value of the square of a Hermitian operator is ≥ 0.

For the Hermitian operator: $H = H^\dagger$. With the results of Exercise 1.9:
$\langle H^2\rangle = \langle\xi'|HH|\xi'\rangle = \xi'^2 \geq 0$.

Exercise 1.11 Further elaborations on the operator H.

-The Hermitian operator H has the property $H^4 = 1$, where 1 is the unity operator. What are the eigenvalues of H?
Reading of section (1.9)-(1.13) is of some help.
$[H, H] = 0 \rightarrow [H, H^4] = 0$.
So, H and H^4 *are simultaneously measurable,* (1.67) page 19. Then, page 18, *the conditions for two observables H and H^4 to be simultaneously measurable is that they should possess simultaneous eigenstates (i.e., every eigenstate of H should also be an eigenstate of H^4).*
H is a Hermitian operator.
What about H^2?

$H^2 = HH = H^\dagger H^\dagger$.
Consequently
$(H^2)^\dagger = (HH)^\dagger = H^\dagger H^\dagger = HH = H^2$.
Simarlily

H^4 is a Hermitian operator.
I define the eigenstate of H^4 to be $|A\rangle$.
So,
$H^4|A\rangle = |A\rangle.$ (C.1.E.16)
I will prove $H^2|A\rangle$ and $H|A\rangle$ to be eigenvectors of H^4.
$H^2|A\rangle \stackrel{\text{def}}{=} |B\rangle \rightarrow H^4|A\rangle = H^2|B\rangle = |A\rangle.$
It follows that
$H^4|B\rangle = H^2|A\rangle = |B\rangle.$
Hence, $|B\rangle$ is an eigenstate of H^4. So, $H^2|A\rangle$ is an eigenstate of H^4.
Now H.
$H|A\rangle \stackrel{\text{def}}{=} |C\rangle \rightarrow H^4|A\rangle = H^3|C\rangle = |A\rangle.$
It follows that
$H^4|C\rangle = H|A\rangle = |C\rangle.$
Hence, $|C\rangle$ is an eigenstate of H^4. So, $H|A\rangle$ is an eigenstate of H^4 .
Since H, H^2 and H^4 commute, they are simultaneously measurable. Every eigenstate of H^4 is an eigenstate of H. Consequently, the eigenvalue of H is 1.

-What are the eigenvalues of H if H is not restricted to being Hermitian? I suppose Fp still assumes $H^4 = 1$, where 1 is the unity operator.
Now the eigenvalues of H can be complex. However, since H, H^2 and H^4 commute, they are simultaneously measurable. Every eigenstate of H^4 is an eigenstate of H. Consequently, the eigenvalue of H is 1.
Remark:
H^4 is the unity operator.
Are H and H^2 unity operators? Well, the other way around: if H is the unity operator, H^2 and H^4 are. However, for with H^4 the unity operator, the conclusion is not unambiguous.
Set for example H^4 to be the 2×2 unity matrix:
$H^4 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$
What do we find for H^2? I shall leave out the details and present to possible 2×2 matrices for H^2:
$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$
and
$\begin{pmatrix} a & \sqrt{1-a^2} \\ \sqrt{1-a^2} & -a \end{pmatrix},$
where $0 < a \leq 1$.
Given the first, unity matrix for H^2, I again found two 2×2 matrices for H:
$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$
and
$\begin{pmatrix} b & \sqrt{1-b^2} \\ \sqrt{1-b^2} & -b \end{pmatrix},$
where $0 < b \leq 1$.
The second matrix for H^2 did produce contradictory results.

On the basis of this latter result, I conclude, given the unity matrix for H^4, H^2 and H are also represented by unit matrices.

Exercise 1.12 The outer product for a continuous range of eigenvalues.

Let ξ be an observable whose eigenvalues, ξ', lie in a continuous range. Let the $|\xi'\rangle$, where
$\langle\xi'|\xi''\rangle = \delta(\xi' - \xi'')$,
be the corresponding eigenkets. Demonstrate that
$\int d\xi' |\xi'\rangle \langle\xi'| = 1,$ (C.1.E.17)
where the integral is over the whole range of eigenvalues, and 1 denotes the unity operator.
Multiply (C.1.E.17) on the left and on the right with $|\xi''\rangle$:
$\int d\xi' \, |\xi'\rangle\langle\xi'|\xi''\rangle = |\xi''\rangle.$ (C.1.E.18)
Then, with $\langle\xi'|\xi''\rangle = \delta(\xi' - \xi'')$, (C.1.E.18) becomes:
$\int d\xi' \, |\xi'\rangle\delta(\xi' - \xi'') = |\xi''\rangle$, or
$|\xi''\rangle = |\xi''\rangle$.

2. Position and Momentum

2.1 Introduction

In this section the roles of position and momentum are investigated.

2.2 Poisson Brackets

In (2.1) and (2.2) the basic equations of Hamiltonian dynamics are presented.
The Hamiltonian for the 1-D case:

$$H = \frac{p^2}{2m} + V(x),$$

The sum of the kinetic and potential energy with classical coordinates, $q = x$, and canonical momentum $p = mv$. The force $F = -\frac{dV}{dx}$.
So,
$\frac{\partial H}{\partial x} = -F = -m\frac{dv}{dt} = -\frac{dp}{dt}$,
and
$\frac{\partial H}{\partial p} = \frac{p}{m} = v = \frac{dx}{dt}$.
in this section the classical Poisson bracket is presented, (2.3).The relation with quantum mechanics is investigated.
Below (2.14), page 26, a quantum mechanical Poisson bracket is defined:
$[u_1u_2, v_1v_2]_{qm}$.
After evaluating this bracket, the expressions given in (2.18) and (2.19) are found. In these two equations i and $\hbar$ pop up. Why, I paraphrase Susskind page 100: "*You may wonder why I put i and $\hbar$ in front of $[u_1, v_1]_{qm}$. These factors are completely arbitrary at this stage. I use them with an eye to the future".*
Since Fp used some language of Dirac, page 86, I hope to find some additional information there.
Fp writes: $\hbar$ commutes with $(u_1v_1 - v_1u_1)$.
Dirac page 86: *$\hbar$ must commute with* $(u_1v_1 - v_1u_1)$.
Both based their conclusion on (2.18):

$u_1v_1 - v_1u_1 = i\hbar[u_1, v_1]_{qm}$.
Suppose $\hbar$ does not commute with $u_1v_1 - v_1u_1$.
Consequently,
$\hbar(u_1v_1 - v_1u_1) \neq (u_1v_1 - v_1u_1)\hbar$.
Is that possible?
Dirac page 24: "*……and is so* $i(\xi\eta - \eta\xi)$*,* (a real number, Nz). This conclusion of Dirac is based on: "*……though if* ξ *and* η*bare real, in general* $\xi\eta$ *is not real".* As mentioned before, I considered this to be a bit mythical. Or better, I could not find an example. However, accepting Dirac's conclusion on $\xi\eta$, $i(\xi\eta - \eta\xi)$ is a real number.
Then,
$[i(\xi\eta - \eta\xi)]^\dagger = -i(\xi\eta - \eta\xi)^\dagger = -i\left(\eta^\dagger\xi^\dagger - \xi^\dagger\eta^\dagger\right) = i(\xi\eta - \eta\xi)$.
Now with (2.18)
$i(u_1v_1 - v_1u_1) = \hbar[u_1, v_1]_{qm}$.
$\hbar[u_1, v_1]_{qm}$ is a real number, as Fp mentioned just below (2.19).
So,
$\hbar(u_1v_1 - v_1u_1) = (u_1v_1 - v_1u_1)\hbar$,
and $\hbar$ commutes with $u_1v_1 - v_1u_1$.
On the middle of page 27 Fp writes: "The notation $[u, v]$ is conventionally reserved for the commutator $uv - vu$ in quantum mechanics."
Hence,
$[u, v] \equiv i\hbar[u, v]_{qm}$, (2.22).

Susskind, section 4.9, demonstrated the connections between commutators and Poisson brackets. On pages 102 and 103, Susskind presented the time dependent Schrödinger equation. Then for the time dependent expectation value of the observable $\boldsymbol{L}$:
$\frac{d}{dt}\langle \boldsymbol{L} \rangle = -\frac{i}{\hbar}\langle [\boldsymbol{L}, \boldsymbol{H}] \rangle$, (4.18) Susskind is derived. $\boldsymbol{H}$ is the Hamiltonian. After the derivation of (4.18) Susskind presented the connection between Poisson brackets and the quantum mechanical commutator.

At the bottom of page 27, Fp writes:" If two dynamical variables, ξ and η, can be written as power series in the q_i and p_j ……. allows $[\xi, \eta]$ to be expressed in terms of the fundamental commutation relations(2.23)-(2.25)."
For example:
$\left[q_i, q_j\right] = 0 \rightarrow q_iq_j - q_jq_i = 0$.
Multiply this expression into the left with q_i:
$q_i^2q_j - q_iq_jq_i = 0$.
Add to the left hand side and the right hand side of the latter expression $q_jq_i^2$:
$q_i^2q_j - q_iq_jq_i + q_jq_i^2 = q_jq_i^2 \rightarrow q_i^2q_j - q_jq_i^2 - q_iq_jq_i + q_jq_i^2 =$
$q_i^2q_j - q_jq_i^2 - \left(q_iq_j - q_jq_i\right)q_i = \left[q_i^2, q_j\right] - \left[q_i, q_j\right]q_i = 0$.
Consequently,
$\left[q_i^2, q_j\right] = 0$.
And so on.

2.3 Wavefunctions

A system with one classical degree of freedom is considered: the Cartesian coordinate x.
The wave function and the standard ket and bra are introduced. Dirac §20 is of some help to appreciate this particular section on the Wavefunctions.
(2.27) is dealt with in Exercise 1.12.
(2.28) has been derived by multiplying (2.27) to the left and to the right hand side of the equality sign with $|A\rangle$.
The wavefunction $\psi_A(x')$ is defined in (2.29).

Dirac nominated this wavefunction to be the representative of $|A\rangle$ for the complete set of commuting observables x'.

In (2.33) the general function $f(x)$ of the observable x given in front of the first integral, (2.33). In the second integral, (2.33), $f(x'')$ is in integrand. How come? A kind of magic? I look into it in more detail.
With (2.28):
$|B\rangle = \int_{-\infty}^{\infty} dx'' \langle x''|B\rangle |x''\rangle$. (C.2.1)
Substitute $|B\rangle = f(x)|A\rangle$ into (C.2.1):
$|B\rangle = \int_{-\infty}^{\infty} dx'' \langle x''|f(x'')|A\rangle |x''\rangle$. (C.2.2)
Since $f(x)$ is a general function, polynomial, of the observable/operator x, $f(x)$ is Hermitian: $[f(x)]^{\dagger} = f(x)$. Operate x on $|A\rangle$, with the result:
$x|A\rangle = x''|A\rangle$,
x'' is a number.
Hence,
$\langle x''|f(x'')|A\rangle = f(x'')\langle x''|A\rangle = f(x'')\psi_A(x'')$.

2.4 Schrödinger Representation.

The system of section 2.3 is considered.
At the top of page 30 Fp writes: “It follows that ……”, and (2.37) is presented:
$\frac{d}{dx}\psi|\rangle = \frac{d\psi}{dx}|\rangle$,
where $|\rangle$ is the standard ket and in (2.37)
$\frac{d}{dx}|\rangle = 0$.
Let’s find out about (2.39):
with (2.27)
$\int_{-\infty}^{\infty} dx'|x'\rangle\langle x'| = 1$,
and (2.29)
$\langle x'|A\rangle = \psi_A(x')$.
Then with (2.38) and $\frac{d}{dx}|\rangle = 0$:
$\int_{-\infty}^{\infty} dx' \left\langle |\phi \frac{d}{dx'}|x'\rangle\langle x'|\psi(x')|\right\rangle = \int_{-\infty}^{\infty} dx'\langle|\phi|x'\rangle\langle x'|\frac{d\psi}{dx'}|\rangle$. (C.2.3)
Use (2.29):
and $\langle x'|A\rangle \equiv \langle x'|\psi(x')|\rangle$, then
$\langle x'|\psi(x')|\rangle = \psi(x')$ (C.2.4)
and

$\langle x'|\frac{d\psi}{dx'}|\rangle = \frac{d\psi}{dx'}$. (C.2.5)

Plug (C.2.4) and (C.2.5) into (C.2.3)→(2.39).

Just below (2.48), page 31, it is mentioned a general function $f(x)$ of the position operator automatically commute with x. $f(x)$ can be expanded in powers of x , a polynomial.

In my note on Poisson brackets, I demonstrated this for:

$[ax^2 + bx, x] = 0.$

At the bottom of page 31: "By definition the standard ket $|\rangle$ satisfies $\langle x'|\rangle = 1$."

Well, (2.35), the general ket state $|A\rangle$ can be written as:

$|A\rangle = \psi_A(x)|\rangle.$

Multiply to the left on both sides with the bra $\langle x'|$:

$\langle x'|A\rangle = \psi_A(x')\langle x'|\rangle.$

Then with (2.29):

$\langle x'|A\rangle = \psi_A(x') \rightarrow \langle x'|\rangle = 1.$

Remark: For convenience I used $|\rangle$ as a general ket.

2.5 Generalized Schrödinger Representation

The scheme in the preceding section of a single operator x is extended in this section.

N generalized coordinates q_i, $i = 1(1)N$, are considered.

On top of page 34 Fp writes:"…..we can derive….."where Dirac, on page 91, writes: "…we have….". Futile?

(2.72) can be written as

$\left[\frac{\partial}{\partial q_i}, \frac{\partial}{\partial q_j}\right] = 0.$ (C.2.6)

What about

$[\frac{\partial}{\partial q_i}, q_j]$?

$\frac{\partial q_j}{\partial q_i} - q_j\frac{\partial}{\partial q_i} = \delta_{ij}.$

Hence

$\left[\frac{\partial}{\partial q_i}, q_j\right] = \delta_{ij}.$ (C.2.7)

Multiply (C.2.7) with $-i\hbar$:

$\left[-i\hbar\frac{\partial}{\partial q_i}, q_j\right] = -i\hbar\delta_{ij}.$

It is possible, according to Dirac page 92, to take $-i\hbar\frac{\partial}{\partial q_i} = p_i$.

Then, (2.74)

$[q_j, p_i] = i\hbar\delta_{ij}.$

Just below (2.74) Fp writes: "It follows from (2.61), (2.68), and (2.74) that….".

I do not understand the role of (2.61).

As mentioned in my notes on section 2.4:

"So, let's look into $\frac{d}{dx}\psi|\rangle$:

$\frac{d}{dx}\psi|\rangle = \frac{d\psi}{dx}|\rangle + \psi\frac{d|\rangle}{dx} = \frac{d\psi}{dx}|\rangle$, (2.37).

Hence

$\frac{d|\rangle}{dx} = 0.$"

Also in (2.68) it is shown
$\frac{\partial|\rangle}{\partial q_i} = 0,$
so,
$p_i|\rangle = 0.$
(2.76) is about representation:
$\frac{\partial\psi(q_1' \ldots\ldots q_N')}{\partial q_i'}$ is the representative of $\left\langle q_1' \ldots\ldots q_N' \middle| \frac{\partial\psi(q_1' \ldots\ldots q_N')}{\partial q_i'} \right\rangle$.
Furthermore
$\langle q_1' \ldots\ldots q_N'|\psi(q_1' \ldots\ldots q_N')\rangle$ is the representative of $\psi(q_1' \ldots\ldots q_N')$.
For this section Dirac's pages 78 and 91-93 are used.

2.6 Momentum Representation

A one degree of freedom system described in the coordinate x and momentum p_x is considered. In the momentum representation a system is represented in terms of the eigenkets of p_x.
Note: I again use for the notation of the standard ket $|\rangle$.
An important result of the momentum representation is given by (2.87):
$x = i\hbar\frac{d}{dp_x}$.
The commutation relation, (2.25), in one dimension:
$xp_x - p_x x = i\hbar.$
Plug $x = i\hbar\frac{d}{dp_x}$ into this commutation relation and the left hand side equals the right hand side.
On page 36 the one degree of freedom is generalized in a system of N coordinates.
Fp concludes this section with the Schrödinger representation to be far better to solve problems than in momentum representation.

2.7 Uncertainty relations.

Fp started this section with the question: how is momentum space wavefunction related to the corresponding coordinate space wavefunction?
(2.27):
$\int_{-\infty}^{\infty} dx'|x'\rangle\langle x'| = 1.$
Plug (2.27) into $\langle p_x'|p_x''\rangle$.
Then, with (2.92) and (2.94)→ (2.95).
Due to the action of the delta function:
$c' = c''.$
To obtain (2.99) and (2.100), use has been made of the equations (2.27), (2.81), (2.96) and the complex conjugate of (2.96)>
To derive (2.102), Fp used (1.83):
$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle \geq \frac{1}{4}|\langle[x, p_x]\rangle|^2.$
The commutation relation in (2.47):
$|[x, p_x]|^2 = \hbar^2.$
Just below (2.102) Fp writes: "It is easily demonstrated ……to Gaussian wave packets….":
$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \frac{1}{4}\hbar^2$.

Easily? In *The Undergraduate Course* , Fp, it took 3 pages to arrive at:
$\Delta k = \frac{1}{2\Delta x}$,(3.68).
A measurement of a particles wave number is equivalent to particles momentum measurement:
$\Delta k = \frac{1}{\hbar}\Delta p$.
Hence,
$\Delta x \Delta p = \frac{\hbar}{2}$,(3.70) *The Undergraduate Course.*
In Exercise 2.3 this result is derived in a slightly different way.
Remark:
I go back to (1.82):
$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \frac{1}{4}|\langle[x, p_x]\rangle|^2 + |\langle\{\Delta x, \Delta p_x\}\rangle|^2$ (C.2.8)
Fp mentioned the final term on the right hand side of (2.8) to be positive definite. The final term represents the anti-commutator $\{\Delta x, \Delta p_x\}$. The expectation value of the anti-commutator is an imaginary number.
The first term on the right hand side of (C.2.8) gives:
$\frac{1}{4}|\langle[x, p_x]\rangle|^2 = \frac{1}{4}|\langle[\Delta x, \Delta p_x]\rangle|^2$.
A Gaussian distribution gives, with (3.70) *The Undergraduate Course*:
$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = (\Delta x \Delta p)^2 = \frac{\hbar^2}{4} = \frac{1}{4}|\langle[x, p_x]\rangle|^2$.
The conclusion to be drawn is: the anti-commutator $\{\Delta x, \Delta p_x\} = 0$ for a Gaussian distribution?

2.8 Displacement operators.

A system with one degree of freedom is considered. This section is dedicated to unitary displacement operations.
Susskind discussed the unitary operator for time evolution.
I suppose the action of the displacement operator is understood. At the beginning of this section one could conclude a displacement just generates a phase factor. This conclusion is formulated by Fp on page 38 between (2.105) and (2.106).
(2.110), with
$D|A\rangle = |Ad\rangle$ and $D^\dagger D|A\rangle = |A\rangle$.
So,
$D^\dagger|Ad\rangle = |A\rangle$.

Remark.
Dirac page 101:
"Since $|Pd\rangle$ can be any ket, we must have $v_d = DvD^{-1}$, Eq. (63)."

Fp, page 39:
"Since this is true for any ket $|Ad\rangle$, we have $v_d = DvD^\dagger$, (2.14)."
DvD^{-1} or $DvD^\dagger$? Does it matter? Well, with (2.128), I conclude it does not:
$[e^{-(ip_x a)/\hbar}]^\dagger = [e^{-(ip_x a)/\hbar}]^{-1}$.
Furthermore
$D^\dagger D = 1 \rightarrow D^\dagger D D^{-1} = D^\dagger \rightarrow D^\dagger = D^{-1}$,

where use has been made of
$DD^{-1} = 1.$
Below (2.114) Fp writes: 'Note that the arbitrary numerical factor in D does not affect either of the results….".
Dirac page 102:
"Note the arbitrary numerical factor of modulus unity in D does not affect…".
I think the addition '*of modulus unity*' is meaningful.
(2.117), with γ tends to zero:
$\lim_{\delta x \to 0} \frac{De^{i\gamma}-1}{\delta x} = \lim_{\delta x \to 0} \frac{D(1+i\gamma)-1}{\delta x}$,
Dirac page 102: "*…D must be made to tend to unity as $\delta x \to 0$ ….."*.
Consequently, $Di\gamma \to i\gamma$, resulting into (2.117).
(2.119): keep in mind δx to be a real number.

The definitions are sometimes confusing:
D is the displacement operator,
v_d is the displaced operator,
d_x is the displacement operator along the x-axis.
(2.120): d_x is anti-Hermitian and consequently an imaginary operator.
(2.118): D is complex, d_x is imaginary and δ_x is a real number.

Just below (2.122) Fp refers to the afore mentioned arbitrary number of modulus unity in relation to the wave function.

Above (2.124), (2.123) with (2.122):
(2.123)→ $\delta x = -(x_d - x)$,
and
$v_d - v = x_d - x.$
With (2.25),
$[q_i, p_j] = i\hbar\delta_{ij}$,
and $i = j$ for the one degree of freedom case,
$[x, i\hbar d_x] = i\hbar$,(2.124).
From this expression and (2.25), (2.125) and (2.126) are obtained. See also Dirac page 103.
From (2.126):
$d_x = -\frac{d}{dx}$.
(2.118) and (2.127):
$D = 1 - i\delta x \frac{p_x}{\hbar}$.
Now the system is displaced over a distance
$\Delta x = N\delta x$ for $N \to \infty$.
Then (2.127) and (2.128) are found and $D^{\dagger}D = 1$.
At the end of this section Fp made some remarks on commutation relations. For example the displacement Δx commutes with the displacement Δy.

So,
$D(\Delta x)D(\Delta y) - D(\Delta y)D(\Delta x) = 0.$
With (2.128)
$\exp\left[-\frac{i(p_x\Delta x + p_y\Delta y)}{\hbar}\right] - \exp\left[-\frac{i(p_y\Delta y + x\Delta x)}{\hbar}\right] = 0.$
Hence the displacement operator creates a phase factor of modulus unity. This represents the eigenvalue of the displacement operator for any ket state.
Plug (2.126) into (2.128) and
$D(\Delta x) = \exp(d_x\Delta x)$,
is obtained.

Exercises

Exercise 2.1 Demonstrate the classical commutators

Demonstrate that
- $[q_i, q_j]_{cl} = 0$.
Given (2.3), the definition of the Poisson Bracket, and:
$\frac{\partial q_i}{\partial q_i} = 1, \frac{\partial q_j}{\partial p_i} = 0, \frac{\partial q_i}{\partial p_i} = 0$ and $\frac{\partial q_i}{\partial q_j} = \delta_{ij}$.
Then $[q_i, q_j]_{cl} = 0$.
- $[p_i, p_j]_{cl} = 0$.
Given (2.3) and:
$\frac{\partial p_i}{\partial p_i} = 1, \frac{\partial p_j}{\partial q_i} = 0, \frac{\partial q_i}{\partial q_j} = \delta_{ij}$ and $\frac{\partial p_i}{\partial p_j} = \delta_{ij}$.
Then $[p_i, p_j]_{cl} = 0.$
- $[q_i, p_j]_{cl} = \delta_{ij}.$
Given (2.3) and:
$\frac{\partial q_i}{\partial q_j} = \delta_{ij}, \frac{\partial p_i}{\partial p_j} = \delta_{ij}, \frac{\partial q_i}{\partial p_i} = 0$ and $\frac{\partial p_j}{\partial q_i} = 0.$
Then $[q_i, p_j]_{cl} = \delta_{ij}.$

Exercise 2.2 Verify various commutation relations

- $[u, v] = -[v, u].$
Use (2.3):
$-[v, u] = [-v, -u] = [u, v].$
- $[u, c] = 0.$
c is a constant. Plug this constant into (2.3) and the result is
$[u, c] = 0.$
- $[u_1 + u_2, v] = [u_1, v] + [u_2, v].$
Replace u by $u_1 + u_2$ in (2.3), then
$[u_1 + u_2, v] = [u_1, v] + [u_2, v].$
- Simarlily $[u, v_1 + v_2] = [u, v_1] + [u, v_2].$
- $[u_1u_2, v] = [u_1, v]u_2 + u_1[u_2, v].$
See Dirac page 86, eq.5 .
- Simarlily $[u, v_1v_2] = [u, v_1]v_2 + v_2[u, v_1].$
$\left[u, [v, w]\right] + \left[v, [w, u]\right] + \left[w, [u, v]\right] = 0$.
By straight forward applying Poisson Brackets and compare the resulting terms, the

expression is verified.
It can be done a bit more simply.
I start with $\left[u,[v,w]\right]$. This expression becomes with the Poisson Brackets:
$\frac{\partial}{\partial p_i}\left([v,w]\frac{\partial u}{\partial q_i}\right)-\frac{\partial}{\partial q_i}([v,w]\frac{\partial u}{\partial p_i})$. (C.E.2.1)
In addition I derived two more similar expression taking into account cyclicality of u,v and w in the expression to be verified:
$\frac{\partial}{\partial p_i}\left([w,u]\frac{\partial v}{\partial q_i}\right)-\frac{\partial}{\partial q_i}([w,u]\frac{\partial v}{\partial p_i})$, (C.E.2.2)
and
$\frac{\partial}{\partial p_i}\left([u,v]\frac{\partial w}{\partial q_i}\right)-\frac{\partial}{\partial q_i}([u,v]\frac{\partial w}{\partial p_i})$. (C.E.2.3)
Evaluate (C.E.2.1)+ (C.E.2.2)+ (C.E.2.3):
$\frac{\partial}{\partial p_i}\left([w,u]\frac{\partial v}{\partial q_i}+[w,u]\frac{\partial v}{\partial q_i}+[u,v]\frac{\partial w}{\partial q_i}\right)-\frac{\partial}{\partial q_i}([v,w]\frac{\partial u}{\partial p_i}+[w,u]\frac{\partial v}{\partial p_i}+[u,v]\frac{\partial w}{\partial p_i})$.
Plug into this expression the Poisson Brackets and the result is 0.

Exercise 2.3 Demonstrate various expectation values for the Gaussian wave packet.

Consider a Gaussian wave packet whose corresponding wave function
$\psi(x')=\psi_0\exp\left[-\frac{(x'-x_0)^2}{4\sigma^2}\right]$, (C.E.2.4)
where ψ_0, x_0 and σ are constants.
With normalization
$\psi_0=\frac{e^{i\phi}}{(2\pi\sigma^2)^{1/4}}$, (4.25) *Undergraduate Course.*
Demonstrate that
(a) $\langle x\rangle = x_0$.
In section 4.4, *Undergraduate Course*, the expectation value has been derived. It is about the evaluation of the integral
$\langle x\rangle = |\psi_0|^2\int_{-\infty}^{\infty}x\exp[-\frac{(x-x_0)^2}{2\sigma^2}]dx$.
The result is:
$\langle x\rangle = x_0$.

(b) $\langle(\Delta x)^2\rangle=\sigma^2$.
$(\Delta x)^2=(x-x_0)^2$.
With (4.29), *Undergraduate Course,*
$\langle(\Delta x)^2\rangle = |\psi_0|^2\int_{-\infty}^{\infty}(x-x_0)^2\exp[-\frac{(x-x_0)^2}{2\sigma^2}]dx$.
This integral is evaluated in section 4.4 *Undergraduate Course*. The result is presented in (4.32):
$\langle(\Delta x)^2\rangle=\sigma^2$.

(c) $\langle p\rangle = 0$.
$\langle p\rangle = -|\psi_0|^2\int_{-\infty}^{\infty}\exp\left[-\frac{(x-x_0)^2}{4\sigma^2}\right]i\hbar\frac{d}{dx}\exp\left[-\frac{(x-x_0)^2}{4\sigma^2}\right]dx$.
This results into
$\langle p\rangle = |\psi_0|^2\frac{i\hbar}{2\sigma^2}\int_{-\infty}^{\infty}(x-x_0)\exp[-\frac{(x-x_0)^2}{2\sigma^2}]dx$.

The integral is zero by symmetry. Consequently
$\langle p\rangle = 0.$

(d) $\langle(\Delta p)^2\rangle = (\frac{\hbar}{2\sigma})^2.$
$\Delta p = p - p_0.$
Since $\langle p\rangle = 0 \rightarrow \langle p_0\rangle = 0$.
Then
$\langle(\Delta p)^2\rangle = \langle(p)^2\rangle.$
So,
$\langle(\Delta p)^2\rangle = \langle(p)^2\rangle = |\psi_0|^2 \int_{-\infty}^{\infty} \exp\left[-\frac{(x-x_0)^2}{4\sigma^2}\right](-i\hbar\frac{d}{dx})^2\exp\left[-\frac{(x-x_0)^2}{4\sigma^2}\right]dx.$
$\langle(\Delta p)^2\rangle = -\frac{|\psi_0|^2\hbar^2}{\sqrt{2\sigma^2}}\int_{-\infty}^{\infty}[\frac{(x-x_0)^2}{2\sigma^2} - 1]\exp[-\frac{(x-x_0)^2}{2\sigma^2}]\frac{d(x-x_0)}{\sqrt{2\sigma^2}}$. (C.E.2.5)

The first integral in (C.E.2.5) equals $\frac{\sqrt{\pi}}{2}$, and the second $\sqrt{\pi}$.
With $|\psi_0|^2 = \frac{1}{\sigma\sqrt{2\pi}}$, (4.25) *Undergraduate Course,*
$\langle(\Delta p)^2\rangle = (\frac{\hbar}{2\sigma})^2.$
Now return to the bottom of page 37 of the section on Uncertainty Relations.
Under (b) of this exercise $\langle(\Delta x)^2\rangle = \sigma^2$ has been derived.
Hence, with the above result for $\langle(\Delta p)^2\rangle = (\frac{\hbar}{2\sigma})^2$, the uncertainty relation for a Gaussian wavefunction is:
$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \frac{\hbar^2}{4}$,(2.102) section 2.7.

Exercise 2.4 The Displacement Operator

Suppose that we displace a one-dimensional quantum mechanical system a distance a along the x-axis. The corresponding displacement operator is
$D(a) =\exp(-\frac{ip_x a}{\hbar})$, (C.E.2.6)
where p_x is the momentum conjugate to the position operator x.
-(a) Demonstrate
$D(a)xD(a)^\dagger = x - a$.
[Hint use the momentum representation , $x = i\hbar\frac{d}{dp_x}$].
I start with the hint:
$D(a)xD(a)^\dagger = D(a)i\hbar\frac{d}{dp_x}D(a)^\dagger.$ (C.E.2.7)
Plug into (C.E.2.7) $D(a) =\exp(-\frac{ip_x a}{\hbar})$:
$\exp\left(-\frac{ip_x a}{\hbar}\right)(-a)\exp\left(\frac{ip_x a}{\hbar}\right) = -a.$
So, the demonstration failed. Now what?
Assume $D(a)xD(a)^\dagger = x - a$ to be correct.
Then
$D(a)xD(a)^\dagger - x = -a \rightarrow D(a)xD(a)^\dagger D - xD = -aD \rightarrow Dx - xD = -aD.$
Multiply $Dx - xD = -aD$ with $D^\dagger$ to the left and with (2.109):
$x - D^\dagger xD = -D^\dagger aD = -aD^\dagger D = -a.$
Then

$D^\dagger x D = x + a.$ (C.E.2.8)

Replace a by $-a$ in (C.E.2.6) and (C.E.2.8)→ $DxD^\dagger = x - a.$

With (2.114) and (2.123):

$x_d = x - a,$

$x_d = DxD^\dagger.$

Then

$DxD^\dagger = x - a.$ (C.E.2.8)

- (b) Demonstrate that

$D(a)x^m D(a)^\dagger = (x-a)^m$.

Let's start with x^2. Multiply (C.E.2.8) with $x - a$:

$(x-a)DxD^\dagger = (x-a)^2.$ (C.E.2.9)

With (C.E.2.8), (C.E.2.9) and $DD^\dagger = 1$, (2.109):

$D^\dagger x D D^\dagger x D = (x-a)^2 \rightarrow Dx^2D^\dagger = (x-a)^2.$

I assume $D(a)x^m D(a)^\dagger = (x-a)^m$ to be correct.

Multiply $D(a)x^m D(a)^\dagger = (x-a)^m$ with $x - a$:

$(x-a)Dx^m D^\dagger = (x-a)^{m+1}.$ (C.E.2.10)

With (C.E.2.8), (C.E.2.10) and $DD^\dagger = 1$, (2.109):

$D^\dagger x D D^\dagger x^m D = (x-a)^{m+1} \rightarrow D(a)x^{m+1}D(a)^\dagger = (x-a)^{m+1}.$

By induction:

$D(a)x^m D(a)^\dagger = (x-a)^m.$

A slightly different approach:

Assume $Dx^m D^\dagger = (x-a)^m$ to be correct. Is this expression correct for $m+1$?

$Dx^{m+1}D^\dagger = (x-a)^{m+1} \rightarrow D^\dagger D x^{m+1} D^\dagger = D^\dagger (x-a)^{m+1}$.

With (2.109):

$D^\dagger D x^{m+1} D^\dagger = D^\dagger (x-a)^{m+1} \rightarrow x D^\dagger D x^m D^\dagger = D^\dagger (x-a)^{m+1}$. Multiply the latter expression with D :

$DxD^\dagger Dx^m D^\dagger = DD^\dagger (x-a)^{m+1}$. Use (2.109) and (C.E.2.16) in this expression:

$(x-a)Dx^m D^\dagger = (x-a)^{m+1} \rightarrow Dx^m D^\dagger = (x-a)^m$, QED.

-(c) Deduce that

$D(a)V(x)D(a)^\dagger = V(x-a).$

I suppose the potential energy operator to be sufficiently smooth function of x.

Consequently, $V(x)$ can be expanded in powers of x : $V(x) = \sum_{i=0}^{\infty} b_i x^i$.

Then, with (C.E.2.10):

$D(a)V(x)D(a)^\dagger = \sum_{i=0}^{\infty} b_i \, D(a)V(x)D(a)^\dagger = \sum_{i=0}^{\infty} b_i (x-a)^i = V(x-a).$

-(d)Let $k = \frac{p_x}{\hbar}$, and let $|k'\rangle$ denote an eigenket of the k operator belonging to the eigenvalue k'. its base kets $|k' + nk_a\rangle$

Demonstrate that

$|A\rangle = \sum_{n=-\infty}^{\infty} c_n \, |k' + nk_a\rangle$, (C.E.2.11)

where the c_n are arbitrary complex coefficients, and $k_a = \frac{2\pi}{a}$, is an eigenket of the $D(a)$ operator belonging to the eigenvalue $\exp(-ik'a)$. Show that the corresponding wavefunction can be written

$\psi_A(x') = e^{ik'x'} u(x')$,

where $u(x' + a) = u(x')$ for all x'.

Dirac, page 99, §25 Displacement operators:

"……., so that if certain states and dynamical variables are connected by some relations, on our displacing them all in a definite way (for example, displacing them all through a distance δx in the direction of the x-axisof Cartesian coordinates), the new states and dynamical variables would have to be connected by the same relation."

Fp at the beginning of section 2.8 Displacement Operations: "……However, we know that the superposition relations between states remain invariant under displacement. …….. ."

As mentioned by Dirac and Fp: "…. The final ket is still not completely determined, because it can be multiplied by a constant phase factor of modulus unity."

$D|A\rangle = \exp\left(-\frac{ip_x a}{\hbar}\right)|A\rangle = \exp(-ika)|A\rangle.$ (C.E.2.12)

where the operator $k = \frac{p_x}{\hbar}$ is substituted.

Now, I have to demonstrate that

$|A\rangle = \sum_{n=-\infty}^{\infty} c_n \, |k' + nk_a\rangle$, (C.E.2.11),

is an eigenket of the D(a) operator belonging to the eigenvalue of $\exp(-ik'a)$.

Given:

$k|k'\rangle = k'|k'\rangle.$

Then,

$k^2|k'\rangle = kk'|k'\rangle = (k')^2|k'\rangle.$ (C.E.2.13)

So, with Maclaurin's series expansion:

$\exp(-ika)|k'\rangle = \sum_{r=0}^{\infty} \frac{(-ika)^r}{r!}|k'\rangle = \sum_{r=0}^{\infty} \frac{(-ik'a)^r}{r!}|k'\rangle = \exp(-ik'a)|k'\rangle.$

Is this result sufficient to demonstrate:

$\exp(-ika) \sum_{n=-\infty}^{\infty} c_n \, |k' + nk_a\rangle = \exp(-ik'a) \sum_{n=-\infty}^{\infty} c_n \, |k' + nk_a\rangle$?

For $n = 0$, I demonstrated above:

$D|A\rangle = \exp(-ik'a)|A\rangle.$

Now, for $n \neq 0$? If $nk_a = 2\pi n/a$ is just a number to be included into $k' + nk_a = k''$,

I am allowed to assume:

$k|k''\rangle = k'|k''\rangle$? I leave it here.

Show that the corresponding wave function can be written as:

$\psi_A(x') = e^{ik'x'} u(x')$, (C.E.2.14)

where $u(x' + a) = u(x')$ for all x'.

I assume $\psi_A(x') = e^{ik'x'} u(x')$ to be correct. Does this lead to a contradiction?

Plug into (C.E.2.14)

$x' \to x' + a.$

Then,

$\psi_A(x'+a) = e^{ik'(x'+a)}u(x'+a) = e^{ik'a}e^{ik'x'}u(x')$,
where $e^{ik'a}$ is a phase factor.

3 Quantum Dynamics

3.1 Schrödinger equation of motion

The time evolution of a quantum mechanical system is evaluated.
In this section it is of some help to use the analysis of displacement operators in section 2.8. (3.7):
$T = 1 + (t - t_0)\tau$,
with (3.5), $T^\dagger T = 1$,
$[1 + (t - t_0)\tau^\dagger][1 + (t - t_0)\tau] = 1.$
Neglect order $(t - t_0)^2$:
$(t - t_0)\tau^\dagger + (t - t_0)\tau = 0$.
Hence
$\tau^\dagger + \tau = 0,$
and τ is anti-Hermitian with imaginary eigenvalue.
Rehearsal:
$\tau|A\rangle = \tau'|A\rangle,$ (C.3.1)
where τ' is the eigenvalue.
Then
$\langle A|\tau^\dagger = \tau'^*\langle A|.$ (C.3.2)
Multiply (C.3.1) with $\langle A|$:
$\langle A|\tau|A\rangle = \tau'\langle A|A\rangle.$ (C.3.3)
Multiply (C.3.2) with $|A\rangle$ and use the anti-Hermitian character of τ :
$\langle A|\tau|A\rangle = -\tau'^*\langle A|A\rangle.$ (C.3.4)
Hence, (C.3.3) and (C.3.4) give:
$\tau' = -\tau'^*,$
and for τ' being a complex number $a + ib \rightarrow a = 0$.
Page 45:
Classical Physics: See for Example Susskind(2) page 145.

3.2 Heisenberg Equation of Motion

In this section another approach for the time evolution of the system is presented.
In (3.17) use has been made of (3.3):
$|At\rangle = T(t, t_0)|At_0\rangle$.
(3.16):
$|A_t\rangle = T^\dagger(t, t_0)|A\rangle.$
With $|A_t\rangle$ and $|At\rangle$, (3.17) is obtained. The first part of (3.17):
$|A_t t\rangle = T^\dagger(t, t_0)T(t, t_0)|At_0\rangle$. (C.3.5)
(3.5)
$T^\dagger T = 1 \rightarrow T^\dagger(t, t_0)T(t, t_0) = 1.$
Hence, (C.3.5) can be written as

$|A_t t\rangle = |At_0\rangle$. (C.3.6)

With (3.16)

$|A_t t\rangle = T^\dagger(t,t_0)|At\rangle \rightarrow |A_t t_0\rangle = T^\dagger(t_0,t_0)|At_0\rangle = |At_0\rangle$.

So,

$|At_0\rangle = |A_t t_0\rangle$. (C.3.7)

Plug (C.3.7) into (C.3.6)

$|A_t t\rangle = |A_t t_0\rangle$, (3.17),

where use has been made of: $T^\dagger(t_0,t_0) = 1$.

The text below (3.17): "Thus, the transformation (3.16) has the effect of bringing all kets representing states of undisturbed motion to rest." Meaning, the operator $T^\dagger$ as a decelerator?

Similar to the displacement operator, the rule for a general observable v is introduced.

The invariance of the expectation value $\langle A|v|A\rangle$ gives:

$\langle A_t|v_t|A_t\rangle = \langle A|v|A\rangle$. (C.3.8)

Plug (3.18), $\langle A_t| = \langle A|T$, and (3.16) into (C.3.8):

$\langle A|Tv_tT^\dagger|A\rangle = \langle A|v|A\rangle \rightarrow v = Tv_tT^\dagger$ →(3.19).

Note: invariance of the expectation value of a dynamic variable has not been mentioned in section 2.8). Let's look into it, page 39:

$\langle Ad|v_d|Ad\rangle = \langle A|v|A\rangle$.

With (2.110):

$\langle A|D^\dagger v_d D|A\rangle = \langle A|v|A\rangle$.

Hence,

$D^\dagger v_d D = v$ →(2.114).

In (3.21) H is introduced in (3.22) and a "bridge" between Heisenberg's and Schrödinger's representation is build.

In (3.23) ,(3.19) is used.

Note, with (3.24),

$T^\dagger vHT = T^\dagger vTT^\dagger HT = v_t H_t$.

Below (3.28) Fp "This operator manifestly commutes with H, …" means:

$[T,H] = 0$, with (3.28):

$\exp\left[-\frac{iH(t-t_0)}{\hbar}\right]H - H\exp\left[-\frac{iH(t-t_0)}{\hbar}\right] = 0$.

Then, with (3.24)

$TH - HT = 0 \rightarrow T^\dagger TH - T^\dagger HT = 0 \rightarrow H - T^\dagger HT = 0 \rightarrow H = H_t$.

Just below (3.30), Fp underlines the relation between the Heisenberg representation and the Schrödinger representation. Suppose

$[v,H] = 0 \rightarrow [v,T] \rightarrow vT - Tv = 0 \rightarrow T^\dagger vT - T^\dagger Tv = 0 \rightarrow v_t = v$.

With the assumption $[v,H] = 0 \rightarrow v_t = v$, where v is the Schrödinger dynamical observable, and (3.25), (3.31) is obtained.

3.3 Ehrenfest's Theorem

In this section the form of the quantum mechanical Hamiltonian is looked for.

In the introductory considerations of this section, Fp mentioned the classical product xp_x and the Hermitian product $(xp_x + p_x x)/2$. See also Fp, Undergraduate Course page 46. Furthermore FP: 'When the system in question has no classical analogue the we are reduced to guessing a form for H that reproduces the observed behaviour of the system." Susskind, page 124, advised some more tools to find the Hamiltonian.

In (3.33) and (3.34), Fp presented two formulae. For example (3.33), see (2.3):

$[x_i, F(\boldsymbol{x}, \boldsymbol{p})]_{cl} = \frac{\partial x_i}{\partial x_i}\frac{\partial F}{\partial p_i} - \frac{\partial x_i}{\partial p_i}\frac{\partial F}{\partial x_i} = \frac{\partial F}{\partial p_i}$.

Then, with (2.22):

$[x_i, F(\boldsymbol{x}, \boldsymbol{p})] = i\hbar\frac{\partial F}{\partial p_i}$,(3.33).

To find (3.33), Fp referred to (3.32). I prefer the above approach.

Yet, I use Fp's approach and the symmetry of (3.32), see (2.87):

$x_i F - F x_i = i\hbar\frac{\partial F}{\partial p_i}$. (C.3.9)

Plug $x_i = i\hbar\frac{\partial}{\partial p_i}$ into (C.3.9) and use the operator character[1] of (C.3.9):

$i\hbar F\frac{\partial}{\partial p_i} + i\hbar\frac{\partial F}{\partial p_i} - \hbar F\frac{\partial}{\partial p_i} = i\hbar\frac{\partial F}{\partial p_i}$.

Similarly, with $p_i = -i\hbar\frac{\partial}{\partial x_i}$, (3.34) is obtained.

To find (3.37), $x_i = i\hbar\frac{\partial}{\partial p_i}$ and (3.33) are used.

(3.40):

$[x_t(t), x_i(0)] = [\frac{p_i(0)t}{m}x_i(0) - x_i(0)\frac{p_i(0)t}{m}]$. (C.3.10)

Then, with the famous commutator (2.25), (C.3.10) delivers

$[x_t(t), x_i(0)] = \frac{i\hbar t}{m}$.

In the commutator of (3.43), $\frac{p^2}{2m}$ $(= \frac{1}{2m}\sum_j p_j^2)$ of (3.42) does not contribute.

In (3.45), (3.25) and (3.44) are used.

Finally for this section: see also Ehrenfest's Theorem Fp, *Undergraduate Course*, Section 4.5.

3.4 Schrödinger Wave Equation.

Now the state of the system is evolving with time.

For convenience I reproduce (3.10):

$i\hbar\frac{d|At\rangle}{dt} = H(t)|At\rangle$.

Note: in this section $H(t) = H$, independent of time.

To obtain (3.48), the time evolving ket $|At\rangle$ has to be multiplied by $\langle x'|$, and with (3.10) (3.50) is found.

In (3.52) the kinetic energy part representation of H, (3.49) is given, where use has been made of:

$\nabla'^2\langle x'| = 0$. Trivial may be, however worthwhile to remember.

Below (3.58) the stationary ket is defined. For stationary kets see also Dirac § 29.

[1] "The operators are assumed to act on everything on their right", Fp, *Undergraduate Course* , Page 45.

Integrating (3.57) produces (3.58). Multiply (3,58) with $\langle x'|$, make use of $\psi(x', t_0) = \langle x' | A t_0 \rangle \rightarrow (3.59)$.
The solutions of Schrödinger's time independent wave equation are found with the conditions given in (3.61) and (3.62).

3.4.1 *Intermezzo* Second order Differential equation

The general solution of
$y'' - ay = 0$,
are
$y = c_1 e^{\sqrt{a}x} + c_2 e^{-\sqrt{a}x}$.
For y to remain finite for $x \rightarrow \infty$, $c_1 = 0$ or $a < 0$.
With $a < 0$, a wave type solution is found.
$a < 0 \rightarrow [V(x') - E] > 0$ in (3.60).
The solutions of the differential equation for y can be found in textbooks or with help of WolframAlpha. The first step to find the above solution for y is to try a solution like $y = e^{\lambda x}$. Of course, $c_1 = 0$ is a valid solution. Then there is no need for $a < 0$. The solution for y is a decaying function of x.
End of Intermezzo.

To find (3.64) reference is made to the 1-D case.
Schrödinger's time independent wave equation (3.55) can be transformed into the conservation equation of the probability density (3.65).
In Fp's *Undergraduate Course* section 4.3 on Normalization of the Wavefunction, the conservation equation has been derived for the 1-D case.
In (3.68) the relation between the probability current and the expectation value of the momentum at time t is presented.
The demonstration of the derivation of (3.68) can be found in Fp's *Undergraduate Course* section 4.5 on Ehrenfest's Theorem.
(3.69) is derived for a potential with an imaginary part.
This can be demonstrated with the 1-D case in section 4.3 *Undergraduate Course.*
Instead of V in (4.13)[2] use $V + \mathrm{Im}(V)$. Now the complex conjugate of (4.13)[2] produces an additional expression $[\mathrm{Im}(V)]^*$. Summation of (4.13)[2] and (4.14)[2] gives the extra term in (3.69): $\frac{2 \cdot \mathrm{Im}(V)}{\hbar} \rho$, ρ defined in (3.63).

Exercises

Exercise 3.1 About commutators expanded in power series.

The demonstration asked for are presented in my notes on section 3.3.

Exercise 3.2 About the complex potential V(**x**).

If the potential $V(\boldsymbol{x})$ is complex, demonstrate ……. In my notes on section 4.3 I paid attention to the relation between the probability current ρ and the imaginary component of the potential $\frac{2 \cdot \mathrm{Im}(V)}{\hbar} \rho$.

[2] This number refers to the *Undergraduate Course.*

Exercise 3.3 Analysis of the one-dimensional harmonic oscillator.

Consider a one-dimensional harmonic oscillator whose Hamiltonian is

$$H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2, \qquad \text{(C.E.3.1)}$$

where x and p_x are conjugate position and momentum operators, respectively, and m, ω are positive constants.

(a) Demonstrate that the expectation value of H is positive definite.

The eigenstates of the Hamiltonian form a complete set of eigenstates $|\lambda_i\rangle$ with eigenvalue λ_i' .

So, the general state

$|B\rangle = \sum_i c_i\,|\lambda_i\rangle$,

and

$|B\rangle$ properly normalized.

Then

$$\langle B|H|B\rangle = \langle \sum_i c_i^*\,\lambda_i|H|\sum_i c_i\,\lambda_i\rangle = \sum_i |c_i|^2\lambda_i' \,. \qquad \text{(C.E.3.2)}$$

λ_i' is positive. See Chapter 5 of Fp's *Graduate Course*:

$\lambda_i' = E = \left(i + \frac{1}{2}\hbar\omega\right)$, (5.104)[2],

where $i = 0,1,2, \ldots$.

Hence the expectation value of the Hamiltonian is definite positive.

(b) Let

$$A = \sqrt{\frac{m\omega}{2\hbar}}\,x + i\frac{p_x}{\sqrt{2m\omega\hbar}}\,. \qquad \text{(C.E.3.4)}$$

Deduce that:

- $[A, A^\dagger] = 1$.

Plug C.E.3.4) into $[A, A^\dagger]$:

$$[A, A^\dagger] = \frac{i}{\hbar}[p_x, x].$$

With (2.25): $[x, p_x] = i\hbar$,

$$[A, A^\dagger] = \frac{i}{\hbar}[p_x, x] = 1.$$

- $H = \hbar\omega(\frac{1}{2} + A^\dagger A)$. $\qquad \text{(C.E.3.5)}$

With (C.E.3.4):

$$A^\dagger A = \frac{1}{2\hbar}m\omega x^2 + \frac{p_x^2}{2m\hbar\omega} - \frac{ixp_x}{2\hbar} + \frac{ip_x x}{2\hbar} = \frac{1}{2\hbar}m\omega x^2 + \frac{p_x^2}{2m\hbar\omega} - \frac{i}{2\hbar}[x, p_x]$$

With $[x, p_x] = i\hbar$:

$$A^\dagger A = \frac{1}{2\hbar}m\omega x^2 + \frac{p_x^2}{2m\hbar\omega} - \frac{1}{2} \rightarrow \hbar\omega\left(\frac{1}{2} + A^\dagger A\right) = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2 = H \,.$$

In addition

$$H = \hbar\omega\left(AA^\dagger - \frac{1}{2}\right) \,. \qquad \text{(C.E.3.6)}$$

- $[H, A] = -\hbar\omega A$.

The toolkit just developed can be used.

So, plug $[A, A^\dagger] = 1$ and $H = \hbar\omega(\frac{1}{2} + A^\dagger A)$ into $[H, A]$. Furthermore, keep in mind the operator character of A and H, then

$[H, A] = -\hbar\omega A$ is obtained.

- $[H, A^\dagger] = \hbar\omega A^\dagger$.

Plug $[A, A^\dagger] = 1$ and $H = \hbar\omega(\frac{1}{2} + A^\dagger A)$ into $[H, A^\dagger]$, then
$[H, A^\dagger] = \hbar\omega A^\dagger$ is obtained.
(c) Suppose $|E\rangle$ is an eigenket of the Hamiltonian whose corresponding energy is E:
i.e.,
$H|E\rangle = E|E\rangle$.
Demonstrate:
- $HA|E\rangle = (E - \hbar\omega)A|E\rangle$.
With $[H, A] = -\hbar\omega A \rightarrow AH - \hbar\omega A$:
$HA|E\rangle = AH|E\rangle - \hbar\omega A|E\rangle = AE|E\rangle - \hbar\omega A|E\rangle = (E - \hbar\omega)A|E\rangle$. (C.E.3.7)
- $HA^\dagger = (E + \hbar\omega)A^\dagger|E\rangle$.
With $[H, A^\dagger] = \hbar\omega A^\dagger$ and similar to the derivation of (C.E.3.7),
$HA^\dagger = (E + \hbar\omega)A^\dagger|E\rangle$, (C.E.3.8)
is found.
Deduce the allowed values of E are:
$E_n = (n + \frac{1}{2})\hbar\omega$, (C.E.3.9)
where $n = 0,1,2, \ldots$.
I start with $H = \hbar\omega(\frac{1}{2} + A^\dagger A)$,(C.E.3.5), and derive the expectation value of
$H - \frac{\hbar\omega}{2} = \hbar\omega A^\dagger A$:
$\left\langle E\left|\hbar\omega A^\dagger A\right|E\right\rangle = \left\langle E\left|H - \frac{\hbar\omega}{2}\right|E\right\rangle = \left(E - \frac{\hbar\omega}{2}\right)\langle E|E\rangle = E - \frac{\hbar\omega}{2}$. (C.E.3.10)
Dirac, page 137:
$\left\langle E\left|\hbar\omega A^\dagger A\right|E\right\rangle$ is the square of the length of the ket $\sqrt{\hbar\omega}A|E\rangle$ and consequently, (C.E.3.10),
$\left\langle E\left|\hbar\omega A^\dagger A\right|E\right\rangle > 0 \rightarrow E > \frac{\hbar\omega}{2}$. (C.E.3.11)
Now, with (C.E.3.7)
$HA|E\rangle = (E - \hbar\omega)A|E\rangle$.
Then,
$A|E\rangle$ is an eigenket of H with eigenvalue of H : $(E - \hbar\omega)$.
With positive eigenvalues and $E \geq \frac{\hbar\omega}{2}$. Consequently, the lowest possible eigenvalue is
$E = \frac{\hbar\omega}{2} \rightarrow E_0$
With (C.E.3.8) another eigenvalue of H, $(E + \hbar\omega)$, is obtained of the ket $A^\dagger|E\rangle$.
Hence,
$E = \frac{\hbar\omega}{2} + \hbar\omega = \hbar\omega\left(1 + \frac{1}{2}\right) \rightarrow E_1$.
is an eigenvalue of H.
Since $(E - \hbar\omega) \equiv E'$ is an eigenvalue of H, $E' - \hbar\omega = E - 2\hbar\omega$ is an eigenvalue of H, etc.
Dirac, page 137: "*…..which cannot extend to infinity, because it would contain eigenvalues contradicting $E \geq \frac{\hbar\omega}{2}$, and can terminate only with the value $\frac{\hbar\omega}{2}$.*"
Similarly, as mentioned above, since $(E + \hbar\omega) \equiv E''$ is an eigenvalue of H, $E'' + \hbar\omega = = E + 2\hbar\omega$,etc.
Consequently, the eigenvalues are:
$E_n = (n + \frac{1}{2})\hbar\omega$.
(d) Let $|E_n\rangle$ be properly normalized (i.e., $\langle E_n|E_n\rangle = 1$) eigenket corresponding to the eigen

value E_n . Show the kets to be defined such that

$A|E_n\rangle = \sqrt{n}|E_{n-1}\rangle$, (C.E.3.12)

and

$A^\dagger|E_n\rangle = \sqrt{n+1}|E_{n+1}\rangle$. (C.E.3.13)

Operate $A^\dagger$ on (C.E.3.12), using (C.3.E.13):

$A^\dagger A|E_n\rangle = \sqrt{n}A^\dagger|E_{n-1}\rangle = \sqrt{n}\sqrt{n}|E_n\rangle = n|E_n\rangle$. (C.E.3.14)

Operate A on (C.E.3.13), using (C.3.E.12):

$AA^\dagger|E_n\rangle = \sqrt{n+1}A|E_{n+1}\rangle = (n+1)|E_n\rangle$. (C.E.3.15)

Then,

$AA^\dagger|E_n\rangle - A^\dagger A|E_n\rangle = [A, A^\dagger]|E_n\rangle = (n+1)|E_n\rangle - n|E_n\rangle = |E_n\rangle$. (C.E.3.16)

Hence,

(C.E.3.16)→ $[A, A^\dagger] = 1$.

So, the definitions of the kets "works".

With (C.E.3.13)

$A^\dagger|E_{n-1}\rangle = \sqrt{n}|E_n\rangle \rightarrow |E_n\rangle = \frac{A^\dagger}{\sqrt{n}}|E_{n-1}\rangle = \frac{(A^\dagger)^2}{\sqrt{n(n-1)}}|E_{n-1}\rangle = \cdots = \frac{(A^\dagger)^n}{\sqrt{n!}}|E_0\rangle$. (C.E.3.17)

Exercise 3.3 Intermezzo Dirac's Ladder Up and Down

I start with the relation between the operators of Dirac and Fp:

$\eta \equiv iA^\dagger$,

and

$\tilde{\eta} \equiv -iA$.

I neglect the imaginary factor.

Dirac, page 137, eq. (9):

$\left[A, \left(A^\dagger\right)^n\right] = n\left(A^\dagger\right)^{n-1}$. (C.E.3.18)

I will proof (C.E.3.18) by induction.

Multiply $\left[A, \left(A^\dagger\right)^n\right] = n\left(A^\dagger\right)^{n-1}$ to the left with $A^\dagger$:

$A^\dagger A\left(A^\dagger\right)^n - \left(A^\dagger\right)^{n+1}A = n\left(A^\dagger\right)^n$. (C.E.3.19)

Plug $A^\dagger A = AA^\dagger - 1$ into (C.E.3.19):

$\left(AA^\dagger - 1\right)\left(A^\dagger\right)^n - \left(A^\dagger\right)^{n+1}A = n\left(A^\dagger\right)^n$,

and the result is

$\left[A, \left(A^\dagger\right)^{n+1}\right] = (n+1)\left(A^\dagger\right)^n$, QED.

On page 137 Dirac demonstrated the operator A to lower the eigenvalue with one unit and the operator $A^\dagger$ to raise the eigenvalue with one unit.

Now, with (C.E.3.18)

$A\left(A^\dagger\right)^n|E_0\rangle - \left(A^\dagger\right)^n A|E_0\rangle = n\left(A^\dagger\right)^{n-1}|E_0\rangle$. (C.E.3.20)

With

$A|E_0\rangle = 0$,

(C.E.3.20) results into

$A\left(A^\dagger\right)^n|E_0\rangle = n\left(A^\dagger\right)^{n-1}|E_0\rangle$. (C.E.3.21)

Multiply (C.E.3.21) to the left with $\langle E_0|A^{n-1}$ and use $[(A^\dagger)^n]^\dagger = A^n$:

$\left\langle E_0\middle|A^n\left(A^\dagger\right)^n\middle|E_0\right\rangle = n\left\langle E_0\middle|A^{n-1}\left(A^\dagger\right)^{n-1}\middle|E_0\right\rangle$. (C.E.3.22)

Then, with (C.E.3.22) and $\langle E_0|E_0\rangle = 1$

$\left\langle E_0\middle|A^n\left(A^\dagger\right)^n\middle|E_0\right\rangle = n(n-1)\left\langle E_0\middle|A^{n-2}\left(A^\dagger\right)^{n-2}\middle|E_0\right\rangle = \cdots = n!\,\langle E_0|E_0\rangle = n!$.

Hence the kets

$\left(A^\dagger\right)^n|E_0\rangle$ have to be multiplied by $(n!)^{1/2}$ to become properly normalized:

$|E_n\rangle = (n!)^{-1/2}\left(A^\dagger\right)^n|E_0\rangle,$ (C.E.3.23)

as already demonstrated in (C.E.3.17).

Let's find out about (C.E.3.13) in a slightly different way.

$A^\dagger|E_n\rangle = \sqrt{n+1}|E_{n+1}\rangle.$

in a slightly different way.

Multiply (C.E.3.23) with $A^\dagger$:

$A^\dagger|E_n\rangle = (n!)^{-\frac{1}{2}}\left(A^\dagger\right)^{n+1}|E_0\rangle.$ (C.E.3.24)

With (C.E.3.24):

$\left(A^\dagger\right)^{n+1}|E_0\rangle = (n!)^{\frac{1}{2}}A^\dagger|E_n\rangle$.

(C.E.3.23) for $(n+1)$:

$|E_{n+1}\rangle = [(n+1)!]^{-1/2}\left(A^\dagger\right)^{n+1}|E_0\rangle.$ (C.E.3.25)

Plug $\left(A^\dagger\right)^{n+1}|E_0\rangle = (n!)^{\frac{1}{2}}A^\dagger|E_n\rangle$ into (C.E.3.25):

$|E_{n+1}\rangle = [(n+1)!]^{-1/2}(n!)^{\frac{1}{2}}A^\dagger|E_n\rangle.$

So,

$A^\dagger|E_n\rangle = (n!)^{-\frac{1}{2}}[(n+1)!]^{1/2}|E_{n+1}\rangle = [n+1]^{1/2}|E_{n+1}\rangle.$

Can I deduce (C.E.3.12) in a direct way with (C.E.3.23)?

With (C.E.3.23):

$|E_{n-1}\rangle = [(n-1)!]^{-1/2}\left(A^\dagger\right)^{n-1}|E_0\rangle \rightarrow |E_{n-1}\rangle = \left(A^\dagger\right)^{-1}\sqrt{n}[n!]^{-1/2}\left(A^\dagger\right)^n|E_0\rangle \rightarrow$

$\rightarrow |E_{n-1}\rangle = \left(A^\dagger\right)^{-1}\sqrt{n}|E_n\rangle$. (C.E.3.26)

The next step is to multiply (C.E.3.26) with $\sqrt{n}$:

$n\left(A^\dagger\right)^{-1}|E_n\rangle = \sqrt{n}|E_{n-1}\rangle.$ (C.E.3.27)

Does the operator $n\left(A^\dagger\right)^{-1}$ in (C.E.3.27) equals A?

I come back to that later on.

I assume (C.E.3.12), $A|E_n\rangle = \sqrt{n}|E_{n-1}\rangle$, to be correct.

With, (C.E.3.23):

$A|E_n\rangle = A(n!)^{-1/2}\left(A^\dagger\right)^n|E_0\rangle.$ (C.E.3.28)

Furthermore, the expression on the left hand side for $|E_{n-1}\rangle$, given in (C.3.E.26),is used:

$|E_{n-1}\rangle = [(n-1)!]^{-1/2}\left(A^\dagger\right)^{n-1}|E_0\rangle.$

Multiply the latter expression with $\sqrt{n}$ and another expression for $A|E_n\rangle$, (C.E.3.12):

$A|E_n\rangle = \sqrt{n}[(n-1)!]^{-1/2}\left(A^\dagger\right)^{n-1}|E_0\rangle.$ (C.E.3.29)

So, there two expressions for $A|E_n\rangle \rightarrow$ (C.E.3.28) and (C.E.3.29).

Equating both expressions:

$\sqrt{n}[(n-1)!]^{-1/2}\left(A^\dagger\right)^{n-1} = A(n!)^{-1/2}\left(A^\dagger\right)^n \rightarrow \sqrt{n}(n!)^{1/2}\left(A^\dagger\right)^{n-1} =$

$= A[(n-1)!]^{1/2}\left(A^\dagger\right)^n \rightarrow n\left(A^\dagger\right)^{n-1} = A\left(A^\dagger\right)^n,$

and
$A\left(A^{\dagger}\right)^{n}|E_0\rangle = n\left(A^{\dagger}\right)^{n-1}|E_0\rangle$, (C.E.3.21),
has been found again.

Next: (C.E.3.18)
$$\left[A,\left(A^{\dagger}\right)^{n}\right] = n\left(A^{\dagger}\right)^{n-1} \rightarrow \left[A\left(A^{\dagger}\right)^{n} - \left(A^{\dagger}\right)^{n}A\right]|E_0\rangle = n\left(A^{\dagger}\right)^{n-1}|E_0\rangle. \quad \text{(C.E.3.30)}$$
With
$A|E_0\rangle = 0$,
(C.E.3.30) results into
$$A\left(A^{\dagger}\right)^{n}|E_0\rangle = n\left(A^{\dagger}\right)^{n-1}|E_0\rangle = n\left(A^{\dagger}\right)^{-1}\left(A^{\dagger}\right)^{n}|E_0\rangle. \quad \text{(C.E.3.31)}$$
Above I raised the question:
does the operator $n\left(A^{\dagger}\right)^{-1}$ equals the operator A?
Let's analyse $n\left(A^{\dagger}\right)^{-1}|E_n\rangle$, (C.E.3.27).
With (C.E.3.23), $n\left(A^{\dagger}\right)^{-1}|E_n\rangle$ can be written as:
$n\left(A^{\dagger}\right)^{-1}|E_n\rangle = n(n!)^{-1/2}\left(A^{\dagger}\right)^{n-1}|E_0\rangle$.
Use (C.3.3.21):
$n\left(A^{\dagger}\right)^{-1}|E_n\rangle = n(n!)^{-1/2}\left(A^{\dagger}\right)^{n-1}|E_0\rangle = (n!)^{-1/2}A\left(A^{\dagger}\right)^{n}|E_0\rangle = A|E_n\rangle$.
$n\left(A^{\dagger}\right)^{-1} = A$, operating on the ket $\left(A^{\dagger}\right)^{n}|E_0\rangle$.

I return to (C.E.3.23):
$|E_n\rangle = (n!)^{-1/2}\left(A^{\dagger}\right)^{n}|E_0\rangle$.
$|E_n\rangle$ is normalized.
Consequently, with (C.E.3.23):
$$\langle E_n|E_n\rangle = 1 = \frac{1}{n!}\left\langle E_0\middle|A^{n}\left(A^{\dagger}\right)^{n}\middle|E_0\right\rangle. \quad \text{(C.E.3.32)}$$
In addition
$\langle E_0|E_0\rangle = 1$.
Hence,
$\frac{1}{n!}A^{n}\left(A^{\dagger}\right)^{n} = 1$, and $n = 1 \rightarrow AA^{\dagger} = 1$.
Reminder:
$[A, A^{\dagger}]\big|E_0\rangle = AA^{\dagger}\big|E_0\rangle = |E_0\rangle$, since $A|E_0\rangle = 0$.
(C.E.3.18):
$A\left(A^{\dagger}\right)^{n}|E_0\rangle - \left(A^{\dagger}\right)^{n}A|E_0\rangle = n\left(A^{\dagger}\right)^{n-1}|E_0\rangle$.
Multiply (C.E.3.18) with A^{n-1} :
$$A^{n}\left(A^{\dagger}\right)^{n}|E_0\rangle - A^{n-1}\left(A^{\dagger}\right)^{n}A|E_0\rangle = nA^{n-1}\left(A^{\dagger}\right)^{n-1}|E_0\rangle \rightarrow n!\,|E_0\rangle. \quad \text{(C.E.3.33)}$$
Then,
$\frac{1}{n!}A^{n}\left(A^{\dagger}\right)^{n}|E_0\rangle = |E_0\rangle$.
Hence, the eigenvalue of the operator
$\frac{1}{n!}A^{n}\left(A^{\dagger}\right)^{n} = 1$.
End of intermezzo.

Exercise 3.3 (e)

(e) Let the $\psi_n(x') = \langle x'|E_n\rangle$ be the wavefunctions of the properly normalized energy eigenkets $|E_n\rangle$.

Given that
$A|E_0\rangle = 0,$
deduce that
$\left(\frac{x'}{x_0} + x_0 \frac{d}{dx'}\right)\psi_0 = 0,$ (C.E.3.34)
where $x_0 = (\hbar/m\omega)^{1/2}$.
With
$A = \sqrt{\frac{m\omega}{2\hbar}}x + i\frac{p_x}{\sqrt{2m\omega\hbar}}$,(C.E.3.4) ,
and
$p_{x'} = -i\hbar\frac{d}{dx'}$,
$\rightarrow A = \frac{1}{\sqrt{2}}\left(\frac{x'}{x_0} + x_0\frac{d}{dx'}\right).$ (C.E.3.35)
Since
$A|E_0\rangle = |0\rangle$, the "null" vector,
$\langle x'|A|E_0\rangle = \langle x'|0\rangle = 0$.
Furthermore
$\psi_0(x') = \langle x'|E_0\rangle.$
What about
$A\psi_0(x') = A\langle x'|E_0\rangle$?
Dirac dealt with this question, page 139, with (C.E.3.35)
$\langle x'|A|E_0\rangle = 0 = \left\langle x'\right|\left(\frac{x'}{x_0} + x_0\frac{d}{dx'}\right)\left|E_0\right\rangle.$ (C.E.3.37)
Actually, Dirac:
$\langle x'|A|E_0\rangle = 0 = \left\langle x'\right|x_0\frac{d}{dx'} + \frac{x'}{x_0}\left|E_0\right\rangle.$ (C.E.3.38)
Is there a difference between (C.E.3.37) and (C.E.3.38)? I do not think so.
Then, with (C.E.3.38):
$x_0\frac{d}{dx'}\langle x'|E_0\rangle + \frac{x'}{x_0}\langle x'|E_0\rangle = \left(\frac{x'}{x_0} + x_0\frac{d}{dx'}\right)\psi_0 = 0,$ (C.E.3.34)
So,
$\left(\frac{x'}{x_0} + x_0\frac{d}{dx'}\right)\psi_0 = 0$, (C.E.3.34).
This differential equation can be solved:
$\frac{d}{dx'}\psi_0 = -\frac{x'}{x_0^2}\psi_0 \rightarrow \psi_0 = Ce^{-\frac{1}{2}(\frac{x'}{x_0})^2}$,
where C is the constant of integration deduced from:
$\int_{-\infty}^{\infty}|\psi_0|^2 d\,x' = 1 \rightarrow C = \frac{1}{\pi^{1/4}x_0^{1/2}}$.
Hence
$\psi_0 = \frac{1}{\pi^{1/4}x_0^{1/2}}e^{-\frac{1}{2}(\frac{x'}{x_0})^2}$.
(C.E.3.23):
$|E_n\rangle = (n!)^{-1/2}\left(A^\dagger\right)^n|E_0\rangle$,
and
$\psi_n(x') = \langle x'|E_n\rangle = (n!)^{-1/2}\langle x'|\left(A^\dagger\right)^n|E_0\rangle.$
Using Dirac's approach:
$\psi_n(x') = (n!)^{-1/2}\left(A^\dagger\right)^n\langle x'|E_0\rangle = (n!)^{-1/2}\left(A^\dagger\right)^n\psi_0(x').$

Furthermore

$A^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}}x - i\frac{p_x}{\sqrt{2m\omega\hbar}}$,(C.E.3.4) ,

and

$p_{x'} = -i\hbar\frac{d}{dx'}$,

$\rightarrow A^{\dagger} = \frac{1}{x_0\sqrt{2}}\left(x' - x_0^2\frac{d}{dx'}\right)$.

Then,

$$\psi_n(x') = \frac{1}{\pi^{1/4}(2^n n!)^{1/2}x_0^{n+1/2}}(x' - x_0^2\frac{d}{dx'})^n e^{-\frac{1}{2}(\frac{x'}{x_0})^2}. \quad \text{(C.E.3.39)}$$

Remark:

- As mentioned by Mahan, the differential equation representing the harmonic oscillator has a solution in terms of Hermite polynomials. This is related with the potential of the oscillator existing for all space. (C.E.3.39) represents the Hermite polynomials (Mahan page 31).
- Susskind, pages 338 and 339, shows the series of solutions for the wavefunctions $\psi_n(x')$ with help of the operator $iA^{\dagger}$, equal to the operator defined by Dirac.

Then, i.e.,

$\psi_1(x') = iA^{\dagger}\psi_0(x')$. The difference with Fp is a phase factor $e^{i\pi/2}$.

Exercise 3.4 The one-dimensional Harmonic oscillator: Matrix elements.

Consider the one-dimensional quantum harmonic oscillator discussed in Exercise 3.3. Let $|n\rangle$ be a properly normalized energy eigenket belonging to the eigenvalue E_n.

Show that:

- $\langle n'|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n}\delta_{n'n-1} + \sqrt{n+1}\delta_{n'n+1})$.

With

$A = \sqrt{\frac{m\omega}{2\hbar}}x + i\frac{p_x}{\sqrt{2m\omega\hbar}}$, (C.E.3.4),

$x = \sqrt{\frac{\hbar}{2m\omega}}(A + A^{\dagger})$.

Consequently

$$\langle n'|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle n'|A + A^{\dagger}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\langle n'|A|n\rangle + \langle n'|A^{\dagger}|n\rangle). \quad \text{(C.E.3.40)}$$

With the information of Exercise 3.3:

$A^{\dagger}|n\rangle = \sqrt{n+1}|n+1\rangle$,

and

$A|n\rangle = \sqrt{n}|n-1\rangle$.

Plug these expressions into (C.E.3.40):

$$\langle n'|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\langle n'|\sqrt{n}|n-1\rangle + \langle n'|\sqrt{n+1}|n+1\rangle). \quad \text{(C.E.3.41)}$$

Since the kets $|n\rangle$ are orthonormal, (C.E.3.41) results into:

$$\langle n'|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n}\delta_{n'n-1} + \sqrt{n+1}\delta_{n'n+1}) . \quad \text{(C.E.3.42)}$$

Furthermore

$\langle x\rangle^3 = \langle n|x|n\rangle = 0$, $\langle A\rangle = 0$ and $\langle A^n\rangle = 0$.

- $\langle n'|p_x|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}(-\sqrt{n}\delta_{n'n-1} + \sqrt{n+1}\delta_{n'n+1})$.

With

$A = \sqrt{\frac{m\omega}{2\hbar}}x + i\frac{p_x}{\sqrt{2m\omega\hbar}}$, (C.E.3.4),

$p_x = i\sqrt{\frac{m\hbar\omega}{2}}(-A + A^\dagger)$.

Consequently,

$$\langle n'|p_x|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\langle n'|-A + A^\dagger|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}(-\langle n'|A|n\rangle + \langle n'|A^\dagger|n\rangle). \quad \text{(C.E.3.43)}$$

The, with results given in (C.E.3.41) and (C.E.3.42), (C.E.3.43) becomes

$$\langle n'|p_x|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}(-\sqrt{n}\delta_{n'n-1} + \sqrt{n+1}\delta_{n'n+1}), \quad \text{(C.E.3.44)}$$

and

$\langle p_x\rangle = 0$.

- $\langle n'|x^2|n\rangle = \frac{\hbar}{2m\omega}[\sqrt{n(n-1)}\delta_{n'n-2} + \sqrt{(n+1)(n+2)}\delta_{n'n+2} + (2n+1)\delta_{n'n}]$.

With

$x = \sqrt{\frac{\hbar}{2m\omega}}(A + A^\dagger)$ and $[A, A^\dagger] = 1$:

$$x^2 = \frac{\hbar}{2m\omega}\left[A^2 + \left(A^\dagger\right)^2 + AA^\dagger + A^\dagger A\right] = \frac{\hbar}{2m\omega}[A^2 + \left(A^\dagger\right)^2 + 2A^\dagger A + 1]. \quad \text{(C.E.3.45]}$$

The job can be done.

However, with (C.E.3.41) and $x = \sqrt{\frac{\hbar}{2m\omega}}(A + A^\dagger)$:

$$\langle n'|x^2|n\rangle = \frac{\hbar}{2m\omega}[\langle n'|(A + A^\dagger)\sqrt{n}|n-1\rangle + \langle n'|(A + A^\dagger)\sqrt{n+1}|n+1\rangle]. \quad \text{(C.E.3.46)}$$

Then again with information of Exercise 3.3

$A^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$,

and

$A|n\rangle = \sqrt{n}|n-1\rangle$:

$\langle n'|x^2|n\rangle = \frac{\hbar}{2m\omega}[\langle n'|A\sqrt{n}|n-1\rangle + \langle n'|A^\dagger\sqrt{n}|n-1\rangle + \langle n'|A\sqrt{n+1}|n+1\rangle +$

$+\langle n'|A^\dagger\sqrt{n+1}|n+1\rangle] = \frac{\hbar}{2m\omega}[\langle n'|\sqrt{n(n-1)}|n-2\rangle + \langle n'|\sqrt{n}\sqrt{n}|n\rangle +$

$+\langle n'|\sqrt{n+1}\sqrt{n+1}|n\rangle + \langle n'|\sqrt{(n+1)(n+2)}|n+2\rangle] \rightarrow$

$\rightarrow \langle n'|x^2|n\rangle = \frac{\hbar}{2m\omega}[\sqrt{n(n-1)}\delta_{n'n-2} + \sqrt{(n+1)(n+2)}\delta_{n'n+2} + (2n+1)\delta_{n'n}]$.

$$\langle x^2\rangle = \frac{\hbar}{2m\omega}(2n+1). \quad \text{(C.E.3.47)}$$

- $\langle n'|{p_x}^2|n\rangle = \frac{m\hbar\omega}{2}\left[-\sqrt{n(n-1)}\delta_{n'n-2} - \sqrt{(n+1)(n+2)}\delta_{n'n+2} + (2n+1)\delta_{n'n}\right]$.

I the result for $\langle n'|p_x|n\rangle$ and rewrite (C.E.3.43)

$$\langle n'|p_x|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}(-\langle n'|\sqrt{n}|n-1\rangle + \langle n'|\sqrt{n+1}|n+1\rangle). \quad \text{(C.E.3.48)}$$

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[3] In chapter 4 *Undergraduate Course* $\langle x\rangle = \int_{-\infty}^{\infty} x|\psi_0|^2 dx = 0$, with the Gaussian distribution centred around $x = 0$.

Plug $p_x = i\sqrt{\frac{m\hbar\omega}{2}}(-A + A^\dagger)$ into (C.E.3.48). Following the procedure applied to (C.E.3.46), results into:

$\langle n'|{p_x}^2|n\rangle = \frac{m\hbar\omega}{2}\left[-\sqrt{n(n-1)}\delta_{n'n-2} - \sqrt{(n+1)(n+2)}\delta_{n'n+2} + (2n+1)\delta_{n'n}\right].$

$\langle {p_x}^2\rangle = \frac{m\hbar\omega}{2}(2n+1).$ (C.E.3.49)

- Deduce that

$\langle(\Delta x)^2\rangle\langle(\Delta p_x)^2\rangle = (n+\frac{1}{2})^2\hbar^2$. (C.E.3.50)

Given:

$\Delta x = x - \langle x\rangle = x,$

and

$\Delta\, p_x = \, p_x - \langle\, p_x\rangle = \, p_x.$

Then, with (C.E.3.47) and (C.E.3.49):

$\langle(\Delta x)^2\rangle\langle(\Delta p_x)^2\rangle = \, \langle x^2\rangle\langle {p_x}^2\rangle = \frac{\hbar}{2m\omega}(2n+1)\frac{m\hbar\omega}{2}(2n+1) = (n+\frac{1}{2})^2\hbar^2.$

In addition, with (C.E.3.45) and (C.E.3.49):

$\langle x^2\rangle = \frac{\hbar}{2m\omega}\langle 2AA^\dagger - 1\rangle = \frac{\hbar}{2m\omega}(2n+1),$

and

$\langle {p_x}^2\rangle = \frac{m\hbar\omega}{2}\langle 2AA^\dagger - 1\rangle = \frac{m\hbar\omega}{2}(2n+1).$

$\langle AA^\dagger\rangle = n + 1,$

and.

$\langle A^\dagger A\rangle = n.$

(C.E.3.5)

$H = \hbar\omega(\frac{1}{2} + A^\dagger A),$

this illustrates the relation between the Hamiltonian and the raising/lowering operators.

In section 2.7 , Fp presented the Heisenberg Uncertainty Relation:

$\langle(\Delta x)^2\rangle\langle(\Delta p_x)^2\rangle \geq \frac{1}{4}\hbar^2, (2.102).$

For the Harmonic oscillator the uncertainty relation is

$\langle(\Delta x)^2\rangle\langle(\Delta p_x)^2\rangle = (n+\frac{1}{2})^2\hbar^2$, (C.E.3.50).

Consequently, for the Gaussian distribution $(n = 0)$, as mentioned by Fp below (2.102), the Uncertainty Relation is:

$\langle(\Delta x)^2\rangle\langle(\Delta p_x)^2\rangle = \frac{1}{4}\hbar^2.$

Exercise 3.5 Analysis of the Hamiltonian of a particle in one dimension.

Consider a particle in one dimension whose Hamiltonian is

$H = \frac{{p_x}^2}{2m} + V(x).$

By calculating $[[H, x], x]$, demonstrate that

$\sum_{n'}|\langle n|x|n'\rangle|^2\,(E_{n'} - E_n) = \frac{\hbar^2}{2m}$, (C.E.3.51)

where $|n\rangle$ is a properly normalized energy eigenket corresponding to the eigenvalue E_n , and the sum is over all eigenkets. $H|n\rangle = E_n|n\rangle$.

$[[H, x], x] = (Hx - xH)x - x(Hx - xH) = Hx^2 - 2xHx + x^2H$. (C.E.3.52)

Reminder: an operator works always on "something", i.e., $|n\rangle$.

So, with ${p_x}^2 = -\hbar^2\frac{d^2}{dx^2}$:

$Hx^2 = -\frac{\hbar^2}{m} + x^2H,$
and
$2xHx = 2x^2H$.
With these results, and (C.E.3.52):
$\big[[H,x],x\big] = -\frac{\hbar^2}{m}$. (C.E.3.53)

Exercise 3.5 *Intermezzo Operator Algebra*

In the section on Conservation of Energy, Susskind mentioned the condition for $\langle Q \rangle$ not to change is:
$[Q,H] = 0$.
Susskind continues: "*We can make the statement stronger. Using the properties of commutators, it's easy to see that if* $[H,Q] = 0$*, then* $[Q^2,H] = 0$*, or even more generally,* $[Q^n,H] = 0$ *, for any* n*. It turns out that we can make a stronger claim: if* Q *commutes with the Hamiltonian, the expectation value of all functions of* Q *are conserved. That's what conservation means in quantum mechanics."* In Noordzij(4), I did prove above the statement.
What about $[H,x^2]$ =?
Taken into account the statement of Susskind, I would expect : $[H,x^2] = 0$.
Alas, I found above, with
$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x),$
$Hx^2 = -\frac{\hbar^2}{m} + x^2H \rightarrow [H,x^2] = -\frac{\hbar^2}{m}$.
End of Intermezzo.

Exercise 3.5 Continued on the application of [[H, x],x].

Now, what about
$\sum_{n'}|\langle n|x|n'\rangle|^2\,(E_{n'} - E_n) = \frac{\hbar^2}{2m}$?
The identity operator, $\sum_{n'}|n'\rangle\langle n'| = 1$, will be used.
$\sum_{n'}|\langle n|x|n'\rangle|^2\,(E_{n'} - E_n) = \sum_{n'}\langle n|x|n'\rangle\langle n'|x|n\rangle\,(E_{n'} - E_n) =$
$= \sum_{n'}\langle n|x|n'\rangle\langle n'|x|n\rangle\,E_{n'} - \langle n|x\sum_{n'}|n'\rangle\langle n'|xE_n|n\rangle =$
$= \sum_{n'}\langle n|x|n'\rangle\langle n'|x|n\rangle\,E_{n'} - \langle n|x^2H|n\rangle$. (C.E.3.54)
The next one:
$\sum_{n'}\langle n|x|n'\rangle\langle n'|x|n\rangle\,E_{n'}$?
$\sum_{n'}\langle n|x|n'\rangle\langle n'|x|n\rangle\,E_{n'} = \sum_{n'}\langle n|xE_{n'}|n'\rangle\langle n'|x|n\rangle = \sum_{n'}\langle n|xH|n'\rangle\langle n'|x|n\rangle$. (C.E.3.55)
With
$[H,x] = 0$, (C.E.3.55) becomes
$\sum_{n'}\langle n|Hx|n'\rangle\langle n'|x|n\rangle = \langle n|Hx^2|n\rangle.$ (C.E.3.56)
(C.E.3.54), (C.E.3.56) and
$\langle n|Hx^2|n\rangle - \langle n|x^2H|n\rangle = \langle n|Hx^2 - x^2H|n\rangle = -\frac{\hbar^2}{m}.$
Alas, this result differs a factor -2 from (C.E.3.51).
Somewhere down the road I made a mistake. I do not know where. The only thing I can think of not to be allowed to use the identity operator in (C.E.3.56).
I will use a different approach for (C.E.3.54).
Plug into (C.E.3.54), $\langle n'|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n}\delta_{n'n-1} + \sqrt{n+1}\delta_{n'n+1})$, for both $E_{n'}$ and E_n:
$\frac{\hbar}{2m\omega}\{[n+(n+1)][E_{n-1} + E_{n+1}] - [n+(n+1)]E_n\}$. (C.E.3.57)
With

$E_n = \hbar\omega\left(n+\frac{1}{2}\right)$,
(C.E.3.57) becomes:
$\frac{\hbar^2}{2m}\left[(2n+1)^2 - \frac{1}{2}(2n+1)^2\right] = \frac{\hbar^2}{2m}(4n^2+4n+1)$. (C.E.3.58)
Nowhere near $\frac{\hbar^2}{2m}$.
There is more. As an alternative I will use for $\langle n|x^2H|n\rangle$ in (C.E.3.54):
$E_n\langle n|x^2|n\rangle$ given in (C.E.3.47)→ $E_n\frac{\hbar}{2m\omega}(2n+1)$. No surprise, this leads to the same result as given in (C.E.3.58).
I leave this exercise.

Exercise 3.6 The Hamiltonian and the Displacement Operator.

Consider a particle in one dimension whose Hamiltonian is
$H = \frac{{p_x}^2}{2m} + V(x)$.
Suppose the potential to be periodic:
$V(x-a) = V(x)$,
for all x. Deduce that
$[D(a), H] = 0$,
where
$D(a) = e^{ip_x a/\hbar}$.
$[D(a), H] \to (DH - HD)\psi(x) \to$
$\to -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}D\psi(x) + D[V(x)\psi(x)] + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}D\psi(x) - V(x)D\psi(x)$. (C.E.3.59)
With $V(x-a) = V(x) \to V(x) = V(x+a)$.
$DV(x)D^\dagger = D^\dagger V(x)D \to DV = VD$. (C.E.3.60)
Plug this into (C.E.3.59), using (2.126), $p_x = i\hbar D$
$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}D\psi(x) + D[V(x)\psi(x)] + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}D\psi(x) - V(x)D\psi(x) = 0$.
Hence, show that the wave function of an energy eigenstate has the general form:
$\psi(x') = e^{ik'x'}u(x')$, (C.E.3.61)
where k' is a real parameter, and $u(x'-a) = u(x')$ for all x'. This result is known as the *Bloch Theorem*.
In Exercise 2.4, I presented the results:
where $u(x'+a) = u(x')$ for all x'.
$u(x'+a) = u(x') \to u(x') = u(x'-a)$.
I assume $\psi(x') = e^{ik'x'}u(x')$ to be correct. Does this lead to a contradiction?
Plug into (C.E.2.14)
$x' \to x'+a$.
Then,
$\psi(x'+a) = e^{ik'(x'+a)}u(x'+a) = e^{ik'a}e^{ik'x'}u(x') = e^{ik'a}\psi(x')$,
where $e^{ik'a}$ is a phase factor.

Remark
$[D(a), H] = 0$,
the displacement operator and the Hamiltonian have the same eigenstates.
Remark:

In Exercise 2.4 I demonstrated $|A\rangle$ to be an eigenket of $D(a)$.
Can the corresponding wave function, $\psi_A(x') = \langle x'|A\rangle$, be written as:
$\psi_A(x') = e^{ik'x'}u(x')$? This is demonstrated by the substitution $x' = x + a$.

Hence the wavefunction of an energy operator is equal to
$\psi' = e^{ik'x'}u(x')$.
This I conclude from $[D(a), H] = 0$.
With
$[D(a), H]\,\psi' = 0$,
this can be demonstrated.

Exercise 3.7 About the Heisenberg equations of motion and the ladder operators.

3.7 Consider the one-dimensional quantum harmonic oscillator discussed in Exercise 3.3.
Show the Heisenberg equations of motion in terms of the ladder operators A and $A^\dagger$.
The ladder operator
$A = \sqrt{\frac{m\omega}{2\hbar}}x + i\frac{p_x}{\sqrt{2m\omega\hbar}}$,
$A(t=0) = \sqrt{\frac{m\omega}{2\hbar}}x(0) + i\frac{p_x(0)}{\sqrt{2m\omega\hbar}}$.
Furthermore, I will use the results of exercise 3.3:
$[H, A] = -\hbar\omega A$,
and
$[H, A^\dagger] = \hbar\omega A^\dagger$.
Using (3.23), displace the general observable and
$[A, H] = \hbar\omega A = i\hbar\frac{dA}{dt}$.
Hence
$\frac{dA}{dt} = -i\omega A \rightarrow A = A(t=0)e^{-i\omega t}$
and
$\frac{dA^\dagger}{dt} = i\omega A^\dagger \rightarrow A^\dagger = A^\dagger(t=0)\,e^{i\omega t}$.
The position operator
$x = \sqrt{\frac{\hbar}{2m\omega}}\left[A(0)e^{-i\omega t} + A^\dagger(0)e^{i\omega t}\right]$.
The momentum operator
$p_x = i\sqrt{\frac{m\omega\hbar}{2}}\left[-A(0)e^{-i\omega t} + A^\dagger(0)e^{i\omega t}\right]$.
Use the goniometric relations and
$p_x(t) = p_x(0)\cos\omega t - x(0)m\omega\sin\omega t$,
$x(t) = x(0)\cos\omega t + \frac{p_x(0)}{m\omega}\sin\omega t$.

Exercise 3.8 About the time independent Schrödinger equation and the Virial Theorem

Consider a one-dimensional bound state. Using the time-independent Schrödinger equation, prove that
$\langle\frac{p_x^2}{2m}\rangle = E - \langle V\rangle$,
and
$\langle\frac{p_x^2}{2m}\rangle = -E + \langle V\rangle + \langle x\frac{dV}{dx}\rangle$.

Fp mentioned the stationary wavefunction to be real.
The Hamiltonian:
$H = \frac{p_x^2}{2m} + V(x).$
Schrödinger equation:
$H\psi = E\psi.$
Then, I find for the expectation value:
$\langle H \rangle = E$:
$\langle \frac{p_x^2}{2m} + V(x) \rangle = E \rightarrow \langle \frac{p_x^2}{2m} \rangle = E - \langle V(x) \rangle.$
Now I evaluate
$[H, xp_x]$.
$[H, xp_x] = Hxp_x - xp_xH = xHp_x - xp_xH + Hxp_x - xHp_x$,
where I added and subtracted xHp_x.
Then
$[H, xp_x] = x[H, p_x] + [H, x]p_x = i\hbar x \frac{dV}{dx} - i\hbar \frac{p_x^2}{m}$,(www.en.m.wikipedia.org ,Virial Theorem).
Now,
$x[H, p_x] + [H, x]p_x = 0.$
Then
$i\hbar x \frac{dV}{dx} - i\hbar \frac{p_x^2}{m} = 0.$
Consequently
$\langle \frac{p_x^2}{2m} \rangle = \frac{1}{2} \langle x \frac{dV}{dx} \rangle.$
In this exercise, I should have proven in the first place
$\langle \frac{p_x^2}{2m} \rangle = -E + \langle V(x) \rangle + \langle x \frac{dV}{dx} \rangle.$
I did not do that.
Subtract
$\langle \frac{p_x^2}{2m} \rangle = E - \langle V(x) \rangle$ from $2 \langle \frac{p_x^2}{2m} \rangle = \langle x \frac{dV}{dx} \rangle$ and
$\langle \frac{p_x^2}{2m} \rangle = -E + \langle V(x) \rangle + \langle x \frac{dV}{dx} \rangle,$
is found.

4 Orbital Angular Momentum

4.1 Orbital Angular Momentum

See *The Undergraduate Course Chapter 8*, Fp.
Consider a particle described by Cartesians coordinates and their conjugate momenta.
The important equations for angular momentum are given in (4.8)-(4.10).
These expressions are summed up by (4.11). Well, to what avail?
To demonstrate (4.16)
$[L_x^2, L_z] = L_xL_xL_z - L_zL_xL_x = L_xL_xL_z - L_xL_zL_x + L_xL_zL_x - L_zL_xL_x \rightarrow$
$\rightarrow L_x[L_x, L_z] + [L_x, L_z]L_x.$
With (4.10), (4.16) is obtained.
The remark on top of page 59 is mathematically summarized on page 104 of *The Undergraduate*

Course. The commutator $[L^2, L_x] = 0$ is presented in Eq.(8.11) of this *Course.*
To demonstrate (4.22), with (4.9), (4.10) and (4.20),
$[L^+, L_z] = [L_x, L_z] + i[L_y, L_z] = -i\hbar L_y - \hbar L_x = -\hbar L^+.$
Since
$[L^2, L_x] = [L^2, L_y] = 0$,
$[L^2, L^+] = [L^2, L^-] = 0$.

4.2 Eigenvalues of Orbital Angular Momentum.

See *The Undergraduate Course Chapter 8*, Fp.
(4.32) is found by using:
$L^2\, L^+ = L^+ L^2$.
This expression is found with the commutators $[L^2, L_x] = 0$ and $[L^2, L_y] = 0$.
(4.33) and (4.34) compare with (8.34) and (8.36) of *The Undergraduate Course.*
Top of page 60:
$\langle B|B\rangle$ as mentioned by Dirac, can be considered as the length of the ket $|B\rangle$. Consequently, $\langle B|B\rangle \geq 0$.
(4.33) implies that
$L^+|l, m\rangle \propto |l, m+1\rangle$.
In *The Undergraduate Course* §8.4, page 106, Fp writes: "We, thus, conclude that when the operator $L_+ (\equiv L^+)$ operates on an eigenstate of L_z corresponding to the eigenvalue $m\hbar$ it converts it to an eigenstate corresponding to the eigenvalue $(m+1)\hbar$. Hence, L_+ is known as the *raising operator* for (L_z). To me, this formulation explains the action of L^+ in a clear way.
(4.35), with (4.23) and (4.25):
$L_z L^-|l, m\rangle = (L^- L_z + [L_z, L^-]|l, m\rangle = (L^- L_z - \hbar L^-)|l, m\rangle = (m-1)\hbar|l, m\rangle,$
explaining the action of the *lowering operator* L^-.
(4.37) follows from
$L^-|0\rangle = |0\rangle,$
since the square of m in (4.31) indicates also a lower bound for m .
(4.44) follows from (4.25) and (4.43).
In (4.48) note
$(\ldots\ldots)^*$.
At the end of section 4.2, Fp summarizes the results of the eigenvalues of orbital angular momentum.

4.3 Rotation Operators

In this section a particle is described by spherical polar coordinates.
Also *Undergraduate Course §8.3 Representation of Angular Momentum,* Fp.
(4.61) is completely similar to (2.127).
At the bottom of page 64, Fp mentioned a rotation about the x-axis does not commute with a rotation about the y-axiswith (4.68) and (4.68) we have
$[R_x, R_y] = \frac{[L_y, L_x]\Delta\varphi_y \Delta\varphi_x}{\hbar^2}$.
Using (4.8) the above expression becomes:

$[R_x, R_y] = \frac{[L_y, L_x]\Delta\varphi_y\Delta\varphi_x}{\hbar^2} = \frac{i}{\hbar} L_z \Delta\varphi_y \Delta\varphi_x$,
illustrating the non-commutating character of the rotation.

4.4 Eigenfunctions of Orbital Angular Momentum.

Fp presented the three components of orbital angular momentum in Cartesian coordinates. The transformations on page 65 can also be found in the *Undergraduate Course* pages 105-106 and for spherical harmonics see pages 110-114.
For the functions discussed in this section see for example Abramowitz, M. and I.A. Stegun and Chisholm, J.S.R., and R.M. Morris.
Spherical harmonics and quantum mechanics are also dealt with by Mahan in chapters 4 and 5.
(4.87), Fp assumed the wave function $\psi(r, \theta, \varphi)$ to be separable.
So, with (4.86),
$L^2\psi(r, \theta, \varphi) = R(r)L^2Y(\theta, \varphi) = \lambda\hbar^2 R(r)Y(\theta, \varphi) \rightarrow L^2Y(\theta, \varphi) = \lambda\hbar^2\, Y(\theta, \varphi)$.(C.4.4.1).
Then, with (4.85) and (C.4.4.1), (4.88) is obtained.
Remark:
(4.89) $P_{l,m}(\cos\varphi)$ should be $P_{l,m}(\cos\theta)$. A typo, I suppose.
I assume this separation works for the Schrödinger equation in spherical coordinates.
As mentioned by Fp, in this section 4.4 the results of section 4.2 have been reproduced.

4.5 Motion in Central Field.

Consider a particle of mass M in a spherical symmetric potential, for example a Coulomb potential.
Fp analysed the Schrödinger representation.
Just below (4.98): $p = -i\hbar\nabla$ instead of $p = -\frac{i}{\hbar}\nabla$. A typo.
(4.102): the Hamiltonian commutes with all three components of angular momentum. For example: $[L_x, H]$. With (4.101), (4.80) operating on $\psi(r, \theta, \varphi) = R(r)Y(\theta, \varphi)$, the result is
$i\hbar[\frac{R(r)}{\hbar r^2}\{L_xL^2 - L^2L_x\}Y(\theta, \varphi)]$.
Since
$L_xL^2 - L^2L_x = 0$,
(4.102) is found.
In the same way (4.103) is obtained. As mentioned by Fp, angular momentum and its magnitude squared are constants of motion: (3.31).
Just below (4.104) Fp states : "…we already know the most general form of the wavefunction …..is $\psi(r, \theta, \varphi) = R(r)Y(\theta, \varphi)$." Well, what I understand is that the separation works.
Plugging (4.105) into (4.101) and use (4.93), the differential equation for the radial component $R(r)$ of the wave function is obtained.
In *The Undergraduate Course* Fp presented in section 9.2 the differential equation for the radial component $R(r)$ of the wave function. In section 9.4 of this *Course*, Fp analysed the central potential for the Hydrogen Atom. Mahan dealt with the subject of Coulomb Potentials in section 5.4.

4.6 Energy Levels of Hydrogen Atom.

The Hydrogen atom is a typical example of a central potential.
Since the orbital eigenfunctions are found, the next step is the evaluation of the radial part of the wave function. See also The Undergraduate Course(Fp) §9.4.
Page 69,(4.112). The exponential function e^{-y} is given here. However, for the behaviour at large r the differential equation (4.109) reduces to

$\frac{d^2P}{dr^2} + \frac{2\mu E}{\hbar^2}P = 0$, $E < 0$.

A meaningful solution of this differential equation is

$P \propto e^{-\sqrt{\frac{2\mu|E|}{\hbar^2}}r} = e^{-r/a}$,

or

$R(r) \propto \frac{1}{r}e^{-\sqrt{\frac{2\mu|E|}{\hbar^2}}r} = \frac{1}{r}e^{-r/a}$

This result for $P = r(Rr)$ represents the exponential part of $P(r)$ of (4.112). See also Mahan, page 120.
Note: this indicates the dependence on the power series $f(y)$ has to vanish for large r .
Keep in mind, there are two terms in (4.115) with y^{n-2} and a coefficient c_{n-1}. This results into the right-hand side of (4.116).
As mentioned by Fp, the series presented in (4.114)must terminate at small n in order to find a physical behaviour for $P(r)$ as presented in (4.112). This results into a $n_{min} = l + 1$. This makes c_{n-1} vanish.
Again, let's analyse the differential equation for small r:

$\frac{d^2P}{dr^2} - \frac{l(l+1)}{r^2}P = 0$.

The meaningful solution of this differential equation is
$P \propto r^{l+1} \rightarrow n_{min} = l + 1$. See also Mahan, page 120.
Now for large values of r. As mentioned above, something must be done with the series y^n in (4.114). So, if not, (4.112),

$\lim_{y\to\infty} f(y)\exp(-y) \rightarrow \infty$.

Consequently, for some maximum value of n, c_n has to vanish.
At the bottom of page 69, Fp presented, for large y, the ratio of successive terms,(4.117), in the series (4.114) according to (4.116). Based on that result Fp obtained the maximum value of n, (4.119).
According to (4.116) I find:

$\frac{c_n}{c_{n-1}} = \frac{2(n-1)-\frac{2\mu e^2 a}{4\pi\epsilon_0\hbar^2}}{n(n-1)-l(l+1)} \equiv \frac{2(n-1)-\frac{2a}{a_0}}{n(n-1)-l(l+1)} (\neq \frac{2}{n})$.

Note: I suppose Fp meant for $n \gg \frac{2a}{a_0}$.
Another approach is to analyse the differential equation (4.113) for large y :

$\frac{d^2f}{dy^2} - 2\frac{df}{dy} = 0$.

The solution for f resulting from this differential equation is:

$\lim_{y\to\infty} f \propto \exp(2y)$.

The series expansion of $\exp(2y)$ gives the tool to find the maximum value of n.
The expansion is presented in (4.118). Now, for $c_n = 0$ in (4.116), (4.119) is obtained:

$n-1=\frac{\mu e^2 a}{4\pi\epsilon_0\hbar^2}$ or $n=\frac{\mu e^2 a}{4\pi\epsilon_0\hbar^2}\equiv\frac{a}{a_0}$, (4.124).
This result gives for c_n:
$c_n[n(n-1)-l(l+1)]=c_{n-1}[2(n-1)-2n]=-c_{n-1}$.
As mentioned above Mahan analysed the cases for $r\to 0$ and $r\to\infty$. Then Mahan defined a function, in the notation of Fp,
$P(y)=y^{l+1}G(y)e^{-y}$,
where
$f(y)=y^{l+1}G(y)e^{-y}$.
$P(y)=y^{l+1}G(y)e^{-y}$ reflects the behaviour of $P(y)$ for small y and large y respectively.
Plugging the expression for $P(y)$ into the Schrödinger's equation results into a standard differential equation which are satisfied by the hypergeometric function(Abramowitz and Stegun). See for this the analysis by Mahan §5.4.2 on Confluent Hypergeometric Functions and §5.4.3 on Hydrogen Eigenfunctions.

Exercises

Exercise 4.1 Application of the fundamental commutators for angular momentum

Demonstrate directly from fundamental commutation relations for angular momentum, (4.11), that
- $[L^2,L_z]=0$.
The general expression for commutators is used:
$[A^2,B]=A^2B-BA^2=A^2B-ABA+ABA-BA^2=A[A,B]+[A,B]A.$
$[L^2,L_z]=\left[L_x^2+L_y^2+L_z^2,L_z\right]=L_x[L_x,L_z]+[L_x,L_z]L_x+L_y\left[L_y,L_z\right]+\left[L_y,L_z\right]L_y+$
$L_z[L_z,L_z]+[L_z,L_z]L_z=L_x[L_x,L_z]+[L_x,L_z]L_x+L_y\left[L_y,L_z\right]+\left[L_y,L_z\right]L_y.$ (C.E.4.1)
With the fundamental relations (4.9) and (4.10), (C.E.4.1) is:
$[L^2,L_z]=i\hbar\left[L_y,L_x\right]+i\hbar\left[L_x,L_y\right]=0.$

- $[L^{\pm},L_z]=\mp\hbar L^{\pm}$.
$[L^{+},L_z]=\left[L_x+iL_y,L_z\right]=[L_x,L_z]-i[L_z,L_y].$ (C.E.4.2)
With (4.9) and (4.10), (C.E.4.2) can be written as
$-\hbar\left(L_x+iL_y\right)=-\hbar L^{+}$.
$[L^{-},L_z]=\left[L_x-iL_y,L_z\right]=[L_x,L_z]+i[L_z,L_y].$ (C.E.4.3)
Then, simarlily to (C.E.4.2), (C.4.1.3) can be written as
$\hbar\left(L_x-iL_y\right)=\hbar L^{-}$.

- $[L^{+},L^{-}]=2\hbar L_z$.
$[L^{+},L^{-}]=\left[\,L_x+iL_y,L_x-iL_y\right]=i\left[L_y,L_x\right]+i\left[L_y,L_x\right]$ →with (4.8) → $2\hbar L_z$.

Exercise 4.2 Orbital Angular Momentum expressed in spherical coordinates.

Demonstrate from Equations (4.74)-(4.79) that the orbital angular momentum components can be expressed in spherical coordinates.
In section 8.3 of *The Undergraduate Course*, Fp writes: "It follows, after some tedious analysis, that ….". Then, Fp presented $\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial z}{\partial z}$,(8.23)-(8.24). A tedious analysis indeed. By

plugging the expression for the derivatives into (4.74)-(4.76) the expressions for the components of orbital momentum in spherical coordinates,(4.80)-(4.82), are obtained.

Exercise 4.3 Expectation values of Angular Momentum Components.

A system is in the state $\psi(\theta,\varphi) = Y_{l,m}(\theta,\varphi)$.
Evaluate:
- $\langle L_x \rangle$. See also Exercise 1 , Chapter 8 of *The Undergraduate Course.*
$\langle L_x \rangle = \oint \psi^* L_x \psi d\Omega$.
L_x is given by Eq.(4.80) 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.(4.82) and (4.85) respectively. 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.(4.20) 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) of *The Undergraduate Course* or *The Graduate Course* (4.55) and (4.56)
Then $\langle L_x \rangle$ becomes, with (4.51), (4.52),(4.55), (4.56){or(4.96) and (4.97)}, and orthogonality:
$\langle L_x \rangle = \oint \psi^* (L^+ + L^-) \frac{1}{2} \psi d\Omega =$
$= \frac{1}{2}[\oint c^+_{l,m} Y^*_{l,m}\, Y_{l,m+1} d\Omega + \oint c^-_{l,m} Y^*_{l,m}\, Y_{l,m-1} d\Omega] = 0$.
Reminder: when using L_x of (4.80), in (4.89) $P_{l,m}(\cos\varphi)$ should be $P_{l,m}(\cos\theta)$.
In addition we conclude $Y_{l,m}(\theta,\phi)$ 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 ?
See section 1.13: Eqs.(1.63)-(1.67).

- $\langle L_y \rangle$.
$L_y = i\frac{L^- - L^+}{2}$.
Similar to $\langle L_x \rangle$, $\langle L_y \rangle = 0$.
Note: operating L_x on $Y_{l,m}(\theta,\varphi)$ with (4.89):
$L_x\, Y_{l,m}(\theta,\varphi) \neq a Y_{l,m}(\theta,\varphi)$,
where a represents an eigenvalue.

- $\langle L_x^2 \rangle$.
$L_x^2 = \frac{1}{4}((L^+)^2 + L^+L^- + L^-L^+ + (L^-)^2)$.
We need to investigate L^+L^- and L^-L^+ .
The other two terms in L_x^2 do not contribute, since $\langle L_x \rangle = 0$.
First , L^+L^- , with Eqs.(4.51), (4.52), (4.96) and (4.97):
$\oint \psi^* (L^+L^-) \frac{1}{4} \psi d\Omega = \frac{1}{4} c^-_{l,m} c^+_{l,m-1}$.
Then , L^-L^+ , with Eqs.(4.51), (4.52), (4.96) and (4.97),:
$\oint \psi^* (L^-L^+) \frac{1}{4} \psi d\Omega = \frac{1}{4} c^+_{l,m} c^-_{l,m+1}$.
Hence $\langle L_x^2 \rangle = \frac{1}{4}\left(c^-_{l,m} c^+_{l,m-1} + c^+_{l,m} c^-_{l,m+1}\right)$.
With Eqs.(8.15) and (8.16) of *The Undergraduate Course*(Fp):

$L^+L^- + L^-L^+ = 2(L^2 - L_z^2)$,
we again find the above result for $\langle L_x^2 \rangle$.
With Eqs.(4.51), (4.52), (4.96) and (4.97), :
$\langle L_x^2 \rangle = \frac{1}{4}\left(c_{l,m}^- c_{l,m-1}^+ + c_{l,m}^+ c_{l,m+1}^-\right) = \frac{1}{2}(l(l+1)\hbar^2 - m^2\hbar^2)$.

- $\langle L_y^2 \rangle$.
$L_y^2 = \frac{1}{4}((L^+)^2 - (L^+L^- + L^-L^+) + (L^-)^2)$.
Hence
$\langle L_y^2 \rangle = -\frac{1}{2}(l(l+1)\hbar^2 - m^2\hbar^2)$.
Rremark:
This exercise could have been done with (4.80) and (4.95).

Exercise 4.4 About the Raising and Lowering Operators and the Spherical Harmonics

Derive Equations (4.96) and (4.97) from Equation (4.95).
To solve this problem I will use the expression in spherical coordinates for the raising and lowering operators respectively, (4.83).
In (4.95)
$\frac{dP_{l\,m}}{d\theta} = \frac{dP_{l\,m}}{d\xi}\frac{d\xi}{d\theta} = -\sin\theta\,\frac{dP_{l\,m}}{d\xi}$.
Since I demonstrate the raising operator L^+, I will use the expression in (4.95) with $P_{l\,m+1}$.
Now,

$$L^+Y_{l\,m} = \hbar e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\varphi}\right)\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-m)!}{(l+m)!}}(-1)^m e^{im\varphi}P_{l\,m}(\cos\theta) \qquad \text{(C.E.4.4)}$$

After performing the differentiation in (C.E.4.4), the result is

$$L^+Y_{l\,m} = -\hbar\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-m)!}{(l+m)!}}(-1)^{m+1}e^{i(m+1)\varphi}P_{l\,m+1}(\cos\theta). \qquad \text{(C.E.4.5)}$$

The last step is to rewrite $\sqrt{\frac{(l-m)!}{(l+m)!}}$ in (C.E.4.5):
$\sqrt{\frac{(l-m-1)!(l-m)!(l+m+1)!}{(l+m+1)!(l-m-1)!(l+m)!}} = \sqrt{\frac{(l-m-1)!}{(l+m+1)}}\sqrt{\frac{(l-m)!(l+m+1)!}{(l+m)!(l-m-1)!}} = \sqrt{\frac{(l-m-1)!}{(l+m+1)}}[(l+m)\big(l-(m+1)\big)]^{1/2}$
and this gives

$$\sqrt{\frac{(l-m-1)!}{(l+m+1)}}[l(l+1) - m(m+1)]^{1/2} = \sqrt{\frac{(l-m)!}{(l+m)!}}. \qquad \text{(C.E.4.6)}$$

Plug (C.E.4.6) into (C.E.4.5) and (4.96) is obtained.
(4.97) for the lowering operator is found in a similar way.

Exercise 4.5 Eigenvalues and eigen functions of L_x

Find the eigenvalues and eigenfunctions (in terms of the angles θ and φ) of L_x.
In Exercise 8.2 of *The Undergraduate Course (UC)* (Fp), the eigenvalues and eigenfunctions of L_x are derived. Some of the results presented there will repeated here.
As found in Exercise (4.3) $Y_{l,m}(\theta,\varphi)$ is not an eigenfunction of L_x.
A general function $F(\theta,\varphi)$ could do the job. It should be a continuous function. In that case $F(\theta,\varphi)$ can be expressed as a series of spherical harmonics, Eq.(C.8.E.5)- *(UC)*:
$L_xF(\theta,\phi) = \frac{1}{2}(L_+ + L_-)\sum_{m=-l}^{m=l} a_m Y_{l,m}(\theta,\phi) =$

$= \frac{1}{2} a_{l-1} \hbar\sqrt{2l} Y_{l,l} + \sum_{m=-l+1}^{m=l-1} \frac{1}{2}(a_{m+1} c_{l,m}^{+} + a_{m-1} c_{l,m}^{-}) Y_{l,m} + \frac{1}{2} a_{-l+1} \hbar\sqrt{2l} Y_{l,-l}.$ (C.E.4.7)

To find the eigenvalues, I define the eigenvalue equation

$L_x F(\theta,\phi) = \hbar A F(\theta,\phi) = \hbar A \sum_{m=-l}^{m=l} a_m Y_{l,m}(\theta,\phi),$ (C.E.4.8)

where A represents the factor for the eigenvalues.

The next step is to equate the coefficients of $Y_{l,m}$ in (C.E.4.7) and (C.E.4.8), with Eqs.(4.51) and (4.52). Then, $2l+1$ equations are obtained:

$A a_l = \frac{1}{2} a_{l-1}\sqrt{2l},$

$A a_{l-1} = \frac{1}{2}(\sqrt{2l} a_l + \sqrt{4l-2} a_{l-2}),$

$A a_{l-2} = \frac{1}{2}(\sqrt{4l-2} a_{l-1} + \sqrt{6l-6} a_{l-3}),$

……,

$A\hbar a_m = \frac{1}{2}(a_{m+1} c_{l,m}^{+} + a_{m-1} c_{l,m}^{-}),$

……,

$A a_0 = \frac{\sqrt{l(l+1)}}{2}(a_1 + a_{-1}),$

……,

$A a_{-l+1} = \frac{1}{2}(\sqrt{4l-2} a_{-l+2} + \sqrt{2l} a_{-l}),$

$A a_{-l} = \frac{1}{2} a_{-l+1}\sqrt{2l}.$

These are $2l+1$ expressions and with $-l \le m \le l$, the eigenvalues are found.

The expression for A is expected to be:

$A(A^2-1)(A^2-4)(A^2-9)\ldots\ldots(A^2-[l-1]^2)(A^2-l^2) = 0,$

with the eigenvalues

$A\hbar = 0, \pm\hbar, \pm 2\hbar, \pm 3\hbar, \ldots\ldots, \pm(l-1)\hbar, \pm l\hbar.$

The results for $l = 1, 2$ are presented

I start with the case for $l = 1$.

Then

$F(\theta,\varphi) = \sum_{m=-1}^{m=1} a_m Y_{1\,m}.$ (C.E.4.9)

Now $L_x F(\theta,\varphi)$ is evaluated where

$L_x = \frac{1}{2}(L^+ + L^-)$ will be used.

The eigenvalue equation is

$L_x F(\theta,\varphi) = \frac{1}{2}(L^+ + L^-) F(\theta,\varphi) = \frac{1}{2}(L^+ + L^-) \sum_{m=-1}^{1} a_m Y_{1\,m} = A\hbar \sum_{m=-1}^{1} a_m Y_{1\,m}$,

where $A\hbar$ is the eigenvalue.

So, A and a_m need to be evaluated.

With (4.96) and (4.97)

$\frac{1}{2}(L^+ + L^-) \sum_{m=-1}^{1} a_m Y_{1\,m} = \frac{1}{2}\sqrt{2}(a_0 Y_{1\,1} + a_{-1} Y_{1\,0} + a_1 Y_{1\,0} + a_0 Y_{1-1})\hbar.$ (C.E.4.10)

Equate the coefficients of the spherical harmonics in

$\frac{1}{2}\sqrt{2}\,\hbar \sum_{m=-1}^{m=1} a_m Y_{1\,m} = \hbar A \sum_{m=-1}^{m=1} a_m Y_{1\,m}.$

The result is

$A a_1 = \frac{1}{2}\sqrt{2} a_0,$

$A a_0 = \frac{1}{2}\sqrt{2}(a_1 + a_{-1})$, and

$A a_{-1} = \frac{1}{2}\sqrt{2} a_0$.

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

$$F(\theta,\varphi)=a_1 Y_{1\,1}+a_1\sqrt{2}Y_{1\,0}+a_1 Y_{1-1}. \quad \text{(C.E.4.11)}$$

and

$$F(\theta,\varphi)=a_1 Y_{1\,1}-a_1\sqrt{2}Y_{1\,0}+a_1 Y_{1-1}, \quad \text{(C.E.4.12)}$$

with eigenvalues $\pm\hbar$.

The eigenfunction for $A=0$ is:

$$F(\theta,\varphi)=a_1 Y_{1\,1}-a_1 Y_{1-1}. \quad \text{(C.E.4.13)}$$

a_1 is found normalising $F(\theta,\varphi)$:

$\int_0^{2\pi}\int_0^{\pi} F^* F \sin\theta d\theta d\varphi$. Plug (C.E.4.11) or (C.E.4.12) into this integral and

$a_1=\frac{1}{2}\sqrt{2}$.

Hence for the eigenfunction $F(\theta,\varphi)$, $A=\pm 1$,the following series of spherical harmonics are found:

$$F(\theta,\varphi)=\frac{1}{2}\sqrt{2}Y_{1\,1}+Y_{1\,0}+\frac{1}{2}\sqrt{2}Y_{1-1}. \quad \text{(C.E.4.14)}$$

and

$$F(\theta,\varphi)=\frac{1}{2}\sqrt{2}Y_{1\,1}-Y_{1\,0}+\frac{1}{2}\sqrt{2}Y_{1-1}. \quad \text{(C.E.4.15)}$$

For the eigenfunction $F(\theta,\varphi)$, $A=0\rightarrow a_1=1$, the following series of spherical harmonics is found:

$$F(\theta,\varphi)=Y_{1\,1}-Y_{1-1}. \quad \text{(C.E.4.16)}$$

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

$L_x F(\theta,\varphi)=\hbar(\frac{1}{2}\sqrt{2}Y_{1\,1}+Y_{1\,0}+\frac{1}{2}\sqrt{2}Y_{1-1})$,

$L_x F(\theta,\varphi)=-\hbar(\frac{1}{2}\sqrt{2}Y_{1\,1}-Y_{1\,0}+\frac{1}{2}\sqrt{2}Y_{1-1})$

and

$L_x F(\theta,\varphi)=0$.

Note: there is no contradiction with $[L^2,L_x]=0$ .The eigenfunction of L_x is also an eigenfunction of L^2.

Other eigenfunctions are obtained by evaluating the series expansion for $l=2$ of the function in, Eq.(C.8.E.5)- *(UC)*:

$L_x F(\theta,\phi)=$

$\frac{1}{2}a_{l-1}\hbar\sqrt{2l}Y_{l,l}+\sum_{m=-l+1}^{m=l-1}\frac{1}{2}(a_{m+1}c_{l,m}^{+}+a_{m-1}c_{l,m}^{-})Y_{l,m}+\frac{1}{2}a_{-l+1}\hbar\sqrt{2l}Y_{l,-l}$.

For $l=2$:

$$F(\theta,\varphi)=\sum_{m=-2}^{m=2}a_m Y_{2\,m}. \quad \text{(C.E.4.17)}$$

$L_x F(\theta,\varphi) = \hbar B \sum_{m=-2}^{m=2} a_m Y_{2\,m}$. (C.E.4.18)

The analysis is the same as for the $l = 1$ series expansion.

So, equate the coefficients of the spherical harmonics in

$L_x \sum_{m=-2}^{m=2} a_m Y_{2\,m} = \frac{1}{2}(L^+ + L^-) \sum_{m=-2}^{m=2} a_m Y_{2\,m} = \hbar B \sum_{m=-2}^{m=2} a_m Y_{2\,m}$.

The result is

$Ba_2 = a_1$,

$Ba_1 = a_2 + \frac{\sqrt{6}}{2} a_0$,

$Ba_0 = \frac{\sqrt{6}}{2}(a_1 + a_{-1})$,

$Ba_{-1} = \frac{\sqrt{6}}{2} a_0 + a_{-2}$ and

$Ba_{-2} = a_{-1}$.

In the first place an equation for B is found:

$B(B^2 - 1)(B^2 - 4) = 0$.

Consequently 5 eigenvalues are found:

$0, \pm\hbar, \pm 2\hbar$.

By plugging B into the above 5 equations for a_m, the coefficients $a_1, .., a_{-2}$ expressed in a_2 for the 5 eigenfunctions are obtained.

For $B = \pm 1$ and the related a_2

$F(\theta,\varphi) = a_2(Y_{2\,2} + Y_{2\,1} - Y_{2-1} - Y_{2-2})$, with eigenvalue ħ,

$F(\theta,\varphi) = a_2(Y_{2\,2} - Y_{2\,1} + Y_{2-1} - Y_{2-2})$, with eigenvalue $-$ħ.

For $B = \pm 2$ and the related a_2

$F(\theta,\varphi) = a_2(Y_{2\,2} + 2Y_{2\,1} + \sqrt{6}Y_{2\,0} + 2Y_{2-1} + Y_{2-2})$, with eigenvalue 2ħ

and

$F(\theta,\varphi) = a_2\left(Y_{2\,2} - 2Y_{2\,1} + \sqrt{6}Y_{2\,0} + 2Y_{2-1} - Y_{2-2}\right)$, with eigenvalue -2ħ.

For $B = 0$ and the related a_2

$F(\theta,\varphi) = a_2\left(Y_{2\,2} - \frac{\sqrt{6}}{3}Y_{2\,0} + Y_{2-2}\right)$, with eigenvalue 0.

a_2 is found by normalization of $G(\theta,\varphi)$,

$\int_0^{2\pi}\int_0^{\pi} G^* G \sin\theta d\theta d\varphi$,

and the $l = 2$ spherical harmonics as presented in (8.94),(8.95) and (8.96) in *The Undergraduate Course*(Fp).

Keep in mind: for $B = \pm 2$, another a_2 is obtained than obtained for the case $B = \pm 1$.

Simarlily for the case $B = 0$.

Exercise 4.6 Measurement and Probabilities 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 what probabilities? In Exercise 4.5 we obtained the eigenfunctions of L_x for $l = 1$. The eigenfunction with the eigenvalue $\hbar$ is

$F(\theta,\varphi) = \frac{1}{2}\sqrt{2}Y_{1\,1} + Y_{1\,0} + \frac{1}{2}\sqrt{2}Y_{1-1}$. (C.E.4.19)

After this measurement L_z has been measured.

The commutator

$[L_x, L_z] \neq 0$.

In Section 1.13 on Compatible Observables this case of non-commuting operators(observables) is discussed.
The eigenstate of L_x is not the eigenstate of L_z.
Now I cite Fp, on the middle of page 18,:"*It is clear that if the observables L_x and L_z do not possess simultaneous eigenstates then if the eigenvalue of L_x is known (i.e., the system is in an eigenstate of L_x) then the eigenvalue of L_z is uncertain (i.e., the system is not in an eigenstate of L_z), and vice versa."*
I suppose: "….then the eigenvalue of L_z is uncertain…" is to interpret as the uncertainty before the measurement L_z .
For L_z we have:
$L_z Y_{1\,m} = m\hbar Y_{1\,m}$
and
$m = 1,0,-1$. These are the eigenvalues to be obtained by a subsequent measurement of L_z.
Furthermore:

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta \text{ and } Y_{1,\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\varphi}. \qquad \text{(C.E.4.20)}$$

These expression are given in Section 8.7 on Spherical Harmonics of *The Undergraduate Course* or can be derived from (4.89) and (4.90).
The probability of a measurement equals the square of the amplitude of the wave function.
So, with (C.E.4.20),
$m = 0: P = \frac{3}{4\pi}\cos^2\theta$,
and
$m = 1: P = \frac{3}{8\pi}\sin^2\theta$.
Or is integration over $0 < \theta < \pi$ necessary?
Repeat the calculations in which the measurement of L_x yields the results 0 and $-\hbar$.
In Exercise 4.5, I found the eigenvalue , 0 and $-\hbar$. For a different eigenfunction of L_x.
The question: "What values will be obtained by a subsequent measurement of L_z , and with what probabilities?" , does lead to the same answers as given above.

Exercise 4.7 The eigenvalues of an axially symmetric operator.

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 with $L^2 = L_x^2 + L_y^2 + L_z^2$:
$H = \frac{L^2-L_z^2}{2I_1} + \frac{L_z^2}{2I_2}$.
So,
$H = \frac{L^2}{2I_1} + \frac{L_z^2(I_1-I_2)}{2I_1I_2}$.
Hence
$HY_{l,m} = (\frac{L^2}{2I_1} + \frac{L_z^2(I_1-I_2)}{2I_1I_2})Y_{l,m}$.

With Eqs.(4.25) and (4.43), the eigenvalues are:
$\frac{\hbar^2 l(l+1)}{2I_1} + \frac{(m\hbar)^2(I_1-I_2)}{2I_1 I_2}$.

Exercise 4.8 The eigenvalues of a function of x and p

The expectation value of $f(\boldsymbol{x},\boldsymbol{p})$ in any stationary state is a constant. Calculate
$0 = \frac{d}{dt}(\langle \boldsymbol{x}\cdot\boldsymbol{p}\rangle) = \frac{i}{\hbar}\langle[H, \boldsymbol{x}\cdot\boldsymbol{p}]\rangle$,
for a Hamiltonian of the form
$H = \frac{p^2}{2m} + V(r)$.
In Exercise 3.8 I presented the result for the 1-D Cartesian coordinate x..
I present the analysis in the 1-D Cartesian coordinate x.
Consider a system in state $|A\rangle$.
In the Schrödinger representation: the state of the system is time dependent.
Then
$\frac{d}{dt}\langle A|\boldsymbol{x}\cdot\boldsymbol{p}|A\rangle = \left\langle \frac{dA}{dt}\middle|\boldsymbol{x}\cdot\boldsymbol{p}\middle|A\right\rangle + \left\langle A\middle|\boldsymbol{x}\cdot\boldsymbol{p}\middle|\frac{dA}{dt}\right\rangle$. (C.E.4.21)
With
$\frac{d|A\rangle}{dt} = -\frac{i}{\hbar}H|A\rangle$ and $\frac{d\langle A|}{dt} = \frac{i}{\hbar}\langle A|H$,
(C.E.4.21) becomes
$0 = \frac{d}{dt}(\langle \boldsymbol{x}\cdot\boldsymbol{p}\rangle) = \frac{i}{\hbar}\langle H\boldsymbol{x}\cdot\boldsymbol{p}\rangle - \frac{i}{\hbar}\langle \boldsymbol{x}\cdot\boldsymbol{p}H\rangle = \frac{i}{\hbar}\langle[H, \boldsymbol{x}\cdot\boldsymbol{p}]\rangle$.
So,
$\frac{i}{\hbar}\langle[H, \boldsymbol{x}\cdot\boldsymbol{p}]\rangle = 0$. (C.E.4.22)
Hence, show that
$\langle\frac{p^2}{2m}\rangle = \frac{1}{2}\langle r\frac{d}{dr}V(r)\rangle$

In stationary state. This is another form of the *Virial Theorem*. (See Exercise 3.8).
For the 1-D case, (C.E.4.22) can be written as
$Hxp_x - xp_xH = xHp_x - xp_xH + Hxp_x - xHp_x = x[H,p_x] + [H,x]p_x = 0$. (C.E.4.23)
Now, plug the expression for
$H = \frac{p_x^2}{2m} + V(x)$ into (C.E.4.23), use $p_x = -i\hbar\frac{d}{dx}$,
$x\frac{p_x^2}{2m}p_x + xV(x)p_x - xp_x\frac{p_x^2}{2m} - xp_xV(x) + \frac{p_x^2}{2m}xp_x + V(x)xp_x - x\frac{p_x^2}{2m}p_x - xV(x)p_x = 0$.
Use in this expression $p_x = -i\hbar\frac{d}{dx}$, a lot of terms cancel. However,
$\frac{p_x^2}{2m}xp_x = \frac{p_x}{2m}(p_xxp_x) = \frac{p_x}{2m}(p_x + xp_x^2) = -\frac{i\hbar}{m}(\frac{p_x^2}{2m} + \frac{p_x^2}{2m}) + xp_x\frac{p_x^2}{2m}$,
and
$xp_xV(x) = -i\hbar x\frac{dV}{dx} + xVp_x$.
Note: a commutator always operates on something.
Then
$i\hbar x\frac{d}{dx}V(x) - i\hbar\frac{p_x^2}{m} = 0$.
Hence
$\langle\frac{p_x^2}{2m}\rangle = \frac{1}{2}\langle x\frac{d}{dx}V(x)\rangle \rightarrow \langle\frac{p^2}{2m}\rangle = \frac{1}{2}\langle r\frac{d}{dr}V(r)\rangle$.

Exercise 4.9 Virial Theorem for an energy eigenvalue of the hydrogen atom

Use the Virial Theorem of exercise 4.8 to prove that

$\langle\frac{1}{r}\rangle = \frac{1}{n^2 a_0}$,

for an energy eigenstate of the hydrogen atom.

The virial Theorem:

$\langle\frac{p^2}{2m}\rangle = \frac{1}{2}\langle r\frac{d}{dr}V(r)\rangle$.

For the hydrogen atom:

$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$.

So,

$r\frac{d}{dr}V(r) = \frac{e^2}{4\pi\epsilon_0 r}$.

Then twice the kinetic energy:

$2\langle\frac{p^2}{2m}\rangle = \frac{e^2}{4\pi\epsilon_0 r} = -\langle V\rangle$,

or

$\langle\frac{p^2}{2m}\rangle = -\frac{1}{2}\langle V\rangle$. (C.E.4.24)

The total energy E_n:

$E_n = \langle\frac{p^2}{2m}\rangle + \langle V\rangle$,

can be written, with (C.E.4.24),

$E_n = -\frac{1}{2}\langle V\rangle + \langle V\rangle = \frac{1}{2}\langle V\rangle$. (C.E.4.25)

With (4.120), $E_n = \frac{E_0}{n^2}$, we find with (C.E.4.25),

$\langle V\rangle = -\langle\frac{e^2}{4\pi\epsilon_0 r}\rangle = 2\frac{E_0}{n^2}$. (C.E.4.26)

With the expressions for E_0 , (4.121), and the Bohr radius $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$, (C.E.4.26) becomes:

$\langle\frac{1}{r}\rangle = \frac{1}{n^2 a_0}$.

Note: $\langle\frac{1}{r}\rangle$ is independent of the quantum number l . See the note on top of page 71. The energy levels are independent of the quantum number l . $\langle\frac{1}{r}\rangle$ is proportional to the potential energy.

$\langle\frac{1}{r}\rangle$ could also be found from: $\left\langle R_{nl}\left|\frac{1}{r}\right|R_{nl}\right\rangle$ using the expressions derived in section 4.6 on Energy Levels of Hydrogen Atom. A tedious job.

Another possibility is to use Laguerre polynomials as presented in Mahan, page 123.

Exercise 4.10 Derivation of the radial wave functions of the hydrogen atom

Demonstrate that the first few properly normalised radial wave functions of the hydrogen atom take the form:

a) $R_{10}(r) = \frac{2}{{a_0}^{3/2}}\exp(-\frac{r}{a_0})$.

For this radial wave function: $n = 1$ and $l = 0$. Furthermore, $a = a_0$

The function

$R(r) = P(r)/r$ has to be evaluated.

$P(r)$ is given by (4.113):

$P\left(\frac{r}{a_0}\right) = f(\frac{r}{a_0})$ exp$(-\frac{r}{a_0})$.

So,

$R(r/a_0) = \frac{a_0}{r}\, f(\frac{r}{a_0})$ exp$(-\frac{r}{a_0})$. (C.E.4.27)

The power-law solution, (4.114), is

$f(y) = \sum_n c_n y^n$.

Hence, $n = 1$,

$f(y) \propto y$.

Plug this result into (C.E.4.27):

$R(r/a_0) \propto \exp\left(-\frac{r}{a_0}\right)$. (C.E.4.28)

The next step is to normalize R given in (C.E.4.28):

$C^2 \int_0^\infty \exp\left(-2\frac{r}{a_0}\right) r^2 dr = 1$.

After integration by parts, the result for the constant C is:

$C = \frac{2}{{a_0}^{3/2}}$ and the radial wave function is:

$R_{10}(r) = \frac{2}{{a_0}^{3/2}}exp(-\frac{r}{a_0})$. (C.E.4.29)

Note: a bit more convenient instead of integration by parts is to use the expression:

$n! = \int_0^\infty y^n\, e^{-y} dy$, (Chisholm and Morris, Chapter 19 , The factorial function).

In Exercise 4.9, using the virial theorem $\langle\frac{1}{r}\rangle = \frac{1}{n^2 a_0}$ is obtained.

This result is found also with $R_{10}(r)$ and $n = 1$.

So,

$\langle\frac{1}{r}\rangle = \int_0^\infty R_{10}\frac{1}{r}R_{10} r^2 dr = \frac{1}{a_0}$? (C.E.4.30)

Plug $R_{10}(r)$ given in (C.E.4.29) into (C.E.4.30), integrate by parts and the result is

$\langle\frac{1}{r}\rangle = \int_0^\infty R_{10}\frac{1}{r}R_{10} r^2 dr = \frac{1}{a_0}$.

b) $R_{20}(r) = \frac{2}{(2a_0)^{\frac{3}{2}}}(1 - \frac{r}{2a_0})exp(-\frac{r}{2a_0})$.

For this radial wave function: $n = 2$ and $l = 0$. Furthermore, $a = 2a_0$.

So, with (4.112),

$P\left(\frac{r}{2a_0}\right) = f(\frac{r}{2a_0})$ exp$(-\frac{r}{2a_0})$.

(C.4.114)

$f(y) = \sum_n c_n y^n = c_1\frac{r}{2a_0} + c_2(\frac{r}{2a_0})^2$.

Hence,

$R(r/2a_0) = \frac{2a_0}{r}[c_1\frac{r}{2a_0} + c_2(\frac{r}{2a_0})^2]$ exp$(-\frac{r}{2a_0})$,

or

$R(r/2a_0) = [c_1 + c_2\frac{r}{2a_0}]$ exp$(-\frac{r}{2a_0})$. (C.E.4.31)

Now, with (4.116), $l = 0$ and $\frac{2a}{a_0} = 4$,

$c_2 = -c_1$.

Plug this result in (C.E.4.31)

$R(r/2a_0) = c_1[1 - \frac{r}{2a_0}]$ exp$(-\frac{r}{2a_0})$. (C.E.4.32)

The next step is to normalize R given in (C.E.4.32):

$c_1^2 \int_0^\infty R^2\, r^2 dr = 1.$

Use $n! = \int_0^\infty y^n\, e^{-y} dy,$

and the result for the constant $c_1 = \frac{2}{(2a_0)^{\frac{3}{2}}}$.

The radial wavefunction becomes

$R_{20}(r) = \frac{2}{(2a_0)^{\frac{3}{2}}}(1 - \frac{r}{2a_0})\exp(-\frac{r}{2a_0}).$

Again with this radial wavefunction

$\langle\frac{1}{r}\rangle = \int_0^\infty R_{20}\frac{1}{r}R_{20}r^2 dr = \frac{1}{a_0}.$

c) $R_{21}(r) = \frac{1}{\sqrt{3}(2a_0)^{\frac{3}{2}}}\frac{r}{a_0}\exp(-\frac{r}{2a_0}).$

For this radial wavefunction $n = 2$ and $l = 1$. Furthermore, $a = 2a_0$.

So, with (4.112),

$P\left(\frac{r}{2a_0}\right) = f(\frac{r}{2a_0})\ \exp(-\frac{r}{2a_0}).$

(4.114):

$f(y) = \sum_n c_n y^n \to c_2(\frac{r}{2a_0})^2, c_1 = 0.$

Hence,

$R(r/2a_0) = \frac{2a_0}{r}[c_2(\frac{r}{2a_0})^2]\ \exp(-\frac{r}{2a_0}).$ (C.E.4.33)

The next step is to normalize R given in (C.E.4.33):

$c_2^2 \int_0^\infty R^2\, r^2 dr = 1.$

Use $n! = \int_0^\infty y^n\, e^{-y} dy,$

and the result for the constant $c_2 = \frac{2}{(a_0)^{\frac{3}{2}}\sqrt{4!}} = \frac{2}{\sqrt{3}(2a_0)^{\frac{3}{2}}}$.

The radial wavefunction is:

$R_{21}(r) = \frac{1}{\sqrt{3}(2a_0)^{\frac{3}{2}}}\frac{r}{a_0}\exp(-\frac{r}{2a_0}).$

Again with this radial wavefunction

$\langle\frac{1}{r}\rangle = \int_0^\infty R_{21}\frac{1}{r}R_{21}r^2 dr = \frac{1}{a_0}.$

So it is to be expected:

$\left\langle R_{nl}\middle|\frac{1}{r}\middle|R_{nl}\right\rangle = \frac{1}{a_0}$,

and the coulomb potential, (4.107),

$\left\langle R_{nl}\middle|-\frac{e^2}{4\pi\epsilon_0 r}\middle|R_{nl}\right\rangle = -\frac{1}{a_0}\frac{m}{\hbar^2}$.

The expression for R_{nl} is obtained with (4.112)

$R(r/na_0) = \frac{na_0}{r}f(\frac{r}{na_0})\ \exp(-\frac{r}{na_0}).$

Then using (4.116), the coefficients c_n are expressed in c_{l+1}.

For example

$c_{l+2} = -c_{l+1}\frac{n-(l+1)}{l+1}$, (C.E.4.34)

and

$c_n = -c_{n-1}\frac{1}{n(n-1)-l(l+1)}$.

Furthermore, the general term for $l+1<k<n$:

$c_k = c_{k-1}\frac{2(n-k+1)}{k(k-1)-l(l+1)}$.

The power-law solution becomes

$$f\left(\frac{r}{na_0}\right) = c_{l+1}\left(\frac{r}{na_0}\right)^{l+1} + \sum_{k=l+2}^{n-1} c_k\left(\frac{r}{na_0}\right)^k - c_{n-1}\frac{1}{n(n-1)-l(l+1)}\left(\frac{r}{na_0}\right)^n , \qquad \text{(C.E.4.35)}$$

and

$R(r/na_0) = \frac{na_0}{r} f\left(\frac{r}{na_0}\right) \exp\left(-\frac{r}{na_0}\right)$.

Exercise 4.10 Epilogue. Relation between Fp's recurrence expression and Laguerre Polynomials

At the end of Exercise 4.10 I derived some values for c_n and indicated that all can be constructed in terms of c_{l+1} with help of the recurrence relation (4.116).

I will go a step further to develop c_k (C.E.4.35) with (4.116).

$$c_k = c_{l+3} = (-1)^{k-(l+1)} c_{l+1}\frac{[n-(l+1)][n-(l+2)]}{(l+1)(2l+3)} . \qquad \text{(C.E.4.36)}$$

$$c_k = c_{l+4} = (-1)^{k-(l+1)} c_{l+1}\frac{[n-(l+1)][n-(l+2)][n-(l+3)]}{(l+1)(2l+3)(3l+6)} . \qquad \text{(C.E.4.37)}$$

$$c_k = c_{l+5} = (-1)^{k-(l+1)} c_{l+1}\frac{[n-(l+1)][n-(l+2)][n-(l+3)][n-(l+4)]}{(l+1)(2l+3)(3l+6)(4l+10)} . \qquad \text{(C.E.4.38)}$$

$$c_k = c_{l+6} = (-1)^{k-(l+1)} c_{l+1}\frac{[n-(l+1)][n-(l+2)][n-(l+3)][n-(l+4)][n-(l+5)]}{(l+1)(2l+3)(3l+6)(4l+10)(5l+15)} . \qquad \text{(C.E.4.39)}$$

Is there a pattern to discover in (C.E.4.34), and (C.E.4.36)-(C.E.4.39)?

The numerator shows:

$$N(n,l,k) \equiv \frac{[n-(l+1)]!}{[n-k]!} = \frac{[n-(l+1)]!}{[n-(l+1)-\{k-(l+1)\}]!} . \qquad \text{(C.E.4.40)}$$

Hence

for $k = l+1 \rightarrow N(n,l,k) = 1$.

The denominator gives:

$$\prod_{i=1}^{k-(l+1)}[il+(1+i)\tfrac{i}{2}] = \left(\frac{1}{2}\right)^{k-(l+1)}[\{k-(l+1)\}!]\prod_{i=1}^{k-(l+1)}(2l+1+i). \qquad \text{(C.E.4.41)}$$

Note: To include the minimum value of $n(k=l+1)$ in (C.E.4.41) some additional work has to be done.

Then , for c_k, with (C.E.4.40) and (C.E.4.41),the following closed expression results:

$$c_k = (-2)^{k-(l+1)} c_{l+1}\binom{n-(l+1)}{k-(l+1)}\frac{2l+1}{\prod_{i=0}^{k-(l+1)}[2l+(1+i)]} =$$

$$= (-2)^{k-(l+1)} c_{l+1}\binom{n-(l+1)}{k-(l+1)}\frac{(2l+1)!}{(l+k)!} . \qquad \text{(C.E.4.42)}$$

This expression applies for $k \geq l+1$. To have $i=0$ in (C.E.4.42), I introduced $(2l+1)$ in numerator. For $k=l+1$ in (C.E.4.42), $c_k = c_{l+1}$.

Induction would complete the evaluation.

Now for

$R\left(\frac{r}{na_0}\right) = \frac{na_0}{r} f\left(\frac{r}{na_0}\right) \exp\left(-\frac{r}{na_0}\right)$,

with

$$f\left(\frac{r}{na_0}\right) = c_{l+1}\left(\frac{r}{na_0}\right)^{l+1} + \sum_{k=l+2}^{n} c_k\left(\frac{r}{na_0}\right)^k . \qquad \text{(C.E.4.43)}$$

Note: I included $c_{n-1}\frac{1}{n(n-1)-l(l+1)}\left(\frac{r}{na_0}\right)^n$ in the summation.

Hence

$$R\left(\frac{r}{na_0}\right)=c_{l+1}(\frac{r}{na_0})^l e^{-\frac{r}{na_0}}\{\sum_{k=l+1}^{n}\left(-\frac{2r}{na_0}\right)^{k-(l+1)}\binom{n-(l+1)}{k-(l+1)}\frac{(2l+1)!}{(l+k)!}\}. \qquad \text{(C.E.4.44)}$$

Example: set in the summation of (C.E.4.44) $n=l+2$,

Then

$$R_{l+2,l}\left(\frac{r}{na_0}\right)=c_{l+1}(\frac{r}{na_0})^l e^{-\frac{r}{na_0}}\left\{1-\frac{1}{l+1}\frac{r}{na_0}\right\}.$$

c_{l+1} is obtained from:

$c_{l+1}^2\int_0^\infty R^2\,r^2dr=1.$

Mahan expressed $R\left(\frac{r}{na_0}\right)$ in associated Laguerre polynomials. What is the relation of these polynomials with (C.E.4.44)?

Mahan Eq.(5.127):

$$R\left(\frac{r}{a_0}\right)=N\left(\frac{r}{a_0}\right)^l e^{-\frac{r}{na_0}}L_{n_r}^{2l+1}\left(\frac{2r}{na_0}\right), \qquad \text{(C.E.4.45)}$$

where

N is a normalization coefficient that depends on the quantum numbers (l,n_r).

Mahan included

$\frac{[n-(l+1)]!}{(n+l)!}(2l+1)!$, in N. I do not do that. Consequently, there is a new normalization coefficient C:

$$C\frac{[n-(l+1)]!}{(n+l)!}(2l+1)!=N. \qquad \text{(C.E.4.46)}$$

Furthermore, the closed form of the Laguerre polynomials:

$$L_{n_r}^{2l+1}\left(\frac{2r}{na_0}\right)=\sum_{i=0}^{n_r}(-1)^i\binom{n_r+2l+1}{n_r-i}\frac{(\frac{2r}{na_0})^i}{i!}, \qquad \text{(C.E.4.47)}$$

and

n_r is the radial quantum number and n is the principal quantum number. n_r represents the number of zero's of the radial wavefunction.

$$n=n_r+l+1. \qquad \text{(C.E.4.48)}$$

So, combining (C.E.4.45) and (C.E.4.46)

$$R\left(\frac{r}{a_0}\right)=C\left(\frac{r}{a_0}\right)^l e^{-\frac{r}{na_0}}\frac{[n-(l+1)]!}{(n+l)!}(2l+1)!\sum_{i=0}^{n_r}(-1)^i\binom{n_r+2l+1}{n_r-i}\frac{(\frac{2r}{na_0})^i}{i!}. \qquad \text{(C.E.4.49)}$$

Translate (C.E.4.49) in Fp notation:

$$R\left(\frac{r}{a_0}\right)=C\left(\frac{r}{a_0}\right)^l e^{-\frac{r}{na_0}}\frac{[n-(l+1)]!}{(n+l)!}(2l+1)!\sum_{k=l+1}^{n}(-1)^{k-(l+1)}\binom{n+l}{n-k}\frac{(\frac{2r}{na_0})^{\{k-(l+1)\}}}{\{k-(l+1)\}!}, \qquad \text{(C.E.4.50)}$$

Now the relation between (C.E.4.44) and the Laquerre polynomials in (C.E.4.50) can be established.

Does $\binom{n-(l+1)}{k-(l+1)}\frac{(2l+1)!}{(l+k)!}$ equals $\frac{[n-(l+1)]!}{(n+l)!}(2l+1)!\binom{n+l}{n-k}\frac{1}{\{k-(l+1)\}!}$?

$\binom{n-(l+1)}{k-(l+1)}\frac{(2l+1)!}{(l+k)!}=\frac{[n-(l+1)]!(2l+1)!}{(n-k)!\{k-(l+1)\}!(l+k)!}$,

and

$\frac{[n-(l+1)]!}{(n+l)!}(2l+1)!\binom{n+l}{n-k}\frac{1}{\{k-(l+1)\}!}=\frac{[n-(l+1)]!(2l+1)!}{(n-k)!\{k-(l+1)\}!(l+k)!}$.
Furthermore,
$c_{l+1}=C$.
So, the relation between the recurrence expression of Fp and the Laguerre polynomials is established.
Remark: Basically, it is about the comparison between the confluent hypergeometric function and the recurrence relation of Fp. For the radial wave function of the hydrogen atom, the confluent hypergeometric function is identical to an associated Laguerre polynomial(Mahan):
$F\left(-n_r,2l+2,\frac{2r}{na_0}\right)=\frac{[n-(l+1)]!(2l+1)!}{(n+l)!}\sum_{k=l+1}^{n}(-1)^{k-(l+1)}\binom{n+l}{n-k}\frac{(\frac{2r}{na_0})^{\{k-(l+1)\}}}{\{k-(l+1)\}!}$,
where the summation represents the associated Laguerre polynomial. Mahan used the expression "identical'. To prevent misunderstanding, I prefer proportional. The factor, $\frac{[n-(l+1)]!(2l+1)!}{(n+l)!}$, making the confluent hypergeometric function identical to the associated Laguerre polynomial is **not** part of the associated Laguerre polynomial.

5 Spin Angular Momentum

5.1 Introduction

In this chapter attention is paid to a particle with an internal angular momentum called spin. It is about spin one-half particles.

5.2 Properties of Spin Angular Momentum

Equation (5.10)
$|+\rangle\langle+|+|-\rangle\langle-|=1$
is presented in the section on Measurements(1.10), Eq.(1.54):
$\sum_i|i\rangle\langle i|=1$.
In my notes on section (1.10), I proved the unitary character of (1.54) .
On page 74 Fp presented the relations for the operators S_x,S_y and S_z ,(5.11)-(5.13) and mentioned these relations satisfy the commutation relations (4.8)-(4.10). For example:
$[S_x,S_y]=i\hbar S_z$. (C.5.2.1)
Plug the expressions given in (5.11) and (5.12) into (C.5.2.1), use (5.8), (5.9) and (5.13), then the equality is demonstrated.
For completeness I present here the relation between the spin angular momentum operator and the Pauli 2×2 matrices:
$S_i=\frac{\hbar}{2}\sigma_i$, (10.47)-(10.50) *Undergraduate Course* Fp. In that chapter 10, Fp presented the raising and lowering operators:
$S_\pm=S_x\pm iS_y$, (10.6).
Now. Look at (5.11) and (5.12):
$S_x+iS_y=\hbar|+\rangle\langle-|$,
and
$S_x-iS_y=\hbar|-\rangle\langle+|$.
Hence

$S_+ = \hbar|+\rangle\langle -|$,
and
$S_- = \hbar|-\rangle\langle +|$.
Furthermore:

$$\hbar|+\rangle\langle -| = \hbar\begin{pmatrix}1\\0\end{pmatrix}(0 \quad 1) = \hbar\begin{pmatrix}0 & 1\\0 & 0\end{pmatrix} = \frac{\hbar}{2}\left[\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} + i\begin{pmatrix}0 & -i\\i & 0\end{pmatrix}\right], \qquad \text{(C5.2.2)}$$

and

$$\hbar|-\rangle\langle +| = \hbar\begin{pmatrix}0\\1\end{pmatrix}(1 \quad 0) = \hbar\begin{pmatrix}0 & 0\\1 & 0\end{pmatrix} = \frac{\hbar}{2}\left[\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} - i\begin{pmatrix}0 & -i\\i & 0\end{pmatrix}\right]. \qquad \text{(C.5.2.3)}$$

See also *Undergraduate Course* Fp.
Something to remember.
Note: $|\pm\rangle$ are the eigenkets of the spin operator S_z. Susskind used $|u\rangle$ and $|d\rangle$ for these eigenkets. Sometimes this is a bit more convenient when doing adding and subtracting as for the verification of (C.5.2.1). In Feynman, et al, you will also find the $|\pm\rangle$ notation for spin one-half particles.
(5.14):
$S^2 = \frac{3\hbar^2}{4}$:
Using (5.2), (5.8), (5.9) and (5.10), S_x^2 is found with (5.11):

$$S_x^2 = \frac{\hbar^2}{4}(|+\rangle\langle -| + |-\rangle\langle +|)(|+\rangle\langle -| + |-\rangle\langle +|)$$

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

The same result can be found for S_y^2 and S_z^2 .
Now, for example, with (5.8) and (5.13),

$$S_z|+\rangle = \frac{\hbar}{2}(|+\rangle\langle +| - |-\rangle\langle -|)|+\rangle = \frac{\hbar}{2}(|+\rangle\langle +|+\rangle - |-\rangle\langle -|+\rangle) = \frac{\hbar}{2}|+\rangle \text{ ,(5.6) .}$$

5.3 Wavefunction of Spin One-Half Particle

Fp introduced the simultaneous eigenstates of the position operators x, y, z and the spin operator S_z. These simultaneous eigenstates are the product states of the positions eigenkets and spin eigenkets. The two wave functions ψ_+ and ψ_- with their normalization condition are presented.

5.4 Rotation operators in Spin Space

Fp started this section with forgetting about spatial position and concentrating on the spin state.
For a general ket is given by a linear combination of the 2 spin vectors:
$|A\rangle = c_+|+\rangle + c_-|-\rangle$.
$c_+ = \langle +|A\rangle$ and $c_- = \langle -|A\rangle$ →(5.23).

So, the effect on rotation on $\langle S_x\rangle$ is given by (5.30).
This expression is derived from (5.28). Then Fp writes below (5.28) : "…or " resulting into (5.29).
Now, (5.30):
$S_x \cos\Delta\varphi - S_y \sin\Delta\varphi$.
Substitute (5.11) and (5.12) into this expression. The result is:

$$\frac{\hbar}{2}[(|+\rangle\langle -|)e^{i\Delta\varphi} + (|-\rangle\langle +|)e^{-i\Delta\varphi}]. \qquad \text{(C.5.4.1)}$$

I suppose to be allowed to rewrite (C.5.4.1) and recapture (5.29). The latter expression follows from (5.28).
The first term in the expression (5.28) is:

$$\frac{\hbar}{2}e^{\frac{iS_z\Delta\varphi}{\hbar}}(|+\rangle\langle-|). \qquad \text{(C.5.4.2)}$$

As mentioned in section 5.2 , $(|+\rangle\langle-|)$ acts as a raising operator on $e^{\frac{iS_z\Delta\varphi}{\hbar}}$. How? Does that change

$\frac{\hbar}{2}e^{\frac{iS_z\Delta\varphi}{\hbar}}(|+\rangle\langle-|)$ into $\frac{\hbar}{2}e^{\frac{i\Delta\varphi}{2}}(|+\rangle\langle-|)e^{\frac{i\Delta\varphi}{2}}$? It looks to me a kind of magic. I do not understand how that could possibly happen.

There are a few questions here:
- S_z in the exponent is the expectation value? I think so. Since, in section 4.3 about the rotational operator and orbital motion, in (4.26), L_z in the exponential is the expectation value $\langle L_z\rangle$.
- what is the rotation all about? I think it is a sort of change in coordinates: θ, φ, r into θ, φ', r. Where $\varphi' = \varphi + \Delta\varphi$. Such a transformation is of no importance: it adds a phase factor to the new wavefunction.
- When S_z in (5.28) is the expectation value: $\frac{\hbar}{2}e^{\frac{iS_z\Delta\varphi}{\hbar}}(|+\rangle\langle-|) = \frac{\hbar}{2}e^{\frac{i\Delta\varphi}{2}}(|+\rangle\langle-|)$.

Consequently, $\frac{\hbar}{2}e^{\frac{i\Delta\varphi}{2}}(|+\rangle\langle-|)e^{\frac{i\Delta\varphi}{2}}$ should be $\frac{\hbar}{2}e^{\frac{i\Delta\varphi}{4}}(|+\rangle\langle-|)e^{\frac{i\Delta\varphi}{4}}$? If so, (5.30) changes into $S_x\cos(\frac{\Delta\varphi}{2}) - S_y\sin(\frac{\Delta\varphi}{2})$. With a rotation of $\Delta\varphi$, this result is not to be expected to say the least. Note: I did use the positive value of the expectation value. That does not matter. Using the negative value, a phase factor $e^{i\pi}$ can be included to obtain (5.28).
- The solution to the rotation conundrum can be found from (4.60)-(4.62). Since it is about the expectation value of the spin operator aligned to the z-axis of the coordinate system I translate (4.60) into the "stationary spin system:

$T_z(\delta\varphi) = 1 - iS_z\delta\varphi/\hbar \rightarrow 1 - i\delta\varphi/2$.

Similar to (4.61), I define $\frac{\delta\varphi}{2} = \frac{\Delta\varphi}{N}$.
With $N \rightarrow \infty$, I obtain for (5.24):

$T_z(\Delta\varphi) = e^{(-i\Delta\varphi)}$.

Then, with this expression for the rotation operator, I found (5.30).

Again, what is the importance of the rotation operator besides creating a phase factor?
Fp presented a second approach to find (5.30) from (5.27) using the *Baker-Hausdorff lemma.* This lemma will be used to evaluate expression (5.27). It is about the expectation value of S_x for a spin system rotated about the z-axis with an angle $\Delta\varphi$.
The Taylor series expansion is used for the exponential.
In general for

$$e^q S_x e^{-q} = (1 + q + \frac{q^2}{2!} + \frac{q^3}{3!} + \cdots)S_x(1 - q + \frac{q^2}{2!} - \frac{q^3}{3!} + \cdots), \qquad \text{(C.5.4.3)}$$

Where

$$q = \frac{iS_z\Delta\varphi}{\hbar}. \qquad \text{(C.5.4.3a)}$$

(C.5.4.3) becomes

$$e^{q}S_{x}e^{-q} = S_{x} + qS_{x} - S_{x}q + \frac{S_{x}q^{2}}{2!} - qS_{x}q + \frac{q^{2}S_{x}}{2!} + \frac{q^{3}S_{x}}{3!} - \frac{q^{2}S_{x}q}{2!} + \frac{qS_{x}q^{2}}{2!} - \frac{S_{x}q^{3}}{3!} + \cdots \quad \text{(C.5.4.4)}$$

So,

$$e^{q}S_{x}e^{-q} = \sum_{l=0}^{\infty}\frac{q^{l}}{l!}S_{x}\sum_{j=0}^{\infty}(-1)^{j}\frac{q^{j}}{j!} = \sum_{l=0}^{\infty}\sum_{j=0}^{\infty}\frac{(-1)^{j}}{l!j!}q^{l}S_{x}q^{j}, \quad \text{(C.5.4.5)}$$

where $\{l, j, n \in \mathbb{N}\}$.

Or, with (C5.4.3a),

$$e^{q}S_{x}e^{-q} = \sum_{l=0}^{\infty}\sum_{j=0}^{\infty}\frac{(-1)^{j}}{l!j!}q^{l}S_{x}q^{j} = \sum_{l=0}^{\infty}\sum_{j=0}^{\infty}\frac{(-1)^{j}}{l!j!}(\frac{i\Delta\varphi}{\hbar})^{l+j}S_{z}^{l}S_{x}S_{z}^{j}. \quad \text{(C.5.4.5a)}$$

This can also be written as:

$$e^{q}S_{x}e^{-q} = \sum_{s=0}^{\infty}\sum_{j=0}^{s}\frac{(-1)^{j}}{(s-j)!j!}q^{s-j}S_{x}q^{j} = \sum_{s=0}^{\infty}\sum_{j=0}^{s}\frac{(-1)^{j}}{(s-j)!j!}(\frac{i\Delta\varphi}{\hbar})^{s}S_{z}^{s-j}S_{x}S_{z}^{j}. \quad \text{(C.5.4.5b)}$$

To evaluate (C.5.4.5), I start with

$q^{0}(\propto \Delta\varphi^{0})$: S_{x} .

$q^{1}(\propto \Delta\varphi)$: $qS_{x} - S_{x}q \equiv [q, S_{x}]$. (C.5.4.6)

So

$$qS_{x} - S_{x}q = \frac{i\Delta\varphi\hbar}{4}\left[\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} - \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right] = \frac{\hbar\Delta\varphi}{2}\begin{pmatrix}0 & i\\ -i & 0\end{pmatrix} = -\Delta\varphi S_{y}\ , \quad \text{(C.5.4.7)}$$

Then for $q^{2}(\propto \Delta\varphi^{2})$

$$\frac{S_{x}q^{2}}{2!} - qS_{x}q + \frac{q^{2}S_{x}}{2!} = \frac{S_{x}q^{2}}{2!} - \frac{qS_{x}q}{2} - \frac{qS_{x}q}{2} + \frac{q^{2}S_{x}}{2!} = \frac{1}{2!}\{q(qS_{x} - S_{x}q) - (qS_{x} - S_{x}q)q\} =$$

$$= \frac{1}{2!}\{q[q, S_{x}] - [q, S_{x}]q\} = \frac{1}{2!}\big[q, [q, S_{x}]\big], \quad \text{(C.5.4.8)}$$

and, with (C.5.4.7) and (C.5.4.8),

$$\frac{S_{x}q^{2}}{2!} - qS_{x}q + \frac{q^{2}S_{x}}{2!} = \frac{1}{2!}(S_{x}q^{2} - 2qS_{x}q + q^{2}S_{x}) = \frac{1}{2!}\big(-q\Delta\varphi S_{y} + \Delta\varphi S_{y}q\big) = -\frac{1}{2!}(\Delta\varphi)^{2}S_{x}, \quad \text{(C.5.4.9)}$$

Next $q^{3}(\propto \Delta\varphi^{3})$

$$\frac{q^{3}S_{x}}{3!} - \frac{q^{2}S_{x}q}{2!} + \frac{qS_{x}q^{2}}{2!} - \frac{S_{x}q^{3}}{3!} = \frac{1}{3!}\{q^{3}S_{x} - 3q^{2}S_{x}q + 3qS_{x}q^{2} - S_{x}q^{3}\}\ .$$

Rewrite this expression:

$$\left\{\frac{q^{3}S_{x}}{3!} - \frac{q^{2}S_{x}q}{3!} - \frac{q^{2}S_{x}q}{3!} - \frac{q^{2}S_{x}q}{3!} + \frac{qS_{x}q^{2}}{3!} + \frac{qS_{x}q^{2}}{3!} + \frac{qS_{x}q^{2}}{3!} - \frac{S_{x}q^{3}}{3!}\right\}, \quad \text{(C.5.4.10)}$$

or,

$$\frac{q^{3}S_{x}}{3!} - \frac{q^{2}S_{x}q}{2!} + \frac{qS_{x}q^{2}}{2!} - \frac{S_{x}q^{3}}{3!} = \frac{1}{3!}\{q(S_{x}q^{2} - 2qS_{x}q + q^{2}S_{x}) - (S_{x}q^{2} - 2qS_{x}q + q^{2}S_{x})q\} \equiv$$

$$\frac{1}{3!}\Big[q, \big[q, [q, S_{x}]\big]\Big], \quad \text{(C.5.4.11)}$$

or, with (C.5.4.9):

$$\frac{q^{3}S_{x}}{3!} - \frac{q^{2}S_{x}q}{2!} + \frac{qS_{x}q^{2}}{2!} - \frac{S_{x}q^{3}}{3!} = \frac{1}{3!}\{q(S_{x}q^{2} - 2qS_{x}q + q^{2}S_{x}) - (S_{x}q^{2} - 2qS_{x}q + q^{2}S_{x})q\} =$$

$$= -\frac{(\Delta\varphi)^{2}}{3!}(qS_{x} - S_{x}q) = \frac{1}{3!}(\Delta\varphi)^{3}S_{y}\ . \quad \text{(C.5.4.12)}$$

And $q^{4}(\propto \Delta\varphi^{4})$

$$\frac{S_{x}q^{4}}{4!} - \frac{qS_{x}q^{3}}{3!} + \frac{q^{2}S_{x}q^{2}}{2!2!} - \frac{q^{3}S_{x}q}{3!} + \frac{q^{4}S_{x}}{4!} =$$

$$= \frac{1}{4!}\{q(q^3S_x - 3q^2S_xq + 3qS_xq^2 - S_xq^3) - (q^3S_x - 3q^2S_xq + 3qS_xq^2 - S_xq^3)q\} \equiv$$
$$\frac{1}{4!}\Big[q,\Big[q,\big[q,[q,S_x]\big]\Big]\Big] = \frac{1}{4!}(\Delta\varphi)^4 S_x. \qquad \text{(C.5.4.13)}$$

The general expression for the left hand side of (C.5.4.13):

For $q^k (\propto \Delta\varphi^k)$, for $k \geq 0$,

$$\sum_{m=0}^{k}(-1)^{k-m}\frac{q^m S_x q^{k-m}}{(k-m)!m!} = \frac{1}{k!}\sum_{m=0}^{k}(-1)^{k-m}\binom{k}{m} q^m S_x q^{k-m} = \qquad \text{(C.5.4.14a)}$$

$(k \geq 1)$

$$= \frac{1}{k!}\Big\{q\Big(\sum_{m=0}^{k-1}(-1)^{k-1-m}\binom{k-1}{m} q^m S_x q^{k-1-m}\Big) +$$
$$- \Big(\sum_{m=0}^{k-1}(-1)^{k-1-m}\binom{k-1}{m} q^m S_x q^{k-1-m}\Big) q\Big\} =$$
$$= \frac{1}{k!}\Big\{\sum_{m=0}^{k-1}(-1)^{k-1-m}\binom{k-1}{m}(q^{m+1}S_x q^{k-1-m} - q^m S_x q^{k-m})\Big\} =$$
$$= \frac{1}{k!}\{\sum_{m=0}^{k-1}(-1)^{k-1-m}\binom{k-1}{m} q^m\,(qS_x - S_xq)q^{k-1-m})\}.$$

With (5.4.7), finally is obtained for q^k:

$$\frac{\Delta\varphi}{k!}\{\sum_{m=0}^{k-1}(-1)^{k-m}\binom{k-1}{m} q^m\, S_y q^{k-1-m})\},$$

or

$$\frac{\Delta\varphi^k}{k!}\left(\frac{i}{\hbar}\right)^{k-1}\sum_{m=0}^{k-1}(-1)^{k-m}\binom{k-1}{m} S_z^m\, S_y S_z^{k-1-m}). \qquad \text{(C.5.4.14b)}$$

In (5.4.14b)

$S_z^m = \left(\frac{\hbar}{2}\right)^m \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$ for m is even,

and

$S_z^m = \left(\frac{\hbar}{2}\right)^m \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ for m is odd.

To demonstrate (5.4.10) once more, (C.5.4.10) can be written as:

$$\Big\{\Big(\frac{q^3S_x}{3!} - \frac{q^2S_xq}{3!}\Big) - \Big(\frac{q^2S_xq}{3!} - \frac{qS_xq^2}{3!}\Big) - \Big(\frac{q^2S_xq}{3!} - \frac{qS_xq^2}{3!}\Big) + \Big(\frac{qS_xq^2}{3!} - \frac{S_xq^3}{3!}\Big)\Big\} =$$
$$= \frac{1}{3!}\{q^2(qS_x - S_xq) - q(qS_x - S_xq)q - q(qS_x - S_xq)q + (qS_x - S_xq)q^2\} =$$
$$\frac{1}{3!}\{(q^2[q,S_x] - q[q,S_x]q) - (q[q,S_x]q - [q,S_x]q^2)\} =$$
$$= \frac{1}{3!}\{q(q[q,S_x] - [q,S_x]q) - (q[q,S_x] - [q,S_x]q)q\} = \frac{1}{3!}\{q\big[q,[q,S_x]\big] - \big[q,[q,S_x]\big]q\} =$$
$$\frac{1}{3!}\Big[q,\big[q,[q,S_x]\big]\Big]. \qquad \text{(C.5.4.15)}$$

To summarize for $n = 4$

$$e^q S_x e^{-q} \rightarrow$$
$$\rightarrow S_x - \frac{1}{2!}(\Delta\varphi)^2 S_x + \frac{1}{4!}(\Delta\varphi)^4 S_x - \Delta\varphi S_y + \frac{1}{3!}(\Delta\varphi)^3 S_y = S_x\Big[1 - \frac{1}{2!}(\Delta\varphi)^2 + \frac{1}{4!}(\Delta\varphi)^4\Big] -$$
$$S_y\Big[\Delta\varphi - \frac{1}{3!}(\Delta\varphi)^3\Big].$$

For q^k and $\{k \in \mathbb{N}\}$, I derived (C.5.4.14a),:

$\sum_{m=0}^{k}(-1)^{k-m}\frac{q^m S_x q^{k-m}}{(k-m)!m!}=\frac{1}{k!}\sum_{m=0}^{k}(-1)^{k-m}\binom{k}{m}q^m S_x q^{k-m}$. (C.5.4.14a)

$\{m\in\mathbb{N}\}$.

With $q=\frac{iS_z\Delta\varphi}{\hbar}$, (C.5.4.14a) can be written as:

$\frac{1}{k!}\sum_{m=0}^{k}(-1)^{k-m}\binom{k}{m}q^m S_x q^{k-m}=\frac{1}{k!}(\frac{i\Delta\varphi}{\hbar})^k\sum_{m=0}^{k}(-1)^{k-m}\binom{k}{m}(S_z)^m S_x (S_z)^{k-m}$, (C.5.4.14c)

or , with (C.5.4.13)

$\frac{1}{k!}\sum_{m=0}^{k}(-1)^{k-m}\binom{k}{m}q^m S_x q^{k-m}=\frac{1}{k!}(\frac{i\Delta\varphi}{\hbar})^k\left[S_z,[S_z,\dots[S_z,S_x]\dots]\right]$. (C.5.4.14d)

Then,

$S_z^m=(\frac{\hbar}{2})^m\begin{pmatrix}1&0\\0&1\end{pmatrix}$ for m is even,

and

$S_z^m=(\frac{\hbar}{2})^m\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ for m is odd,

in (C.5.4.14.c)

$m=2l$ and $\{l\in\mathbb{N}\}$:

$\frac{1}{k!}(\frac{i\Delta\varphi}{\hbar})^k\sum_{m=0}^{k}(-1)^{k-m}\binom{k}{m}(S_z)^m S_x (S_z)^{k-m}=S_x(-1)^k\frac{(\Delta\varphi)^{2k}}{(2k)!}$,

and $m=2l+1$ and $\{l\in\mathbb{N}\}$:

$\frac{1}{k!}(\frac{i\Delta\varphi}{\hbar})^k\sum_{m=0}^{k}(-1)^{k-m}\binom{k}{m}(S_z)^m S_x (S_z)^{k-m}=-S_y(-1)^k\frac{(\Delta\varphi)^{2k+1}}{(2k+1)!}$.

Hence

$e^q S_x e^{-q}\to\sum_{k=0}^{n}\frac{1}{k!}\sum_{m=0}^{k}(-1)^{k-m}\binom{k}{m}q^m S_x q^{k-m}=$

$S_x\sum_{l=0}^{n}(-1)^l\frac{(\Delta\varphi)^{2l}}{(2l)!}-S_y\sum_{l=0}^{n}(-1)^l\frac{(\Delta\varphi)^{2l+1}}{(2l+1)!}$. (C.5.4.16)

Consequently, for $n\to\infty$ (C.5.4.16) is:

$e^q S_x e^{-q}=S_x\cos\Delta\varphi-S_y\sin\Delta\varphi$, (5.34). (C.5.4.17)

The general expression for (C.5.4.4) is (C.5.4.5) or (C.5.4.17).

To evaluate (5.40), the effect of the rotation operator on the general spin state $|A\rangle$, I calculated

$\langle A|T_z^\dagger T_z|A\rangle$.

Plug (5.40) into this expression of which the result is:

$|\langle+|A\rangle|^2+|\langle-|A\rangle|^2=1$,

as it should be. However, this is not conclusive.

In (5.40):

$T_z=e^{-iS_z\Delta\varphi/\hbar}$.

Furthermore

$S_z|\pm\rangle=\pm\frac{\hbar}{2}|\pm\rangle$.

With these two expressions (5.40) is obtained.

(5.40) can be written as:

$T_z|A\rangle=(e^{-\frac{i\Delta\varphi}{2}}|+\rangle\langle+|+e^{\frac{i\Delta\varphi}{2}}|-\rangle\langle-|)|A\rangle$.

The operators $|+\rangle\langle+|$ and $|-\rangle\langle-|$ are Hermitian.

For example $|+\rangle\langle+|$:

$$|+\rangle\langle+| = \begin{pmatrix}1\\0\end{pmatrix}(1 \quad 0) = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}.$$

So

$$T_z^\dagger T_z = |+\rangle\langle+| + |-\rangle\langle-| = 1,$$

as it should be.

5.5 Magnetic Moments

Consider a particle of electric charge q and speed v performing a circular orbit of radius r in the x-y plane. See also Chapter 10 Spin Precession of The Undergraduate Course, Fp.
Fp expected the relation between the magnetic moment μ and the orbital angular momentum L for classical mechanics, (5.43), to hold for quantum mechanics as well.
See also Chapter 10 of *The Undergraduate Course*, Fp.
Addition of angular momentum, spin and orbital, and the effect on magnetic moment is presented in (5.44). The subject matter is also dealt with in Chapter 11 of *The Undergraduate Course*, Fp.

5.6 Spin Precession

In (5.47) the Hamiltonian for an electron at rest in a magnetic field is presented.
(See also Section 10.6 on Spin Precession *The Undergraduate Course*, Fp).
The Hamiltonian is time independent. So, it is about an electron in a static magnetic field.

5.7 Pauli Two-Component formalism

See section 10.5 of *The Undergraduate Course.*
To find (5.66):
with (5.60) and (5.64)

$$|A'\rangle = S_k|A\rangle = S_k|+\rangle\langle+|A\rangle + S_k|-\rangle\langle-|A\rangle\ . \qquad \text{(C.5.7.1)}$$

Then multiply (C.5.7.1) $\langle+|$ and $\langle-|$ and (5.66)-(5.68) is obtained.
Use, e. g., (5.11)

$$S_x = \frac{\hbar}{2}(|+\rangle\langle-| + |-\rangle\langle+|).$$

Plug (5.11) into (5.68), by using (5.8) and (5.9), the Pauli matrix σ_1, (5.70), is found.
(5.74):

$$\langle S_k\rangle = \langle A|S_k|A\rangle = (\langle A|+\rangle, \quad \langle A|-\rangle)S_k\begin{pmatrix}\langle+|A\rangle\\\langle-|A\rangle\end{pmatrix}. \qquad \text{(C.5.7.2)}$$

Plug $S_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$ into (C.5.7.2):

$$\langle S_x\rangle = \frac{\hbar}{2}(\langle A|+\rangle\langle-|A\rangle + \langle A|-\rangle\langle+|A\rangle\ . \qquad \text{(C.5.7.3)}$$

(C.5.7.3) shows again:
$\langle+|S_x|+\rangle = 0$, and $\langle-|S_x|-\rangle = 0$.
The same result is found for S_y :
$\langle+|S_y|+\rangle = 0$, and $\langle-|S_y|-\rangle = 0$.
For S_z :
$\langle-|S_z|+\rangle = 0$, and $\langle+|S_z|-\rangle = 0$.
I did look for these elements of the 2×2 matrix in (5.68) in order to find out how to interpret the summation in (5.74):
$\langle S_k\rangle = \langle A|S_k|A\rangle = \sum_\pm \langle A|\pm\rangle\langle\pm|S_k|\pm\rangle\langle\pm|A\rangle$,(5.74).

Using (5.60) and (5.61) in $\langle A|S_k|A\rangle$ 4 terms are found. There are four matrix elements in (5.68). I conclude the expression $\sum_{\pm}\langle A|\pm\rangle\langle\pm|S_k|\pm\rangle\langle\pm|A\rangle$ not to be helpful.
(Another approach for the Pauli matrices can be found in, a.o., Susskind).
As mentioned by Fp, (5.81) is easily obtained when use is made of the fact the spin operator S_k commutes with the eigen bras $\langle x',y',z'|$. I interpret this as S_k operates on spin states and not on the basis kets(and bras) of position space. Knowing this, I start with (5.66):
$\langle +|A'\rangle = \langle +|S_k|A\rangle = \langle +|S_k|+\rangle\langle +|A\rangle + \langle +|S_k|-\rangle\langle -|A\rangle$, (5.66)
Since S_k operates on spin states, $\langle x',y',z'|$ can be multiplied into (5.66):
$\langle x',y',z'||\langle +|A'\rangle\rangle = \langle +|S_k|+\rangle\langle x',y',z'|\langle +||A\rangle\rangle + \langle +|S_k|-\rangle\langle x',y',z'|\langle -||A\rangle\rangle$, (5.81).
Simarlily, (5.82) I obtained.
Remark: the left hand side of (5.81) should read $\langle x',y',z'||\langle +|A'\rangle\rangle$ instead of $\langle x',y',z'|\langle +|A'\rangle\rangle$. A typo.
(5.86) and (5.87) are derived with Equation (2.78). For completeness I present (2.78):
$\langle q_1' \dots q_N' \left| p_i = -i\hbar\frac{\partial}{\partial q_i'}\langle q_1' \dots q_N' \right|$,
where $q_1 \dots q_N$ are generalized coordinates with a continuous range of eigen values $q_1' \dots q_N'$.
Ket space is spanned by the eigenkets of $q_1 \dots q_N$: $|q_1' \dots q_N'\rangle$.
(5.91) is found using the Pauli matrices (5.70)-(5.72).
Fp derived (5.92) with help of the commutation and anti-commutation relations (5.75) and (5.76).
I evaluated (5.92) using (5.70)-(5.72) and the summation in (5.91) :

$$(\boldsymbol{\sigma}\cdot\boldsymbol{a})(\boldsymbol{\sigma}\cdot\boldsymbol{b}) = \begin{pmatrix} a_3 & a_1 - ia_2 \\ a_1 + ia_2 & -a_3 \end{pmatrix}\begin{pmatrix} b_3 & b_1 - ib_2 \\ b_1 + ib_2 & -b_3 \end{pmatrix}. \qquad \text{(C.5.7.4)}$$

After matrix multiplication of the matrices in (C5.7.4)

$$(\boldsymbol{\sigma}\cdot\boldsymbol{a})(\boldsymbol{\sigma}\cdot\boldsymbol{b}) = \begin{pmatrix} \boldsymbol{a}\cdot\boldsymbol{b} + i(a_1b_2 - a_2b_1) & -a_1b_3 + a_3b_1 + i(a_2b_3 - a_3b_2) \\ a_1b_3 - a_3b_1 + i(a_2b_3 - a_3b_2) & \boldsymbol{a}\cdot\boldsymbol{b} - i(a_1b_2 - a_2b_1) \end{pmatrix}, \qquad \text{(C.5.7.5)}$$

(C.5.7.5) represents 4 matrices:

$$\begin{pmatrix} \boldsymbol{a}\cdot\boldsymbol{b} & 0 \\ 0 & \boldsymbol{a}\cdot\boldsymbol{b} \end{pmatrix} + i\sigma_1(a_2b_3 - a_3b_2) + i\sigma_2(a_3b_1 - a_1b_3) + i\sigma_3(a_1b_2 - a_2b_1), \qquad \text{(C.5.7.6)}$$

where use has been made of (5.70)-(5.72).
Since,

$$\begin{pmatrix} \boldsymbol{a}\cdot\boldsymbol{b} & 0 \\ 0 & \boldsymbol{a}\cdot\boldsymbol{b} \end{pmatrix} = \boldsymbol{a}\cdot\boldsymbol{b}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

(C.5.7.6) results into (5.92).
In (5.94), Fp indicated $\boldsymbol{n}$ to be a trivial position operator. I suppose Fp meant $|\boldsymbol{n}|^2 = 1$.
Then, with (5.92), the rules (5.96) and (5.97) are obtained.
Since $\boldsymbol{n}\times\boldsymbol{n} = 0$ and with rules (5.96)-(5.97), (5.98) is found.
(5.98) can be written as:

$$\cos\left(\tfrac{\Delta\varphi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - i\sin\left(\tfrac{\Delta\varphi}{2}\right)\left[n_x\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + n_y\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + n_z\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \rightarrow \text{(5.99)}.$$

Keep in mind, in (5.98)

$$\cos\left(\tfrac{\Delta\varphi}{2}\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \equiv \cos\left(\tfrac{\Delta\varphi}{2}\right)\begin{pmatrix} n_x^2 + n_y^2 + n_z^2 & 0 \\ 0 & n_x^2 + n_y^2 + n_z^2 \end{pmatrix},$$

since changing the axis of rotation aligned with the unit vectors n_x, n_y and n_z respectively

$\cos\left(\frac{\Delta\varphi}{2}\right)\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \equiv \cos\left(\frac{\Delta\varphi}{2}\right)\begin{pmatrix}n_x^2(=1) & 0\\ 0 & n_x^2(=1)\end{pmatrix}$, etc.

Recapitulate (5.74):

$\langle S_k\rangle = \left(\frac{\hbar}{2}\right)\chi^\dagger\sigma_k\chi$,

and (10.74) *The Undergraduate Course*, (5.73):

$S_k = \frac{\hbar}{2}\sigma_k$ (10.74) or $S_k \to \frac{\hbar}{2}\sigma_k$ (5.73).

Remark, I consider the use of " →" by Fp confusing. Does it mean: "is equal" or "under rotation"?

(5.38):

$\langle S_k\rangle \to \sum_l R_{kl}\,\langle S_l\rangle$.

Furthermore

$\langle S_l\rangle = \left(\frac{\hbar}{2}\right)\chi^\dagger\sigma_l\chi$.

Then (5.38) can be written as:

$\langle S_k\rangle \to \left(\frac{\hbar}{2}\right)\sum_l R_{kl}\,\chi^\dagger\sigma_l\chi$.

Hence, under rotation (5.101):

$\langle S_k\rangle = \left(\frac{\hbar}{2}\right)\left(\chi^\dagger\sigma_k\chi\right)' = \left(\frac{\hbar}{2}\right)\sum_l R_{kl}\,\chi^\dagger\sigma_l\chi$.

Fp mentioned R_{kl} to be the elements of the conventional rotation matrix:

Let's look into it.

With (5.100)

$\chi' = \exp\left(-i\boldsymbol{\sigma}\cdot\boldsymbol{n}\frac{\Delta\varphi}{2}\right)\chi$,

$\left(\chi^\dagger\sigma_k\chi\right)'$ becomes:

$\chi^\dagger\sigma_k \exp\left(-i\boldsymbol{\sigma}\cdot\boldsymbol{n}\frac{\Delta\varphi}{2}\right)\chi.$ (C.5.7.7)

Here a question arises.

$\exp\left(-i\boldsymbol{\sigma}\cdot\boldsymbol{n}\frac{\Delta\varphi}{2}\right)$ results into the 2×2 matrix (5.99), where use has been made of the Taylor series. Let's denote this matrix by

$A = \begin{pmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix}$, (C.5.7.8)

the elements A_{ij} given by (5.99).

The question:

$\exp\left(+i\boldsymbol{\sigma}\cdot\boldsymbol{n}\frac{\Delta\varphi}{2}\right) = A^\dagger$? I suppose so.

Rewrite (5.100):

$\chi' = A\chi$. (C.5.7.9)

Then, I have for (5.101)

$\langle\sigma_k\rangle_{\Delta\varphi} = \chi^\dagger A^\dagger\sigma_k A\chi = \sum_l R_{kl}\,\langle\sigma_l\rangle$. (C.5.7.10)

Another question: does (5.102) follow from (5.101)/(C.5.7.10)?

(5.102) is proportional to (5.34). The factor is $\frac{\hbar}{2}$.

Fp denotes R_{kl} to be the elements of a conventional rotation matrix. Conventional? In the classical interpretation? I do not know. In 3-D the rotation matrix is a 3×3 matrix in homogeneous coordinates.

I suppose R_{kl} to be the elements of a 2×2 matrix.

Let's start with (C.5.7.10) and set $k = 1$. With (5.7.8),

$$\sigma_1 A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} A_{21} & A_{22} \\ A_{11} & A_{12} \end{pmatrix}. \quad \text{(C.5.7.11)}$$

Another question: is the left-hand side of (C.5.7.10) correct? Look at (5.26), translate this into (C.5.7.10):

$$\langle \sigma_k \rangle_{\Delta\varphi} = \chi^\dagger A^\dagger \sigma_k A \chi = \sum_l R_{kl} \langle \sigma_l \rangle, \quad \text{(C.5.7.12)}$$

since,

$$(A\chi)^\dagger = \chi^\dagger A^\dagger.$$

Now I have to evaluate, with (C.5.7.8) and (C.5.7.11) :

$$A^\dagger \sigma_1 A = \begin{pmatrix} A_{11}^* & A_{21}^* \\ A_{12}^* & A_{22}^* \end{pmatrix} \begin{pmatrix} A_{21} & A_{22} \\ A_{11} & A_{12} \end{pmatrix} \equiv \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}. \quad \text{(C.5.7.13)}$$

For convenience I reproduce the elements of (5.99)

$$A_{11} = \cos\left(\frac{\Delta\varphi}{2}\right) - i n_z \sin\left(\frac{\Delta\varphi}{2}\right),$$

$$A_{12} = \left(-i n_x - n_y\right) \sin\left(\frac{\Delta\varphi}{2}\right),$$

$$A_{21} = \left(-i n_x + n_y\right) \sin\left(\frac{\Delta\varphi}{2}\right),$$

$$A_{22} = \cos\left(\frac{\Delta\varphi}{2}\right) + i n_z \sin\left(\frac{\Delta\varphi}{2}\right).$$

So, for the case $k = 1$ (C.5.7.13) I obtain for the elements of the matrix B:

$$B_{11} = A_{11}^* A_{21} + A_{21}^* A_{11} = \left[\cos\left(\frac{\Delta\varphi}{2}\right) + i n_z \sin\left(\frac{\Delta\varphi}{2}\right)\right] \left(-i n_x + n_y\right) \sin\left(\frac{\Delta\varphi}{2}\right) +$$

$$+\left(i n_x + n_y\right) \sin\left(\frac{\Delta\varphi}{2}\right) \left[\cos\left(\frac{\Delta\varphi}{2}\right) - i n_z \sin\left(\frac{\Delta\varphi}{2}\right)\right]. \quad \text{(C.5.7.14)}$$

Using orthogonality of the unit vectors n_i, (C.5.7.14) results into

$$B_{11} = n_y \sin\Delta\varphi\ . \quad \text{(C.5.7.15)}$$

Next

$$B_{12} = A_{11}^* A_{22} + A_{21}^* A_{12} = \left[\cos\left(\frac{\Delta\varphi}{2}\right) + i n_z \sin\left(\frac{\Delta\varphi}{2}\right)\right] \left[\cos\left(\frac{\Delta\varphi}{2}\right) + i n_z \sin\left(\frac{\Delta\varphi}{2}\right)\right] +$$

$$+\left(i n_x + n_y\right) \sin\left(\frac{\Delta\varphi}{2}\right) \left(-i n_x - n_y\right) \sin\left(\frac{\Delta\varphi}{2}\right) = \cos\Delta\varphi + \left(n_y^2 + i n_z\right) \sin\Delta\varphi \rightarrow$$

$$B_{12} = \cos\Delta\varphi + \left(n_y^2 + i n_z\right) \sin\Delta\varphi. \quad \text{(C.5.7.16)}$$

Then

$$B_{21} = A_{12}^* A_{21} + A_{22}^* A_{11} = \left(i n_x - n_y\right) \sin\left(\frac{\Delta\varphi}{2}\right) \left(-i n_x + n_y\right) \sin\left(\frac{\Delta\varphi}{2}\right) +$$

$$\left[\cos\left(\frac{\Delta\varphi}{2}\right) - i n_z \sin\left(\frac{\Delta\varphi}{2}\right)\right] \left[\cos\left(\frac{\Delta\varphi}{2}\right) - i n_z \sin\left(\frac{\Delta\varphi}{2}\right)\right] = \cos\Delta\varphi + \left(n_x^2 - i n_z\right) \sin\Delta\varphi \rightarrow$$

$$B_{21} = \cos\Delta\varphi + \left(n_x^2 - i n_z\right) \sin\Delta\varphi. \quad \text{(C.5.7.17)}$$

Finally

$$B_{22} = A_{12}^* A_{22} + A_{22}^* A_{12} = \left(i n_x - n_y\right) \sin\left(\frac{\Delta\varphi}{2}\right) \left[\cos\left(\frac{\Delta\varphi}{2}\right) + i n_z \sin\left(\frac{\Delta\varphi}{2}\right)\right] +$$

$$\left[\cos\left(\frac{\Delta\varphi}{2}\right) - i n_z \sin\left(\frac{\Delta\varphi}{2}\right)\right] \left(-i n_x - n_y\right) \sin\left(\frac{\Delta\varphi}{2}\right) = -n_y \sin\Delta\varphi \rightarrow$$

$$B_{22} = -n_y \sin\Delta\varphi. \quad \text{(C.5.7.18)}$$

So, the rotation matrix for $\langle \sigma_x \rangle_{\Delta\varphi}$ is:

$$B = \begin{pmatrix} n_y \sin\Delta\varphi & \cos\Delta\varphi + \left(n_y^2 + i n_z\right) \sin\Delta\varphi \\ \cos\Delta\varphi + \left(n_x^2 - i n_z\right) \sin\Delta\varphi & -n_y \sin\Delta\varphi \end{pmatrix}. \quad \text{(C.5.7.19)}$$

In the same way the rotation matrices for σ_y and σ_z can be found.

Let us return to (C.5.7.12). With matrix B:

$$\chi^{\dagger}B\chi = \sum_l R_{kl}\,\langle\sigma_l\rangle = R_{11}\langle\sigma_1\rangle + R_{12}\langle\sigma_2\rangle + R_{13}\langle\sigma_3\rangle = \chi^{\dagger}\begin{pmatrix} R_{13} & R_{11}-iR_{12} \\ R_{11}+iR_{12} & -R_{13}\end{pmatrix}\chi\,, \tag{C.5.7.20}$$

Then,

$$B = \begin{pmatrix} R_{13} & R_{11}-iR_{12} \\ R_{11}+iR_{12} & -R_{13}\end{pmatrix} = \begin{pmatrix} R_{13} & R_{11}-iR_{12} \\ R_{11}+iR_{12} & -R_{13}\end{pmatrix}. \tag{C.5.7.21}$$

Keep in mind B represents the effect of rotation, for a general rotation axis, on $\langle\sigma_1\rangle$. In the same way the rotation matrices for σ_y and σ_z can be found.

Now can I recover (5.102)? Well, I can. Since in that case the axis of rotation is the z-axis. Hence, with (C.5.7.19) and $n_z = 1(n_x^2, n_y^2 = 0)$:

$$B = \begin{pmatrix} 0 & \cos\Delta\varphi + i\sin\Delta\varphi \\ \cos\Delta\varphi - i\sin\Delta\varphi & 0\end{pmatrix} = \sigma_1\cos\Delta\varphi - \sigma_2\sin\Delta\varphi \;\text{, (5.102).}$$

and , with the axis of rotation aligned with n_z,

$$A = \begin{pmatrix} \cos\left(\frac{\Delta\varphi}{2}\right) - i\sin\left(\frac{\Delta\varphi}{2}\right) & 0 \\ 0 & \cos\left(\frac{\Delta\varphi}{2}\right) + i\sin\left(\frac{\Delta\varphi}{2}\right)\end{pmatrix} = \begin{pmatrix} e^{-i\varphi/2} & 0 \\ 0 & e^{i\varphi/2}\end{pmatrix}. \tag{C.5.7.22}$$

With respect to the permutations mentioned by Fp, I will derive the matrix for the effect of rotation along the z-axis$[n_z = 1(n_x^2, n_y^2 = 0)]$ on σ_2 (or $k = 2$).

With (C.5.7.11)

$$\sigma_2 A = \begin{pmatrix} 0 & -i \\ i & 0\end{pmatrix}\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22}\end{pmatrix} = i\begin{pmatrix} -A_{21} & -A_{22} \\ A_{11} & A_{12}\end{pmatrix}. \tag{C.5.7.23}$$

With (C.5.7.13)

$$A^{\dagger}\sigma_2 A = i\begin{pmatrix} A_{11}^* & A_{21}^* \\ A_{12}^* & A_{22}^*\end{pmatrix}\begin{pmatrix} -A_{21} & -A_{22} \\ A_{11} & A_{12}\end{pmatrix} \equiv \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22}\end{pmatrix}. \tag{C.5.7.24}$$

So, for the case $k = 2$ (C.5.7.24) I obtain for the elements of the matrix C:

$$C_{11} = -iA_{11}^*A_{21} + iA_{21}^*A_{11} = \left[\cos\left(\frac{\Delta\varphi}{2}\right) - in_z\sin(\frac{\Delta\varphi}{2})\right]\left(-n_x + in_y\right)\sin\left(\frac{\Delta\varphi}{2}\right) +$$
$$+\left(-n_x + in_y\right)\sin\left(\frac{\Delta\varphi}{2}\right)\left[\cos\left(\frac{\Delta\varphi}{2}\right) - in_z\sin\left(\frac{\Delta\varphi}{2}\right)\right] = 0 \rightarrow$$
$$C_{11} = 0. \tag{C.5.7.25}$$

Next

$$C_{12} = -iA_{11}^*A_{22} + iA_{21}^*A_{12} = -\left[i\cos\left(\frac{\Delta\varphi}{2}\right) - n_z\sin\left(\frac{\Delta\varphi}{2}\right)\right]\left[\cos\left(\frac{\Delta\varphi}{2}\right) + in_z\sin\left(\frac{\Delta\varphi}{2}\right)\right] +$$
$$-\left(in_x + n_y\right)\sin\left(\frac{\Delta\varphi}{2}\right)\left(-n_x + in_y\right)\sin\left(\frac{\Delta\varphi}{2}\right) = -i\cos\Delta\varphi + \sin\Delta\varphi \rightarrow$$
$$C_{12} = -i\cos\Delta\varphi + \sin\Delta\varphi. \tag{C.5.7.26}$$

Then

$$C_{21} = -iA_{12}^*A_{21} + iA_{22}^*A_{11} = \left(n_x + in_y\right)\sin\left(\frac{\Delta\varphi}{2}\right)\left(-in_x + n_y\right)\sin\left(\frac{\Delta\varphi}{2}\right) +$$
$$\left[i\cos\left(\frac{\Delta\varphi}{2}\right) + n_z\sin\left(\frac{\Delta\varphi}{2}\right)\right]\left[\cos\left(\frac{\Delta\varphi}{2}\right) - in_z\sin\left(\frac{\Delta\varphi}{2}\right)\right] = i\cos\Delta\varphi + \sin\Delta\varphi \rightarrow$$
$$C_{21} = i\cos\Delta\varphi + \sin\Delta\varphi\,. \tag{C.5.7.27}$$

Finally

$$C_{22} = -iA_{12}^*A_{22} + iA_{22}^*A_{12} = -\left(-n_x - in_y\right)\sin\left(\frac{\Delta\varphi}{2}\right)\left[\cos\left(\frac{\Delta\varphi}{2}\right) + in_z\sin\left(\frac{\Delta\varphi}{2}\right)\right] +$$
$$-\left[\cos\left(\frac{\Delta\varphi}{2}\right) - in_z\sin\left(\frac{\Delta\varphi}{2}\right)\right]\left(-n_x + in_y\right)\sin\left(\frac{\Delta\varphi}{2}\right) = 0 \rightarrow$$
$$C_{22} = 0. \tag{C.5.7.28}$$

Hence

$$C=\begin{pmatrix}0 & -i\cos\Delta\varphi+\sin\Delta\varphi\\ i\cos\Delta\varphi+\sin\Delta\varphi & 0\end{pmatrix}=\sigma_2\cos\Delta\varphi-\sigma_1\sin\Delta\varphi. \qquad \text{(C.5.7.29)}$$

Compare $B=\sigma_1\cos\Delta\varphi-\sigma_2\sin\Delta\varphi$,(5.102), and $C=\sigma_2\cos\Delta\varphi-\sigma_1\sin\Delta\varphi$,(C.5.7.29), and the "cyclic permutation" as mentioned by Fp on top of page 85 is illustrated.

In summary:

(5.98) $\exp\left(-i\boldsymbol{\sigma}\cdot\boldsymbol{n}\frac{\Delta\varphi}{2}\right)=\exp[-i\left(\sigma_x n_x+\sigma_y n_y+\sigma_z n_z\right)\frac{\Delta\varphi}{2}]$. (C.5.7.30)

The rotation axis aligned with the x-axis, $n_x=1(n_z^2,n_y^2=0)$,

$$\exp\left[-i(\sigma_x)\frac{\Delta\varphi}{2}\right]\rightarrow\begin{pmatrix}\cos\left(\frac{\Delta\varphi}{2}\right) & -i\sin\left(\frac{\Delta\varphi}{2}\right)\\ -i\sin\left(\frac{\Delta\varphi}{2}\right) & \cos\left(\frac{\Delta\varphi}{2}\right)\end{pmatrix}. \qquad \text{(C.5.7.31)}$$

The rotation axis aligned with the y-axis, $n_y=1(n_z^2,n_y^2=0)$,

$$\exp\left[-i\left(\sigma_y\right)\frac{\Delta\varphi}{2}\right]\rightarrow\begin{pmatrix}\cos\left(\frac{\Delta\varphi}{2}\right) & -\sin\left(\frac{\Delta\varphi}{2}\right)\\ \sin\left(\frac{\Delta\varphi}{2}\right) & \cos\left(\frac{\Delta\varphi}{2}\right)\end{pmatrix}. \qquad \text{(C.5.7.32)}$$

The axis of rotation aligned with z-axis, $n_z=1(n_x^2,n_y^2=0)$,

$$\exp[-i(\sigma_z)\frac{\Delta\varphi}{2}]\rightarrow\begin{pmatrix}\cos\left(\frac{\Delta\varphi}{2}\right)-i\sin\left(\frac{\Delta\varphi}{2}\right) & 0\\ 0 & \cos\left(\frac{\Delta\varphi}{2}\right)+i\sin\left(\frac{\Delta\varphi}{2}\right)\end{pmatrix}. \qquad \text{(C.5.7.22)}$$

Keep in mind, using (C.5.7.6):

$$\exp\left[-i(\sigma_x)\frac{\Delta\varphi}{2}\right]\cdot\exp\left[-i\left(\sigma_y\right)\frac{\Delta\varphi}{2}\right]\cdot\exp\left[-i(\sigma_z)\frac{\Delta\varphi}{2}\right]=\exp[-i\left(\sigma_x n_x+\sigma_y n_y+\sigma_z n_z\right)\frac{\Delta\varphi}{2}]\rightarrow$$

$$\rightarrow\begin{pmatrix}n_x^2\cos\left(\frac{\Delta\varphi}{2}\right) & -i\,n_x\sin\left(\frac{\Delta\varphi}{2}\right)\\ -i\,n_x\sin\left(\frac{\Delta\varphi}{2}\right) & n_x^2\cos\left(\frac{\Delta\varphi}{2}\right)\end{pmatrix}+\begin{pmatrix}n_y^2\cos\left(\frac{\Delta\varphi}{2}\right) & -n_y\sin\left(\frac{\Delta\varphi}{2}\right)\\ n_y\sin\left(\frac{\Delta\varphi}{2}\right) & n_y^2\cos\left(\frac{\Delta\varphi}{2}\right)\end{pmatrix}+$$

$$+\begin{pmatrix}n_z^2\cos\left(\frac{\Delta\varphi}{2}\right)-i\,n_z\sin\left(\frac{\Delta\varphi}{2}\right) & 0\\ 0 & n_z^2\cos\left(\frac{\Delta\varphi}{2}\right)+i\,n_z\sin\left(\frac{\Delta\varphi}{2}\right)\end{pmatrix}=$$

$$=\begin{pmatrix}(n_x^2+n_y^2+n_z^2)\cos\left(\frac{\Delta\varphi}{2}\right)-i\,n_z\sin\left(\frac{\Delta\varphi}{2}\right) & (-i\,n_x-n_y)\sin\left(\frac{\Delta\varphi}{2}\right)\\ (-i\,n_x+n_y)\sin\left(\frac{\Delta\varphi}{2}\right) & (n_x^2+n_y^2+n_z^2)\cos\left(\frac{\Delta\varphi}{2}\right)+i\,n_z\sin\left(\frac{\Delta\varphi}{2}\right)\end{pmatrix}, \qquad \text{(C.5.7.33)}$$

Since $(n_x^2+n_y^2+n_z^2)=1$, (C.5.7.33) equals (5.99).

With the expressions (C.5.7.31) and (C.5.7.32), I can evaluate

$\exp\left[i(\sigma_x)\frac{\Delta\varphi}{2}\right]\sigma_{y,z}\exp\left[-i(\sigma_x)\frac{\Delta\varphi}{2}\right]$,

and

$\exp\left[i\left(\sigma_y\right)\frac{\Delta\varphi}{2}\right]\sigma_{z,x}\exp\left[-i\left(\sigma_y\right)\frac{\Delta\varphi}{2}\right]$.

5.8 Spin Greater Than One-Half Systems

In this section Fp refers to (5.83) for the two wavefunctions $\psi_{\pm}(\boldsymbol{x}')$.

On page 86 above(5.109) Fp writes: "*In this case, the Hamiltonian represented as a* 2×2 *matrix of complex numbers in the Schrodinger/Pauli scheme[see Equation (5.73)], and the spinor eigenvalue equation reduces to a straightforward matrix eigenvalue problem.*":

$S_k\rightarrow\frac{\hbar}{2}\sigma_k$,(5.73), $H\chi=E\chi$,(5.10).

On the middle of page 86,Fp mentioned spin one or a spin three-halves particle. Three-

halves particle? Well, below (5.110) Fp defines a spin three-halves particle to be represented by a four-component spinor.
On page 87 Fp derived the Pauli matrices. See also *Undergraduate Course*, Fp. On page 88 the spin one matrices are given.
On the other hand by writing for: $S^- = \begin{pmatrix} a\ b\ c \\ d\ e\ f \\ g\ h\ i \end{pmatrix}$ and operate this matrix on the column vector representations of the three states, you will find the elements of the lowering operator. Keep in mind the raising and lowering operators being mutual Hermitian conjugates. An example of the exercise is: $S^- \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$.
Then:
$\begin{pmatrix} a\ b\ c \\ d\ e\ f \\ g\ h\ i \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow c = f = i = 0$,
next
$\begin{pmatrix} a\ b\ 0 \\ d\ e\ 0 \\ g\ h\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \rightarrow b = e = 0, h = 1,$
and
$\begin{pmatrix} a\ 0\ 0 \\ d\ 0\ 0 \\ g\ 1\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \rightarrow a = g = 0, d = 1$
Hence
$S^- = \begin{pmatrix} 0\ 0\ 0 \\ 1\ 0\ 0 \\ 0\ 1\ 0 \end{pmatrix}$, I neglect the constant factor.
Simarlily, the raising operator is found:
$S^+ = \begin{pmatrix} 0\ 1\ 0 \\ 0\ 0\ 1 \\ 0\ 0\ 0 \end{pmatrix}$.
With (5.116):
$$S_x = \frac{1}{2}(S^+ + S^-) = \frac{1}{2}\begin{pmatrix} 0\ 1\ 0 \\ 1\ 0\ 1 \\ 0\ 1\ 0 \end{pmatrix}, \qquad \text{(C.5.8.1)}$$
and
$$S_y = -\frac{i}{2}(S^+ - S^-) = \frac{1}{2}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}. \qquad \text{(C.5.8.2)}$$
Again neglected constant factors in the above matrices for S_x and S_y. To complete this exercise, I need to multiply (C.5.81) and C.5.8.2) with $\hbar\sqrt{2}$.
So, including the constant $\hbar\sqrt{2}$ in the lowering and raising operators,
$S^- = \hbar\sqrt{2}\begin{pmatrix} 0\ 0\ 0 \\ 1\ 0\ 0 \\ 0\ 1\ 0 \end{pmatrix}$ and $S^+ = \hbar\sqrt{2}\begin{pmatrix} 0\ 1\ 0 \\ 0\ 0\ 1 \\ 0\ 0\ 0 \end{pmatrix}$
Then with (5.112) the extended Pauli matrices (5.124) and (5.125) are found.
With the commutator (4.24),

$[S^+, S^-] = 2\hbar S_z$,

$$S_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Exercises

Exercise 5.1 Demonstrate the spin operators to be Hermitian.

5.1 Demonstrate that the operators defined in Equations (5.11)-(5.13) are Hermitian, and satisfy the commutation relations (5.1).

Let's start with

$S_x = \frac{\hbar}{2}(|+\rangle\langle -| + |-\rangle\langle +|)$, (5.11).

Then

$S_x^\dagger = \frac{\hbar}{2}[(|+\rangle\langle -|)^\dagger + (|-\rangle\langle +|)^\dagger] = \frac{\hbar}{2}(|-\rangle\langle +| + |+\rangle\langle -|) = \frac{\hbar}{2}(|+\rangle\langle -| + |-\rangle\langle +|)$, (5.11).

On the other hand, with matrix representation:

$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = S_x^\dagger$.

Next

$S_y = \frac{i\hbar}{2}(-|+\rangle\langle -| + |-\rangle\langle +|)$, (5.12).

So,

$S_y^\dagger = -\frac{i\hbar}{2}[-(|+\rangle\langle -|)^\dagger + (|-\rangle\langle +|)^\dagger] = \frac{i\hbar}{2}(-|+\rangle\langle -| + |-\rangle\langle +) = S_y$.

With matrix representation:

$S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = S_y^\dagger$.

Simarlily:

$S_z = S_z^\dagger$.

The commutation relation:

$[S_x, S_y] = i\hbar S_z$.

Using (5.11) and (5.12)

$S_x S_y - S_y S_x = \frac{i\hbar^2}{4}[(|+\rangle\langle -| + |-\rangle\langle +|)(-|+\rangle\langle -| + |-\rangle\langle +|) +$

$-(-|+\rangle\langle -| + |-\rangle\langle +|)(|+\rangle\langle -| + |-\rangle\langle +|)]$. (C.5.E.1)

With (5.8), (5.9) and (5.13)

$[S_x, S_y] = i\hbar S_z$.

As an example:

$S_x S_y \propto (|+\rangle\langle -| + |-\rangle\langle +|)(-|+\rangle\langle -| + |-\rangle\langle +|) = -0 + |+\rangle\langle -||-\rangle\langle +| +$

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

Simarlily, the other two commutation relations are obtained.

Exercise 5.2 Proof of the Baker-Hausdorff lemma

See my notes on Section 5.4. (5.4a Proof of Baker-Hausdorff lemma and the CBA convention).

The Baker-Hausdorff Lemma:

$$f(\lambda) = e^{iG\lambda} A e^{-iG\lambda} = A + i\lambda[G, A] + \left(\frac{i^2\lambda^2}{2!}\right)[G, [G, A]] + \left(\frac{i^3\lambda^3}{3!}\right)[G, [G, [G, A]]] + \cdots \quad (5.31)$$

The Taylor's series expansion:

$f(\lambda) = \lim_{n\to\infty} \sum_{r=0}^{n} \frac{\lambda^r}{r!} f^{(r)}(0)$. Based on Taylor' Theorem. I assume Taylor's Theorem need not to be proven.

For convenience, I will use the CBA-convention as presented in my notes on section 5.4 *On Rotation operators in Spin Space* :

$e^q A e^{-q} = \sum_{k=0}^{\infty} \frac{1}{k!} ([q,)^k A(])^k$, (C.5.4.18),

where

$k = 0$: $([G,)^k A(])^k = A$, 2^k terms,

$k = 1$: $([G,)^k A(])^k = [G, A]$, 2^k terms,

$k = 2$: $([G,)^k A(])^k = [q, [G, A]]$, 2^k terms, ...

Now, in general with (5.31):

$$e^{iG\lambda} A e^{-iG\lambda} = \sum_{p=0}^{\infty} \frac{(iG\lambda)^p}{p!} A \sum_{q=0}^{\infty} \frac{(-iG\lambda)^q}{q!} = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} (-)^q \frac{(i\lambda)^{p+q}}{p!q!} G^p A G^q =$$

$$\sum_{s=0}^{\infty} \sum_{r=0}^{s} (-)^r \frac{(i\lambda)^s}{r!(s-r)!} G^{s-r} A G^r. \qquad \text{(C.5.E.2)}$$

With (C.5.E.2), (5.31) can be written as

$$f(\lambda) = e^{iG\lambda} A e^{-iG\lambda} = A + i\lambda[G, A] + \left(\frac{i^2\lambda^2}{2!}\right) ([G,)^2 A(])^2 + \left(\frac{i^3\lambda^3}{3!}\right) ([G,)^3 A(])^3 + \cdots +$$

$$\left(\frac{i^n\lambda^n}{n!}\right) \sum_{k=0}^{n} (-)^k \binom{n}{k} G^{n-k} A G^k. \qquad \text{(C.5.E.3)}$$

Now I have to prove:

$$\sum_{k=0}^{n} (-)^k \binom{n}{k} G^{n-k} A G^k = ([G,)^n A(])^n. \qquad \text{(C.5.E.4)}$$

Using induction, so,

$$([G,)^{n+1} A(])^{n+1} = ([G,)^n [G, A]\ (])^n. \qquad \text{(C.5.E.5)}$$

Now, instead of A in (C.5.E.4) there appears $[G, A]$. Consequently (C.5.E.5) becomes:

$$([G,)^{n+1} A(])^{n+1} = \sum_{k=0}^{n} (-)^k \binom{n}{k} G^{n-k} [G, A] G^k =$$

$$= \sum_{k=0}^{n} (-)^k \binom{n}{k} G^{n+1-k} A G^k - \sum_{k=0}^{n} (-)^k \binom{n}{k} G^{n-k} A G^{k+1} =$$

$$= G^{n+1} A + \sum_{k=1}^{n} (-)^{k-1} \binom{n}{k-1} G^{n+1-k} A G^k - \sum_{k=1}^{n} (-)^k \binom{n}{k} G^{n+1-k} A G^k +$$

$$+ (-)^{n+1} A G^{n+1}. \qquad \text{(C.5.E.6)}$$

Plug

$\binom{n}{k} + \binom{n}{k-1} = \binom{n+1}{k}$, into (C.5.E.6):

$$G^{n+1} A + \sum_{k=1}^{n} (-)^k \binom{n+1}{k} G^{n+1-k} A G^k + (-)^{n+1} A G^{n+1} =$$

$$= \sum_{k=0}^{n+1} (-)^k \binom{n+1}{k} G^{n+1-k} A G^k. \qquad \text{(C.5.E.7)}$$

Hence, with induction it follows, with (C.5.E.8):

$$e^{iG\lambda} A e^{-iG\lambda} = A + i\lambda[G, A] + \left(\frac{i^2\lambda^2}{2!}\right) ([G,)^2 A(])^2 + \left(\frac{i^3\lambda^3}{3!}\right) ([G,)^3 A(])^3 + \cdots +$$

$$+ \left(\frac{i^n\lambda^n}{n!}\right) ([G,)^n A(])^n + \cdots$$

See also www.math.stackexchange.com .

Another approach for the proof of Baker-Hausdorff lemma.

$f(i\lambda) = e^{iG\lambda} A e^{-iG\lambda} = f(i\lambda) = \sum_{k=0}^{\infty} \frac{a_k}{k!} (i\lambda)^k$,

where $a_k = \frac{d^k f}{d(i\lambda)^k}$ at $i\lambda = 0$ and $a_0 = A$.

$\frac{df}{di\lambda} = [G, f]$. (C.5.E.8)

In addition

$\frac{df}{di\lambda} = \sum_{k=1}^{\infty} \frac{a_k}{(k-1)!}(i\lambda)^{k-1}$. (C.5.E.9)

Plug $f(i\lambda) = \sum_{k=0}^{\infty} \frac{a_k}{k!}(i\lambda)^k$ into (C.5.E.8):

$\frac{df}{di\lambda} = \left[G, \sum_{k=0}^{\infty} \frac{a_k}{k!}(i\lambda)^k\right] = \sum_{k=0}^{\infty} \frac{1}{k!}[G, a_k](i\lambda)^k$. (C.5.E.10)

The two identical expressions (C.5.E.9) and (C.5.E.10):

$\sum_{k=1}^{\infty} \frac{a_k}{(k-1)!}(i\lambda)^{k-1} = \sum_{k=0}^{\infty} \frac{1}{k!}[G, a_k](i\lambda)^k$. (C.5.E.11)

In the left hand side: $k \to k+1$, then, equating the coefficients of $(i\lambda)^k$:

$\sum_{k=0}^{\infty} \frac{a_{k+1}}{k!}(i\lambda)^k = \sum_{k=0}^{\infty} \frac{1}{k!}[G, a_k](i\lambda)^k \to$

$a_{k+1} = [G, a_k]$, (C.5.E.12)

a recurrence relation.

Then $a_1 = [G, a_0] = [G, A]$.

Hence

$a_{k+1} = \left[G, [G, a_{k-1}]\right] = \cdots = ([G,)^{k+1} A(])^{k+1}$. (C.5.E.13)

See www.webhome.phy.duke.edu , *Notes on Baker-Campbell-Hausdorff Formulae*.

In Noordzij(3), Homework 1, a proof is presented.

Exercise 5.3 Pauli Representations of Spin Eigenstates

Find the Pauli representations of the normalized eigenstates of S_x and S_y for a spin-1/2 particle.

The Pauli representation can be read about in Section 10.5 of *The Undergraduate Course*, Fp. I will use the notation of Section 10.5.

The spin operators are, $i = 1,2,3$ corresponding to x, y, z:

$S_i = \frac{\hbar}{2}\sigma_i$,

where σ_i the Pauli-matrices.

- Let's start with S_x.

For the eigenvector in Pauli representation I choose:

$\chi = \begin{pmatrix} a \\ b \end{pmatrix}$. (C.5.E.14)

Then

$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \pm\frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}$. (C.5.E.15)

With the positive eigenvalue, $+1$, of the Pauli-matrix, the eigenvector is $\begin{pmatrix} a \\ a \end{pmatrix}$.

Normalization results into:

$|a| = \frac{1}{\sqrt{2}}$.

Neglecting the phase factor, the eigenvector is:

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}. \quad \text{(C.5.E.16)}$$

Now for the negative eigenvalue -1, the eigenvector is $\begin{pmatrix} a \\ -a \end{pmatrix}$.

With normalization and neglecting the phase factor, the other eigenvector of S_x:

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

- The normalized eigenstates of the operator S_y.

Then

$$\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \pm\frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}.$$

With the positive eigenvalue, $+1$, of the Pauli-matrix, the eigenvector is $\begin{pmatrix} a \\ ia \end{pmatrix}$.

Normalization and neglecting the phase factor gives for the eigenvector:

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}. \qquad \text{(C.5.E.17)}$$

For the negative eigenvalue -1, the eigenvector is $\begin{pmatrix} a \\ -ia \end{pmatrix}$.

With normalization and neglecting the phase factor, the other eigenvector of S_y:

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix}. \qquad \text{(C.5.E.18)}$$

Exercise 5.4 Probabilities of a Measurement of S_z

Suppose a spin-1/2 particle has a spin that 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 probability $\cos^2(\frac{\theta}{2})$ and $-\hbar/2$ with probability $\sin^2(\frac{\theta}{2})$.

Let's start with a spin vector in a direction represented by the normalized vector $\bar{n} = (n_x, n_y, n_z)$.

Then

$$S_n = \frac{\hbar}{2}\begin{pmatrix} n_z & (n_x - in_y) \\ (n_x + in_y) & -n_z \end{pmatrix}. \qquad \text{(C.5.E.19)}$$

See for example Susskind.

Or in spherical coordinates, (C.5.E.19):

$$S_n = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta\cos\phi - i\sin\theta\sin\phi \\ \sin\theta\cos\phi + i\sin\theta\sin\phi & -\cos\theta \end{pmatrix}. \qquad \text{(C.5.E.20)}$$

Now I set $\phi = 0$, the x-z plane.

Hence,

$$S_n = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}. \qquad \text{(C.5.E.21)}$$

The eigenvalues are found by the determinant (Chisholm and Morris)

$\begin{vmatrix} cos\theta - \lambda & sin\theta \\ sin\theta & -cos - \lambda \end{vmatrix} = 0$, for nontrivial solutions.

Hence, the eigenvalues are $\lambda = \pm 1$.

Assume the general eigenvector A to be

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

The spin eigenstates:

$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, (10.45) and (10.46) respectively. *The Undergraduate Course.*

Then

$$\frac{\hbar}{2}\begin{pmatrix}\cos\theta & \sin\theta\\ \sin\theta & -\cos\theta\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix}=\pm\frac{\hbar}{2}\begin{pmatrix}a\\ b\end{pmatrix}. \quad \text{(C.5.E.22)}$$

With the positive eigenvalue, $+1$:

$$\frac{a}{b}=\frac{\sin\theta}{1-\cos\theta}=\frac{\cos\frac{\theta}{2}}{\sin\frac{\theta}{2}}. \quad \text{(C.5.E.23)}$$

Consequently, with normalization and neglecting the phase factor:

$$a=\cos\frac{\theta}{2},$$

and

$$b=\sin\frac{\theta}{2}.$$

The eigenvector with positive eigenvalue is:

$$A_1=\begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}\end{pmatrix}. \quad \text{(C.5.E.24)}$$

Or, with the spin eigenstates:

$$A_1=\cos\frac{\theta}{2}\begin{pmatrix}1\\ 0\end{pmatrix}+\sin\frac{\theta}{2}\begin{pmatrix}0\\ 1\end{pmatrix}. \quad \text{(C.5.E.25)}$$

$\langle A_1|\chi_+\rangle=\cos\frac{\theta}{2}$ and $\langle A_1|\chi_-\rangle=\sin\frac{\theta}{2}$.

The, with the spinor properly normalized (10.56), *The Undergraduate Course*:

$$A_1^\dagger A_1=\cos^2\frac{\theta}{2}+\sin^2\frac{\theta}{2}=1. \quad \text{(C.5.E.26)}$$

Fp: "*In this case, we can interpret $cos^2\frac{\theta}{2}$ as the probability that an observation of S_z will yield the result $+\hbar/2$, and $sin^2\frac{\theta}{2}$ as the probability that an observation of S_z will yield the result $-\hbar/2$.*", page 135 *The Undergraduate Course.*

Remark:

The negative eigenvalue, -1:

$$\frac{a}{b}=\frac{-sin\theta}{1+cos\theta}=-\frac{sin\frac{\theta}{2}}{cos\frac{\theta}{2}}. \quad \text{(C.5.E.27)}$$

Consequently, with normalization and neglecting the phase factor:

$$a=-\sin\frac{\theta}{2}$$

and

$$b=\cos\frac{\theta}{2}.$$

The eigenvector with negative eigenvalue is:

$$A_2=\begin{pmatrix}-\sin\frac{\theta}{2}\\ \cos\frac{\theta}{2}\end{pmatrix}. \quad \text{(C.5.E.28)}$$

Or, with the spin eigenstates:

$$A_2=-\sin\frac{\theta}{2}\begin{pmatrix}1\\ 0\end{pmatrix}+\cos\frac{\theta}{2}\begin{pmatrix}0\\ 1\end{pmatrix}. \quad \text{(C.5.E.29)}$$

With the spinor properly normalized (10.56), *The Undergraduate Course*:

$$A_2^\dagger A_2=\sin^2\frac{\theta}{2}+\cos^2\frac{\theta}{2}=1. \quad \text{(C.5.E.30)}$$

How to interpret this? $|c_+|^2$ and $|c_-|^2$ changed position. The conclusion is still the same?

Well, the probability to observe the positive eigenvalue is:

$|\langle\chi_+|A_1\rangle|^2 = \cos^2\frac{\theta}{2}$,

and the probability to observe the negative eigenvalue is:

$|\langle\chi_-|A_2\rangle|^2 = \sin^2\frac{\theta}{2}$.

Exercise 5.5 Normalizing of a spin state. Measurement of S_x, S_y, and S_z. Calculate expectation values

An electron is in the spin-state

$$\chi = A\begin{pmatrix}1-2i\\2\end{pmatrix}$$

in the Pauli representation. 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.

See also exercise 4 of Chapter 10 *The Undergraduate Course,* Fp.

- A:

Normalization of $\chi \rightarrow$

$$\chi^\dagger\chi = 1 = A^2(1+2i \quad 2)\begin{pmatrix}1-2i\\2\end{pmatrix} = A^2.9 \rightarrow A = \pm\frac{1}{3}.$$

So, with the positive value of A and neglect phase ambiguity.

$$\chi = \tfrac{1}{3}(1-2i)\begin{pmatrix}1\\0\end{pmatrix} + \tfrac{2}{3}\begin{pmatrix}0\\1\end{pmatrix}.$$

- A measurement of S_z :

$$\chi = \tfrac{1}{3}\begin{pmatrix}1-2i\\2\end{pmatrix} = c_+\begin{pmatrix}1\\0\end{pmatrix} + c_-\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}c_+\\c_-\end{pmatrix}$$

I express χ in the normalized eigenstates of S_z, Eqs.(5.56) and (5.62):

$$\chi = \tfrac{1}{3}\begin{pmatrix}1-2i\\2\end{pmatrix} = c_+\begin{pmatrix}1\\0\end{pmatrix} + c_-\begin{pmatrix}0\\1\end{pmatrix}.$$

Equate the elements of the column vectors:

$c_+ = \frac{1}{3}(1-2i)$, (C.5.E.31)

and

$c_- = \frac{2}{3}$. (C.5.E.32)

Bottom of page 135, *The Undergraduate Course,*

"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.5.E.24) and (C.5.E.25):

$|\langle\chi|\chi_+\rangle|^2 = |c_+|^2 = \frac{5}{9}$, and

$|\langle\chi|\chi_-\rangle|^2 = |c_-|^2 = \frac{4}{9}$.

- 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,:

$$\chi = \frac{1}{3}\begin{pmatrix} 1-2i \\ 2 \end{pmatrix} = c_{x+}\chi_{x+} + c_{x-}\chi_{x-} = c_{x+}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} + c_{x-}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}. \quad \text{(C.5.E.33)}$$

Now equate the elements of the column vectors:

$$c_{x+} = \frac{1}{3\sqrt{2}}(3-2i)\,, \quad \text{(C.5.E.34)}$$

and

$$c_{x-} = -\frac{1}{3\sqrt{2}}(1+2i)\,. \quad \text{(C.5.E.35)}$$

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.5.E.27):

$$|\langle\chi|\chi_{x+}\rangle|^2 = |c_{x+}|^2 = \frac{13}{18}\,,$$

and with (C.5.E.28):

$$|\langle\chi|\chi_{x-}\rangle|^2 = |c_{x-}|^2 = \frac{5}{18}\,.$$

- The expectation value of S_x :

$$\langle S_x\rangle = \chi^\dagger S_x\chi = \frac{\hbar}{18}(1+2i\ \ 2)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1-2i \\ 2 \end{pmatrix} = \frac{2\hbar}{9}\,.$$

- Next a measurement of S_y :

I express χ in the normalized eigenstates of S_y, see exercise 2,:

$$\chi = \frac{1}{3}\begin{pmatrix} 1-2i \\ 2 \end{pmatrix} = c_{y+}\chi_{y+} + c_{y-}\chi_{y-} = c_{y+}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} + c_{y-}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix}. \quad \text{(C.5.E.36)}$$

Now equate the elements of the column vectors:

$$c_{y+} = \frac{1}{3\sqrt{2}}(1-4i)\,, \quad \text{(C.5.E.37)}$$

and

$$c_{y-} = \frac{\sqrt{2}}{6}. \quad \text{(C.5.E.38)}$$

Bottom of page 135, *The Undergraduate Course*:

"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.31):

$$|\langle\chi|\chi_{y+}\rangle|^2 = |c_{y+}|^2 = \frac{17}{18}\,,$$

and with (C.10.E.32):

$$|\langle\chi|\chi_{y-}\rangle|^2 = |c_{y-}|^2 = \frac{1}{18}\,.$$

- The expectation value of S_y :

$$\langle S_y\rangle = \chi^\dagger S_y\chi = \frac{\hbar}{18}(1+2i\ \ 2)\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1-2i \\ 2 \end{pmatrix} = \frac{4\hbar}{9}\,.$$

Remark: In the exercises 2 and 4 of Chapter 10, *The Undergraduate Course,* I paid attention to phase ambiguity.

Exercise 5.6 The Probability of a measurement of S_y for a given spinor

Consider a spin-1/2 system represented by the normalized spinor

$$\chi = \begin{pmatrix} \cos\alpha \\ [\sin\alpha]e^{i\beta} \end{pmatrix}$$

in the Pauli representation, where α and β are real. 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 5.3:

$$\chi = \begin{pmatrix} \cos\alpha \\ \sin\alpha\ \exp(\mathrm{i}\delta) \end{pmatrix} = c_{y+}\chi_{y+} + c_{y-}\chi_{y-} = c_{y+}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} + c_{y-}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{pmatrix}. \qquad \text{(C.5.E.39)}$$

Now equate the elements of the column vectors:

$$c_{y+} = \frac{1}{\sqrt{2}}(\cos\alpha - \sin\alpha e^{i(\delta+\frac{\pi}{2})}), \qquad \text{(C.5.E.40)}$$

and

$$c_{y-} = \frac{1}{\sqrt{2}}(\cos\alpha + \sin\alpha e^{i(\delta+\frac{\pi}{2})}). \qquad \text{(C.5.E.41)}$$

- The probability

With (C.5.E.41):

$$|\langle\chi|\chi_{y-}\rangle|^2 = |c_{y-}|^2 = 1 - \sin 2\alpha \sin\delta\ . \qquad \text{(C.5.E.42)}$$

Remark:

Now I like to remind the discussion of exercise 4, Chapter 10 *The Undergraduate Course*, 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 to be answered: does it matter setting $\beta = 0$?

Exercise 5.7 The analysis of an electron at rest in an oscillating magnetic field

An electron is at rest in an oscillating magnetic field

$$\boldsymbol{B} = B_0 \cos(\omega t)\, \boldsymbol{e}_z,$$

where B_0 and ω are real positive constants.

(a) Find the Hamiltonian of the system.

The Hamiltonian is given by Eqs.(10.61) and (10.62), *The Undergraduate Course* Ch. 10,

$H = \Omega S_z$, (10.61),

and

$$\Omega = \frac{geB_0\cos(\omega t)}{2m_e} = \Omega_0\cos(\omega t). \qquad \text{(C.5.E.43)}$$

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 5.3, (C.5.E.16).

Schrödinger's equation

$$i\hbar \frac{\partial \chi}{\partial t} = H\chi \qquad \text{(C.5.E.44)}$$

The state vector in Pauli representation

$$\chi = \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix}. \qquad \text{(C.5.E.45).}$$

Plug this state vector in to (C.5.E.44), (10.65) *The Under Graduate Course*:

$$\frac{dc_\pm}{dt} = \mp i \frac{\Omega}{2} c_\pm, \qquad \text{(C.5.E.46)}$$

where Ω is given in (C.5.E.43), a function of time.

The solutions for both differential equations, (C.5.E.46), are

$$c_+(t) = c_+(0)\ \exp[-i \frac{\Omega_0}{2\omega} \sin(\omega t)], \qquad \text{(C.5.E.47)}$$

and

$$c_-(t) = c_-(0)\ \exp[i \frac{\Omega_0}{2\omega} \sin(\omega t)]. \qquad \text{(C.5.E.48)}$$

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)

$$\chi(t=0) = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} c_+(0) \\ c_-(0) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \qquad \text{(C.5.E.49)}$$

Then,

$$c_+(t) = \frac{1}{\sqrt{2}} \exp[-i \frac{\Omega_0}{2\omega} \sin(\omega t)], \qquad \text{(C.5.E.50)}$$

and

$$c_-(t) = \frac{1}{\sqrt{2}} \exp[i \frac{\Omega_0}{2\omega} \sin(\omega t)]. \qquad \text{(C.5.E.51)}$$

- Find the probability that a measurement of S_x yields the result $-\hbar/2$.

To this end I express the state vector $\chi(t)$

$$\chi(t) = \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix} = c_{x+} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} + c_{x-} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}. \qquad \text{(C.5.E.52)}$$

Hence, with (C.5.E.50) and (C.5.E.51),

$$c_{x+} = \cos[\frac{\Omega_0}{2\omega} \sin(\omega t)], \qquad \text{(C.5.E.53)}$$

and

$$c_{x-} = -i \sin[\frac{\Omega_0}{2\omega} \sin(\omega t)]. \qquad \text{(C.5.E.54)}$$

The probability

$$|c_{x-}|^2 = \sin^2[\frac{\Omega_0}{2\omega} \sin(\omega t)]. \qquad \text{(C.5.E.55)}$$

- 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.

$$\langle S_x \rangle = ((c_+(t))^*, \left(c_-(t) \right)^*) \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix}. \qquad \text{(C.5.E.56)}$$

With (C.5.E.50) and (C.5.E.51):

$\langle S_x \rangle = \frac{\hbar}{2}\cos[\frac{\Omega_0}{\omega}\sin(\omega t)]$. (C.5.E.57)

Then, rewrite (C.5.E.55) with (C.5.E.57)

$|c_{x-}|^2 = \frac{1}{2}(1 - \frac{2}{\hbar}\langle S_x \rangle)$. (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 $\frac{\Omega_0}{2\omega} \geq \frac{\pi}{2}$

$B_0 \geq \frac{2m_e\pi\omega}{ge}$.

6 Addition of Angular Momentum(No sections layout)

No sections.

See also chapter 11 of The *Undergraduate Course*, Fp.

For example (6.3)→(11.3), and $J_{1i} \rightarrow L_i$, $J_{2i} \rightarrow S_i$ etc.

On the middle of page 92, Fp mentioned the two alternate groups of mutually commutating operators, similar to those mentioned on page 143 of *The Undergraduate Course.*

Just a reminder: in (6.18) with orbital momentum and angular momentum(spin): $j = l + s$.

In (6.12) – (6.19):

$|j_1, j_2; m_1, m_2\rangle$,

and

$|j_1, j_2; j, m\rangle$,

are the basic kets.

(6.24):

$J_z = J_{1z} + J_{2z}$ and with the results of the operators given in (6.14), (6.15) and (6.19), (6.25) is obtained. Then it follows, given $m \neq m_1 + m_2$, the CGC's(Clebsch-Gordan[4] Coefficients) to be zero.

(6.26):

$j \leq j_1 + j_2$, follows from the implication of the largest possible value of $j = j_1 + j_2$, bottom of page 93. Now,

$j \geq |j_1 - j_2|$. This follows from the fact that there are just $(2j_1 + 1)(2j_2 + 1)$ independent kets. Then,

$\sum_{j=|j_1-j_2|}^{j_1+j_2}(2j + 1) = (2j_1 + 1)(2j_2 + 1)$, (6.27).

Well, as mentioned by Fp, without loss of generality, set $j_1 \geq j_2$, the summation consists of $(2j_2 + 1)$ terms.

The first term in the summation is

[4] Gordan or Gordon?

$2(j_1 - j_2) + 1,$
and the last term in the summation is
$2(j_1 + j_2) + 1.$
The summation in (6.27) is an arithmetic series, so
$\sum_{j=|j_1-j_2|}^{j_1+j_2}(2j+1) = \frac{1}{2}(2j_2+1)[2(j_1-j_2)+1+2(j_1+j_2)+1] = (2j_1+1)(2j_2+1).$

(6.28) is defined to be the normalization condition.
Another one can be found. To this end I use the other completeness relation presented in (6.21) by multiplying $|j_1, j_2; m_1, m_2\rangle$ into (6.21):
$|j_1, j_2; m_1, m_2\rangle = \sum_j \sum_m \langle j_1, j_2; j, m | j_1, j_2; m_1, m_2\rangle |j_1, j_2; j, m\rangle$. (C.6.1)
Then, multiply (C.6.1) with the bra $\langle j_1, j_2; m_1, m_2|$:
$\langle j_1, j_2; m_1, m_2 | j_1, j_2; m_1, m_2\rangle = \sum_j \sum_m |\langle j_1, j_2; j, m | j_1, j_2; m_1, m_2\rangle|^2 = 1,$ (C.6.2)
where
$\langle j_1, j_2; j, m | j_1, j_2; m_1, m_2\rangle$ are the invers CGC's.
At the bottom of page 94 and at the top of page 95, Fp explained the CGC's and inverse CGC's to be identical. This is of importance in discussing the tables presented on the pages 95-97.

6.1 *Intermezzo Notation*

Notation,
referring to *The Undergraduate Course*,
$m_j = m = m_1 + m_2 = m_{s_1} + m_{s_2},$
$m_{s_1} = \pm\frac{1}{2}$ and $m_{s_2} = \pm\frac{1}{2}$,
$-j \le m_j \le j$,
$j = j_1 + j_2 = s_1 + s_2,$
$|s_1 - s_2| \le j \le s_1 + s_2.$
End of Intermezzo.

Let's anticipate an example given by Fp: a two spin one-half system.
For given j, using (6.28):
$m = 1,$
summing over all the possible values of m_1 and m_2, with the constraint $m = m_1 + m_2$, one term remains and leaving out the labels j_1, j_2
$\left|\left\langle \frac{1}{2}, \frac{1}{2} \middle| 1,1 \right\rangle\right|^2 = 1.$ (C.6.3)
$m = 0,$
$\left|\left\langle \frac{1}{2}, -\frac{1}{2} \middle| 1,0 \right\rangle\right|^2 + \left|\left\langle -\frac{1}{2}, \frac{1}{2} \middle| 1,0 \right\rangle\right|^2 = 1.$
$m = -1,$
$\left|\left\langle -\frac{1}{2}, -\frac{1}{2} \middle| 1,-1 \right\rangle\right|^2 = 1.$ (C.6.4)
(6.30):
$J^{\pm}$ represent the raising and lowering operators for total angular momentum.
(6.32):
the "$\pm$" in the right-hand side of (6.31) changes into "$\mp$" using orthonormality by multiplying the right-hand side of (6.31) with $\langle j_1, j_2; m_1, m_2|$

giving the following expression for the first term on the right-hand side of (6.31)
$\langle j_1, j_2; m_1, m_2 | j_1, j_2; m_1' \pm 1, m_2' \rangle = \delta_{m_1 m_1' \pm 1} \delta_{m_2 m_2'}$.
So, in order to contribute
$m_1 = m_1' \pm 1 \rightarrow m_1' = m_1 \mp 1$ and $m_2' = m_2$.
Simarlily for the second term on the right-hand side
$m_2 = m_2' \pm 1 \rightarrow m_2' = m_2 \mp 1$ and $m_1' = m_1$.
Just below the table on top of page 96, Fp writes:
The normalization condition (6.28) implies that the sum of the squares of all the rows and columns of the above table must be unity. This is a bit confusing, since (6.28) is about summing over all the possible values of m_1 and m_2, of which I presented the example of the two-spin one-half system. This means the sum of the squares of the columns. What about the sum of the squares of the rows? This is about summing of all values of j and m . In (C.6.2) this summation has been derived.

Now I will investigate (6.35) to find out about the CGC's.
Reminder: the " $-$ " sign on the left-hand side of (6.32) goes together with the " $+$ " sign on the right-hand side, and vice versa. Just above (6.35), Fp writes: " $m_1 = m_2 = \pm\frac{1}{2}$ *taking the upper/lower sign".* Meaning? I suppose since $m = 0$ is analysed: $m_1 = \pm\frac{1}{2}$ and $m_2 = \mp\frac{1}{2}$.
On the other hand, on the left-hand side of (6.32) in the inner product $m \pm 1$ is obtained.
So, $m_1 = \pm\frac{1}{2}$ and $m_2 = \pm\frac{1}{2}$. Furthermore, $m_1 = m_2$ is confusing. However, by analysing the two spin one-half system the expression: $m_1 = m_2 = \pm\frac{1}{2}$, becomes clear.
In the Intermezzo below, I will summarize and discus the C-G Coefficients for the two spin one-half system.

6.2 Intermezzo the Angular Momentum of Two Spin One-half Systems at rest.

Note: see the above Intermezzo on Notation.
First in (6.32):
$m = m_j$, and $m_i = m_{j_i}$
So :
$j = s_1 + s_2 = 1$, $s_1 = s_2 = \frac{1}{2}$, the constraint $m_j = m = m_1 + m_2$, and $m_1, m_2 = \pm\frac{1}{2}$.
I start with:
$j = 1, m = 1, m_1, m_2 = \frac{1}{2}$.
The left hand side of (6.32), for the upper sign,
$\sqrt{2-2}\left\langle \frac{1}{2}, \frac{1}{2} \middle| 1,2 \right\rangle = 0$,
as it should be: $\left\langle \frac{1}{2}, \frac{1}{2} \middle| 1,2 \right\rangle$ does not exist.
The right hand side of (6.32),for the upper sign, becomes:
$$\sqrt{\frac{3}{4} - \frac{1}{2}\left(-\frac{1}{2}\right)}\left\langle -\frac{1}{2}, \frac{1}{2} \middle| 1,1 \right\rangle + \sqrt{\frac{3}{4} - \frac{1}{2}\left(-\frac{1}{2}\right)}\left\langle \frac{1}{2}, -\frac{1}{2} \middle| 1,1 \right\rangle = 0.$$
What about the coefficients $\left\langle -\frac{1}{2}, \frac{1}{2} \middle| 1,1 \right\rangle$ and $\left\langle \frac{1}{2}, -\frac{1}{2} \middle| 1,1 \right\rangle$?
Well, both coefficients are equal 1.
In fact, J^+ has been used. So, m is "raised by 1. I think this to be meaningless, since m has to

be 1 instead of 2, on the left hand side.
What about J^-?
The left hand side becomes:
$\sqrt{2}\left\langle \frac{1}{2},\frac{1}{2}\middle|1,0\right\rangle$.
The right hand side of (6.32) is 0.
Now ,what to do?
There is just 1 coefficient for the constraint $m = m_1 + m_2 = 1$ and $m_1 = m_2 = \frac{1}{2}$, with (6.22):
$\left\langle \frac{1}{2},\frac{1}{2}\middle|1,1\right\rangle$,
and (6.28)
$|\left\langle \frac{1}{2},\frac{1}{2}\middle|1,1\right\rangle|^2 = 1$.
So,
$\left\langle \frac{1}{2},\frac{1}{2}\middle|1,1\right\rangle = 1.$
Note: this result cannot be obtained with the recursion relations (6.32).
Next,
$m_1 = \frac{1}{2}$, $m_2 = -\frac{1}{2}$ and $m_j = m = 0$,
the upper sign, left hand side of (6.32), resulting into:
$\sqrt{2}\left\langle \frac{1}{2},-\frac{1}{2}\middle|1,1\right\rangle$.
In (6.35), the right hand side, Fp presents this to be $\sqrt{2}\left\langle \frac{1}{2},\frac{1}{2}\middle|1,1\right\rangle$.
Well, for $m = 1$ there is just one possibility: $m_1, m_2 = \frac{1}{2}$,(6.22).
Now, $m_1 = \frac{1}{2}$, $m_2 = -\frac{1}{2}$ and $m = 0$, for the right hand side, the upper sign,
$\left\langle -\frac{1}{2},-\frac{1}{2}\middle|1,0\right\rangle + 0 \cdot \left\langle \frac{1}{2},-\frac{3}{2}\middle|1,0\right\rangle$. (C.6.5)
Again: $m = 0$. Consequently, the bra-parts of $\left\langle -\frac{1}{2},-\frac{1}{2}\middle|1,0\right\rangle$ and $\left\langle \frac{1}{2},-\frac{3}{2}\middle|1,0\right\rangle$ are not correct. The bra's should comply with comply with $m = 0$.
So, the C-G-coefficients are:
$\left\langle \frac{1}{2},-\frac{1}{2}\middle|1,0\right\rangle$, and $\left\langle -\frac{1}{2},\frac{1}{2}\middle|1,0\right\rangle$.
What about the "0" in front of $\left\langle \frac{1}{2},-\frac{3}{2}\middle|1,0\right\rangle$ in (C.6.5)? I assume this "0" to be 1. There is no difference between $\left\langle \frac{1}{2},-\frac{1}{2}\middle|1,0\right\rangle$ and $\left\langle -\frac{1}{2},\frac{1}{2}\middle|1,0\right\rangle$.

Remark 1:
I do have a problem here with the recursion relation:
- the constraint $m = m_1 + m_2$. If $m \neq m_1 + m_2$, the CGC is zero.
- on the other hand, for, i.e., $m = 0$, $m_1 = \frac{1}{2}$ and $m_2 = -\frac{1}{2}$ works.

So, what to choose? I choose: the CGC's to be $\left\langle \frac{1}{2},-\frac{1}{2}\middle|1,0\right\rangle$ and $\left\langle -\frac{1}{2},\frac{1}{2}\middle|1,0\right\rangle$. The recursion relation is not of much help? With (6.22):

$|1,0\rangle = \left\langle \frac{1}{2}, -\frac{1}{2}\middle|1,0\right\rangle |\frac{1}{2}, -\frac{1}{2}\rangle + \left\langle -\frac{1}{2}, \frac{1}{2}\middle|1,0\right\rangle | -\frac{1}{2}, \frac{1}{2}\rangle.$

Then, (6.29):

$|\left\langle \frac{1}{2}, -\frac{1}{2}\middle|1,0\right\rangle|^2 + |\left\langle -\frac{1}{2}, \frac{1}{2}\middle|1,0\right\rangle|^2 = 1,$

and symmetry

$\left\langle \frac{1}{2}, -\frac{1}{2}\middle|1,0\right\rangle = \left\langle -\frac{1}{2}, \frac{1}{2}\middle|1,0\right\rangle = \frac{1}{\sqrt{2}}.$

The zero's in the table at the top of page 96, result from

$m \neq m_1 + m_2$,Fp, bottom of page 95.

Remark 2:

(6.38) should read $\left\langle \frac{1}{2}, \frac{1}{2}\middle|1,1\right\rangle = \left\langle -\frac{1}{2}, -\frac{1}{2}\middle|1,-1\right\rangle = \pm 1$.

The following case:

$j = 1, m = -1, m_1, m_2 = -\frac{1}{2}.$

Similar to the $j = 1, m = 1, m_1, m_2 = \frac{1}{2}$,

$\left\langle -\frac{1}{2}, -\frac{1}{2}\middle|1,-1\right\rangle = 1$,

the result I already presented above.

The remaining case,

$j = 0, m = 0, m_1 = \frac{1}{2}, m_2 = -\frac{1}{2}$ or $m_1 = -\frac{1}{2}, m_2 = +\frac{1}{2}.$

At the top of page 97, Fp presented an easier method to find out about the CGC's:

"The dot product of a row with any other row must be zero. Likewise, for the dot product of a column with any other column."

The result of this approach is presented in the table at page 97.

In (C.6.3)-(C.6.4), I presented the results as obtained from (6.28).

In (C.6.3):

$\left\langle \frac{1}{2}, \frac{1}{2}\middle|1,1\right\rangle = \pm 1,$ and due to the constraint $m = 1 : m_1 = m_2 = +\frac{1}{2}$

Here I shall repeat some of the results already discussed above for the left hand side of (6.35) or the right hand of (6.32).

Again suppressing the j_1 and j_2 labels, with $m = m_1 + m_2$, the summation in (6.31), the upper sign, the " $m_1 = \frac{1}{2}, m_2 = -\frac{1}{2}$ and $m = 0$ " cell(page 95) and the inner product with $\langle m_1, m_2|$:

$\langle m_1, m_2| \sum_{m_1'} \sum_{m_2'} \{\sqrt{j_1(j_1+1) - m_1'(m_1'+1)}\, |m_1'+1, m_2'\rangle +$

$+\sqrt{j_2(j_2+1) - m_2'(m_2'+1)}|m_1', m_2'+1\rangle\}\langle m_1', m_2'|j, m\rangle.$ (C.6.6)

The summation in (C.6.6) is over all possible dummy variables $m_1' = \pm\frac{1}{2}$ and $m_2' = \pm\frac{1}{2}$, with the constraint: $m' = m_1' + m_2'$.

Hence, with the inner product

$\sum_{m_1'} \sum_{m_2'} \{\sqrt{j_1(j_1+1) - m_1'(m_1'+1)}\, \langle m_1, m_2|m_1'+1, m_2'\rangle +$

$+\sqrt{j_2(j_2+1) - m_2'(m_2'+1)}\langle m_1, m_2|m_1', m_2'+1\rangle\}\langle m_1', m_2'|j, m\rangle.$ (C.6.6a)

Keep in mind: the summation is over all possible dummy variables.

The inner product in (C.6.6a) is $\neq 0$ for

$m_1 = m_1' \pm 1 \rightarrow m_1' = m_1 \mp 1$ and $m_2' = m_2$ for the first term in the summation,

and
simarlily for the second term on the right-hand side of (C.6.6a)
$m_2 = m_2' \pm 1 \rightarrow m_2' = m_2 \mp 1$ and $m_1' = m_1$.
So, for the upper sign , (C.6.6.a) results into
$\sqrt{j_1(j_1+1) - m_1(m_1-1)}\langle m_1 - 1, m_2|j,m\rangle +$
$+\sqrt{j_2(j_2+1) - m_2(m_2-1)}\langle m_1, m_2 - 1|j,m\rangle$. (C.6.6b)
Then, for completeness, (6.32) for the upper sign
$\sqrt{j(j+1) - m(m+1)}\langle m_1, m_2|j,m+1\rangle =$
$\sqrt{j_1(j_1+1) - m_1(m_1-1)}\langle m_1 - 1, m_2|j,m\rangle +$
$+\sqrt{j_2(j_2+1) - m_2(m_2-1)}\langle m_1, m_2 - 1|j,m\rangle$,(6.32).

In addition, I will apply the method used in Noordzij(3),page 61.
(6.22), suppressing the j_1 and j_2 labels:
$|j,m\rangle = \sum_{m_1,m_2}\langle m_1, m_2|j,m\rangle\,|m_1,m_2\rangle$, (C.6.7)
where
$\langle m_1, m_2|j,m\rangle$ are the CGC's(C_i).
I shall analyse $j = 1$ and $m = 0$, the case I failed to analyse above.
With (C.6.7), tensor product notation and $m = 0$,
$|1,0\rangle = C_1\,|\frac{1}{2}\rangle \otimes |-\frac{1}{2}\rangle + C_2\,|-\frac{1}{2}\rangle \otimes |\frac{1}{2}\rangle$. (C.6.8)
So, in column representation, e.g.,
$$|\tfrac{1}{2}\rangle \otimes |-\tfrac{1}{2}\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}$$
Next I will operate the lowering operator on $|1,1\rangle$, using (4.55)-(4.56),
$\sqrt{j(j+1) - m(m-1)} = \sqrt{2}$,
$J^-|1,1\rangle = \sqrt{2}|1,0\rangle$, (C.6.9)
and with the chain rule or with J_1^- (operating on m_1) and J_2^-(operating on m_2),
$\sqrt{j_1(j_1+1) - m_1(m_1-1)} = 1$ and $\sqrt{j_2(j_2+1) - m_2(m_2-1)} = 1$,
$J^-|1,1\rangle = J^-\left(|\frac{1}{2}\rangle \otimes |\frac{1}{2}\rangle\right) = |-\frac{1}{2}\rangle \otimes |\frac{1}{2}\rangle + |\frac{1}{2}\rangle \otimes |-\frac{1}{2}\rangle$. (C.6.10)
In (6.10), I made use of the CGC$= 1$ for the first cell in the first column. Consequently, there are two terms at the right hand side of (C.6.10).
Keep in mind, on the left hand side of (C.6.10): $m = 1$.
Combine (C.6.9) and (C.6.10):
$|1,0\rangle = \frac{1}{\sqrt{2}}(|-\frac{1}{2}\rangle \otimes |\frac{1}{2}\rangle) + \frac{1}{\sqrt{2}}(|\frac{1}{2}\rangle \otimes |-\frac{1}{2}\rangle)$. (C.6.11)
Consequently, from (C.6.8) and (C.6.11), the CGC's are:
$C_1 = \frac{1}{\sqrt{2}} = \frac{\sqrt{j_1(j_1+1)-m_1(m_1-1)}}{\sqrt{j(j+1)-m(m-1)}}$ and $C_2 = \frac{1}{\sqrt{2}} = \frac{\sqrt{j_2(j_2+1)-m_2(m_2-1)}}{\sqrt{j(j+1)-m(m-1)}}$.
A bit closer to Fp's approach.
(6.22):
$|1,0\rangle = C_1\,|\frac{1}{2},-\frac{1}{2}\rangle + C_2|-\frac{1}{2},\frac{1}{2}\rangle$. (C.6.12)

Next, use the lowering operator for the $|1,1\rangle$ state
$J^-|1,1\rangle = \sqrt{2}|1,0\rangle$, (C.6.9).
(6.22), suppressing the $j_1 = \frac{1}{2}$ and $j_2 = \frac{1}{2}$ labels:
$|1,1\rangle$ =CGC($|\frac{1}{2},\frac{1}{2}\rangle$). Again with the lowering operator, CGC= 1[5] and with (C.6.9):

$$J^-|1,1\rangle = J_1^-\,|\tfrac{1}{2},\tfrac{1}{2}\rangle + J_2^-\,|\tfrac{1}{2},\tfrac{1}{2}\rangle = |-\tfrac{1}{2},\tfrac{1}{2}\rangle + |\tfrac{1}{2},-\tfrac{1}{2}\rangle = \sqrt{2}|1,0\rangle. \qquad \text{(C.6.13)}$$

With (6.13)

$$|1,0\rangle = \tfrac{1}{\sqrt{2}}|-\tfrac{1}{2},\tfrac{1}{2}\rangle + \tfrac{1}{\sqrt{2}}|\tfrac{1}{2},-\tfrac{1}{2}\rangle\,. \qquad \text{(C.6.14)}$$

Hence, from (C.6.12) and (C.6.14), the CGC's are:
$C_1 = \frac{1}{\sqrt{2}}$ and $C_2 = \frac{1}{\sqrt{2}}$.
This completes my analysis of the two spin one-half system.
Conclusion about the use of the recursion relations I (6.32):
It is not about a straight forward application of these recursion relations to find out about the CGC's, to say the least.
End of Intermezzo.

At the top of page 97 Fp presented an easy way to complete the table at the bottom of page 96: the rows and columns of the table must all be mutually orthogonal. For example, the dot product of a row with any other row must be zero. So, suppressing the j_1 and j_2 labels, with (C.6.1):

$$\langle m_1', m_2'|m_1, m_2\rangle = \delta_{m_1' m_1}\delta_{m_2' m_2} = \langle m_1', m_2'|\{\textstyle\sum_j \sum_m \langle j,m|m_1,m_2\rangle|j,m\rangle\}. \qquad \text{(C.6.8)}$$

Exercises

Exercise 6.1 Calculate the CGC's for adding spin one-half to spin one.

This exercise can also be found in Chapter 11 of *The Undergraduate Course*, Fp.
I will use the advice of Fp to use a table to collect all the possible CGC's.
See the table below. Below the table, the numbers in the table are calculated.

m_1	m_2	1	2	3	4	5	6
1	$1/2$	1	0	0	0	0	0
1	$-1/2$	0	$1/\sqrt{3}$	0	0	$\sqrt{2}/\sqrt{3}$	0
0	$1/2$	0	$\sqrt{2}/\sqrt{3}$	0	0	$-1/\sqrt{3}$	0
0	$-1/2$	0	0	$-1/\sqrt{3}$	0	0	$\sqrt{2}/\sqrt{3}$
-1	$1/2$	0	0	$\sqrt{2}/\sqrt{3}$	0	0	$1/\sqrt{3}$
-1	$-1/2$	0	0	0	1	0	0
$j_1 = 1$ $j_2 = 1/2$	$j =$ $j_1 \pm j_2$	$3/2$	$3/2$	$3/2$	$3/2$	$1/2$	$1/2$
	$m =$	$3/2$	$1/2$	$-1/2$	$-3/2$	$1/2$	$-1/2$

[5] This leads to the result: $|1,1\rangle = |\frac{1}{2},\frac{1}{2}\rangle$. It is about two spaces of states having two identical states.

	m_1+m_2						

I start with the first column[6]: use $m = m_1 + m_2 = 3/2$. Only the first cell does contribute. Consequently, the first cell of the column is equal to 1. The other cells in the first column are zeroes according to (6.29).
The same reasoning applies to the last column and the last row: $m = m_1 + m_2 = -3/2$. The other cells in the last column produce zeroes according to (6.29).
On the basis of $m = m_1 + m_2$, I plug into the other columns the zeroes.

The second(2) column:
$m = m_1 + m_2 = 1/2.$
I need to find the CGC's for: $j = \frac{3}{2}, m = \frac{1}{2}$ and $m_1 = 1, 0;\ m_2 = -\frac{1}{2}, \frac{1}{2}$ respectively.
The second and third cell in the second(2) column. Consequently, I need to find two CGC's. Again I could apply for the tensor- and column vector approach. I will stay close to the approach of this chapter. So, I will use the result of just one CGC in the first(1) column and the lowering operator J^-.
(6.22):

$$|\tfrac{3}{2},\tfrac{1}{2}\rangle = C_1\,|1,-\tfrac{1}{2}\rangle + C_2\,|0,\tfrac{1}{2}\rangle. \qquad \text{(C.6.E.1)}$$

Next, use the lowering operator for the $|\frac{3}{2},\frac{3}{2}\rangle$ state with (4.55)-(4.56):

$$J^-\,|\tfrac{3}{2},\tfrac{3}{2}\rangle = \sqrt{3}\,|\tfrac{3}{2},\tfrac{1}{2}\rangle\,. \qquad \text{(C.6.E.2)}$$

(6.22), suppressing the $j_1 = 1$ and $j_2 = \frac{1}{2}$ labels, gives

$$|\tfrac{3}{2},\tfrac{3}{2}\rangle = \text{CGC}|1,\tfrac{1}{2}\rangle = |1,\tfrac{1}{2}\rangle,$$

where CGC$= 1$, normalization (6.28), the first(1) column of the table above.
With the lowering operator,

$$J^-\,|\tfrac{3}{2},\tfrac{3}{2}\rangle = J_1^-\,|1,\tfrac{1}{2}\rangle + J_2^-\,|1,\tfrac{1}{2}\rangle = \sqrt{2}|0,\tfrac{1}{2}\rangle + |1,-\tfrac{1}{2}\rangle = \sqrt{3}\,|\tfrac{3}{2},\tfrac{1}{2}\rangle. \qquad \text{(C.6.E.3)}$$

From (C.6.E.3):

$$|\tfrac{3}{2},\tfrac{1}{2}\rangle = \tfrac{\sqrt{2}}{\sqrt{3}}|0,\tfrac{1}{2}\rangle + \tfrac{1}{\sqrt{3}}|1,-\tfrac{1}{2}\rangle. \qquad \text{(C.6.E.4)}$$

Hence, from (C.6.E.1) and (C.6.E.4), the CGC's are:

$$C_1 = \tfrac{1}{\sqrt{3}} \text{ and } C_2 = \tfrac{\sqrt{2}}{\sqrt{3}}\,. \qquad \text{(C.6.E.5)}$$

The third(3) column:
$m = m_1 + m_2 = 1/2.$
I need to find the CGC's for: $j = \frac{1}{2}, m = \frac{1}{2}$ and $m_1 = 1{,}0;\ m_2 = -\frac{1}{2}, \frac{1}{2}$.
The same analysis as used above can be applied. A bit more complicated however, since the machinery of the lowering operator works on two terms instead of one. I use the remark made by Fp at the top of page 97: *"…….Likewise for the dot product of a column with any other column*." So, the dot product of the third column with the second column needs to be zero. The only possible way is for the unknown CGC's in the third column to be equal and opposite. The result is presented in the table above.

[6] The numbers of the columns are given in the first row of the table.

The fifth(5) column. I will pay attention to the fourth(4) column later.
It is convenient, not to say, practical to do this. In this way I can make use of the single CGC $= 1$ in the sixth(6) column. In addition, I will use the raising operator.
$m = m_1 + m_2 = -1/2.$
I need to find the CGC's for: $j = \frac{3}{2}, m = -\frac{1}{2}$ and $m_1 = 0, -1;\ m_2 = -\frac{1}{2}, \frac{1}{2}$.
(6.22):

$$|\tfrac{3}{2}, -\tfrac{1}{2}\rangle = C_1\,|0, -\tfrac{1}{2}\rangle + C_2\,|-1, \tfrac{1}{2}\rangle. \qquad \text{(C.6.E.6)}$$

Next, use the raising operator for the $|\frac{3}{2}, -\frac{3}{2}\rangle$ state with (4.55)-(4.56):

$$\sqrt{j(j+1) - m(m+1)} = \sqrt{3}$$

$$J^+\,|\tfrac{3}{2}, -\tfrac{3}{2}\rangle = \sqrt{3}\,|\tfrac{3}{2}, -\tfrac{1}{2}\rangle. \qquad \text{(C.6.E.7)}$$

With J_1^+ (operating on m_1) and J_2^+(operating on m_2),
$\sqrt{j_1(j_1+1) - m_1(m_1+1)} = 1$ and $\sqrt{j_2(j_2+1) - m_2(m_2+1)} = 1,$

$$J^+\,|\tfrac{3}{2}, -\tfrac{3}{2}\rangle = J_1^+\,|-1, -\tfrac{1}{2}\rangle + J_2^+\,|-1, -\tfrac{1}{2}\rangle = \sqrt{2}|0, -\tfrac{1}{2}\rangle + |-1, \tfrac{1}{2}\rangle = \sqrt{3}\,|\tfrac{3}{2}, -\tfrac{1}{2}\rangle, \qquad \text{(C.6.E.8)}$$

Then

$$|\tfrac{3}{2}, -\tfrac{1}{2}\rangle = \tfrac{\sqrt{2}}{\sqrt{3}}|0, -\tfrac{1}{2}\rangle + \tfrac{1}{\sqrt{3}}|-1, \tfrac{1}{2}\rangle. \qquad \text{(C.6.E.9)}$$

Hence, from (C.6.E.6) and (C.6.E.8), the CGC's are:
$C_1 = \frac{\sqrt{2}}{\sqrt{3}}$ and $C_2 = \frac{1}{\sqrt{3}}$.
This result is presented in the fifth column of the table above.

The fourth(4) column.
With the same reasoning as presented for the third column:
So, the dot product of the fifth column with the fourth column needs to be zero. The only possible way is for the unknown CGC's in the fourth column to be equal and opposite. The result is presented in the table above.
This table is also presented on page 147 of *The Undergraduate Course*, Fp.

Exercise 6.2 Calculate the Clebsch-Gordon coefficients (CGC's) for adding spin 1 to spin 1.

I will make use of the Fp table. There are 81 entries and at least 62 zeroes.

m	m_1	m_2	1	2	3	4	5	6	7	8	9
2	1	1	1	0	0	0	0	0	0	0	0
1	1	0	0	$1/\sqrt{2}$	0	0	0	$-1/\sqrt{2}$	0	0	0
0	1	-1	0	0	$1/\sqrt{6}$	0	0	0	$1/\sqrt{2}$	0	$1/\sqrt{3}$
1	0	1	0	$1/\sqrt{2}$	0	0	0	$1/\sqrt{2}$	0	0	0
0	0	0	0	0	$2/\sqrt{6}$	0	0	0	0	0	$-1/\sqrt{3}$
-1	0	-1	0	0	0	$1/\sqrt{2}$	0	0	0	$-1/\sqrt{2}$	0
0	-1	1	0	0	$1/\sqrt{6}$	0	0	0	$-1/\sqrt{2}$	0	$1/\sqrt{3}$
-1	-1	0	0	0	0	$1/\sqrt{2}$	0	0	0	$1/\sqrt{2}$	0
-2	-1	-1	0	0	0	0	1	0	0	0	0
	$j_1 = 1$ $j_2 = 1$	$j_{max} = 2$ $j_{min} = 0$	2	2	2	2	2	1	1	1	0
		m	2	1	0	-1	-2	1	0	-1	0

The first column(1)[7]:
I start with the first column: use $m = m_1 + m_2 = 2$. Consequently, the first cell of the column is equal to 1. The other cells in the first column are zeroes according to (6.29).
The same reasoning applies to the fifth(5) column and the row: $m = m_1 + m_2 = -2$.
The other cells in the last column(5) produce zeroes according to (6.29).
On the basis of $m = m_1 + m_2$, I plug into the other columns the zeroes.

The second column(2):
$m = m_1 + m_2 = 1.$
I need to find the CGC's for: $j = 2, m = 1$ and $m_1 = 1, 0;\ m_2 = 0,1$.
(6.22):
$|2,1\rangle = C_1|1,0\rangle + C_2|0,1\rangle.$ (C.6.E.10)
Next, use the lowering operator for the $|2,2\rangle$ state with (4.55)-(4.56):
$\sqrt{j(j+1) - m(m-1)} = 2$
$J^-|2,2\rangle = 2|2,1\rangle$. (C.6.E.11)
With the lowering operator on (6.22), $|2,2\rangle$, J_1^- (operating on m_1) , J_2^-(operating on m_2) and (C.6.E.11)
$\sqrt{j_1(j_1+1) - m_1(m_1-1)} = \sqrt{2}$ and $\sqrt{j_2(j_2+1) - m_2(m_2-1)} = \sqrt{2}$,
$J^-|2,2\rangle = J_1^-|1,1\rangle + J_2^-|1,1\rangle = \sqrt{2}|0,1\rangle + \sqrt{2}|1,0\rangle = 2|2,1\rangle,$ (C.6.E.12)
Then
$|2,1\rangle = \frac{1}{\sqrt{2}}|0,1\rangle + \frac{1}{\sqrt{2}}|1,0\rangle.$ (C.6.E.13)
Hence, from (C.6.E.10) and (C.6.E.13), the CGC's are:
$C_1 = \frac{1}{\sqrt{2}}$ and $C_2 = \frac{1}{\sqrt{2}}$.
This result is presented in the table above.

The sixth column(6):
$m = m_1 + m_2 = 1.$
I need to find the CGC's for: $j = 1, m = 1$ and $m_1 = 1,0;\ m_2 = 0,1$.
The same analysis as used above can be applied. A bit more complicated, however. I use the remark made by Fp at the top of page 97: *"…….Likewise for the dot product of a column with any other column.*" So, the dot product of the sixth(6) column with the second(2) column needs to be zero. The only possible way is for the unknown CGC's in the sixth column to be equal and opposite. The result is presented in the table above.

The fourth column(4):
$m = m_1 + m_2 = -1.$
I need to find the CGC's for: $j = 2, m = -1$ and $m_1 = 0, -1;\ m_2 = -1,0$.
(6.22):
$|2,-1\rangle = C_1|0,-1\rangle + C_2|-1,0\rangle.$ (C.6.E.14)
Next, use the raising operator for the $|2,-2\rangle$ state with (4.55)-(4.56):
$\sqrt{j(j+1) - m(m+1)} = 2$
$J^+|2,-2\rangle = 2|2,-1\rangle$. (C.6.E.15)
With J_1^+ (operating on m_1) and J_2^+(operating on m_2), using (C.6.E.15)

[7] The numbers of columns are indicated in the first row of the table.

$\sqrt{j_1(j_1+1)-m_1(m_1+1)}=\sqrt{2}$ and $\sqrt{j_2(j_2+1)-m_2(m_2+1)}=\sqrt{2}$,

$J^+|2,-2\rangle = J_1^+|-1,-1\rangle + J_2^+|-1,-1\rangle = \sqrt{2}|0,-1\rangle + \sqrt{2}|-1,0\rangle = 2|2,-1\rangle$, (C.6.E.16)

Then

$|2,-1\rangle = \frac{1}{\sqrt{2}}|0,-1\rangle + \frac{1}{\sqrt{2}}|-1,0\rangle$. (C.6.E.17)

Hence, from (C.6.E.14) and (C.6.E.17), the CGC's are:

$C_1 = \frac{1}{\sqrt{2}}$ and $C_2 = \frac{1}{\sqrt{2}}$.

This result is presented in the table above.

The eighth column(8):

$m = m_1 + m_2 = -1$.

I need to find the CGC's for: $j = 1, m = -1$ and $m_1 = 1,0;\ m_2 = 0,1$.

The same analysis as used above can be applied. A bit more complicated, however. I use the remark made by Fp at the top of page 97: *".....Likewise for the dot product of a column with any other column."* So, the dot product of the eighth(8) column with the fourth(4) column needs to be zero. The only possible way is for the unknown CGC's in the eighth column to be equal and opposite. The result is presented in the table above.

The third column(3):

$m = m_1 + m_2 = 0$.

I need to find the CGC's for: $j = 2, m = 0$ and $m_1 = 1,0,-1;\ m_2 = -1,0,1$.

(6.22):

$|2,0\rangle = C_1|1,-1\rangle + C_2|0,0\rangle + C_3|-1,1\rangle$. (C.6.E.18)

Next, use the raising operator for the $|2,-1\rangle$ state with (4.55)-(4.56):

$\sqrt{j(j+1)-m(m+1)}=\sqrt{6}$,

$J^+|2,-1\rangle = \sqrt{6}|2,0\rangle$. (C.6.E.19)

(C.6.E.17):

$|2,-1\rangle = \frac{1}{\sqrt{2}}|0,-1\rangle + \frac{1}{\sqrt{2}}|-1,0\rangle$.

Now I operate $J^+ = J_1^+ + J_2^+$ on the right hand side of (C.6.E.17).

With J_1^+ (operating on m_1) and J_2^+(operating on m_2),

$\sqrt{j_1(j_1+1)-m_1(m_1+1)}=\sqrt{2}$ and $\sqrt{j_2(j_2+1)-m_2(m_2+1)}=\sqrt{2}$,

and find four expressions, with (C.6.E.19):

$J^+|2,-1\rangle = J_1^+\frac{1}{\sqrt{2}}|0,-1\rangle + J_1^+\frac{1}{\sqrt{2}}|-1,0\rangle + J_2^+\frac{1}{\sqrt{2}}|0,-1\rangle + J_2^+\frac{1}{\sqrt{2}}|-1,0\rangle =$

$|1,-1\rangle + |0,0\rangle + |0,0\rangle + |-1,1\rangle = \sqrt{6}|2,0\rangle$. (C.6.E.20)

Then

$|2,0\rangle = \frac{1}{\sqrt{6}}|1,-1\rangle + \frac{2}{\sqrt{6}}|0,0\rangle + \frac{1}{\sqrt{6}}|-1,1\rangle$. (C.6.E.21)

Hence, with (C.6.E.18) and (C.6.E.21)

$C_1 = \frac{1}{\sqrt{6}}$, $C_2 = \frac{2}{\sqrt{6}}$ and $C_3 = \frac{1}{\sqrt{6}}$.

These results are plugged into the table above.

Now, what about column 7 and 9?

The rules of orthogonality of the columns and rows and in addition normalisation are not that easily applied. Since these rules lead to 6 equations for six unknowns.

I will use instead the raising operator for column 8.

The seventh column(7):
$m = m_1 + m_2 = 0.$
I need to find the CGC's for: $j = 1, m = 0$ and $m_1 = 1,0,-1;\ m_2 = -1,0,1$.
(6.22):
$|1,0\rangle = C_1|1,-1\rangle + C_2|0,0\rangle + C_3|-1,1\rangle.$ (C.6.E.22)
Next, use the lowering operator for the $|1,1\rangle$ state with (4.55)-(4.56):
$\sqrt{j(j+1) - m(m-1)} = \sqrt{2}$
$J^+|1,1\rangle = \sqrt{2}|1,0\rangle$. (C.6.E.23)
Use the results of the sixth column:
$|1,1\rangle = -\frac{1}{\sqrt{2}}|1,0\rangle + \frac{1}{\sqrt{2}}|0,1\rangle.$ (C.6.E.24)
Now I operate $J^- = J_1^- + J_2^-$ on the right hand side of (C.6.E.24).
With J_1^- (operating on m_1) and J_2^-(operating on m_2),
$\sqrt{j_1(j_1+1) - m_1(m_1-1)} = \sqrt{2}$ and $\sqrt{j_2(j_2+1) - m_2(m_2-1)} = \sqrt{2}$,
and find four expressions, with (C.6.E.24):
$J^-|1,1\rangle = J_1^- \frac{-1}{\sqrt{2}}|1,0\rangle + J_1^- \frac{1}{\sqrt{2}}|0,1\rangle + J_2^- \frac{-1}{\sqrt{2}}|1,0\rangle + J_2^- \frac{1}{\sqrt{2}}|0,1\rangle =$
$= -|0,0\rangle + |-1,1\rangle - |1,-1\rangle + |0,0\rangle = \sqrt{2}|1,0\rangle.$ (C.6.E.25)
Then
$|1,0\rangle = \frac{1}{\sqrt{2}}|-1,1\rangle - \frac{1}{\sqrt{2}}|1,-1\rangle.$ (C.6.E.26)
Hence, with (C.6.E.22) and (C.6.E.26)
$C_1 = \frac{1}{\sqrt{2}}$, $C_2 = 0$ and $C_3 = -\frac{1}{\sqrt{2}}$.
These results are plugged into the table above.

The last column(9):
Is there information to calculate the CGC's easily using orthogonality and normalization?
$m = m_1 + m_2 = 0.$
I need to find the CGC's for: $j = 1, m = 0$ and $m_1 = 1,0,-1;\ m_2 = -1,0,1$.
(6.22):
$|1,0\rangle = C_1|1,-1\rangle + C_2|0,0\rangle + C_3|-1,1\rangle.$ (C.6.E.27)
The orthogonality of the columns 7 and 9, leads to the conclusion:
$\frac{1}{\sqrt{2}}C_1 - \frac{1}{\sqrt{2}}C_3 = 0 \rightarrow C_1 = C_3$,
and the orthogonality of the columns 3 and 9
$C_1 = -C_2.$
Furthermore normalization
$C_2 = \pm\sqrt{1 - 2C_1^2}.$
Hence:
$C_1 = C_3 = \frac{1}{\sqrt{3}}$ and $C_2 = -\frac{1}{\sqrt{3}}$.
These results are plugged into the table above.
The raising and lowering operators cannot be applied.

Exercise 6.3 An electron in a hydrogen atom occupies the combined spin and position state.

This exercise is about a central potential. The eigenfunction can be separated into a radial part, $R(r)$, and into a spherical harmonic, $Y_{l,m}$. Take care of the subscripts since this exercise is not about stationary electrons. It is about orbital - and spin angular momentum. l and m are quantum numbers of orbital motion, m_s the spin angular momentum quantum number. n the quantum number for the radial wave function, the principal quantum number.

The wave function:

$$\psi = R_{21}(r)[\tfrac{1}{\sqrt{3}}Y_{10}(\theta,\varphi)\chi_+ + \tfrac{\sqrt{2}}{\sqrt{3}}Y_{11}(\theta,\varphi)\chi_-], \qquad \text{(C.6.E.28)}$$

where

$n = 2, l = 1$ and $m = 1,0$.

$n > l \geq m_j$, and $m_j = m + m_s$, see Eqs. (11.22) and (11.23) of *The Undergraduate Course.*

$R_{21}(r) = \frac{1}{(2a_0)^{3/2}\sqrt{3}}\frac{r}{a_0}e^{-r/(2a_0)}$, the radial part of the wave function,

$Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta,$

$Y_{11}(\theta,\varphi) = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\varphi},$

$\chi_+ = \begin{pmatrix}1\\0\end{pmatrix}, \chi_- = \begin{pmatrix}0\\1\end{pmatrix}$

and

$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$, the Bohr radius.

a) What values would a measurement of L^2 yield, and with what probabilities?

So,

$L^2\,\psi$? L^2 operates on the orbital part, $Y_{l,m}$ of the wave function ψ, Eq(4.43):

$$L^2\,\psi = 2\hbar^2\psi = 2\hbar^2 R_{21}(r)[\tfrac{1}{\sqrt{3}}Y_{10}(\theta,\varphi)\chi_+ + \tfrac{\sqrt{2}}{\sqrt{3}}Y_{11}(\theta,\varphi)\chi_-]. \qquad \text{(C.6.E.29)}$$

This measurement gives one value for $L^2 \to 2\hbar^2$, with a probability of 1.

b) What values would a measurement of L_z yield, and with what probabilities?

L_z operates on the orbital part, $Y_{l,m}$ of the wave function ψ, Eq.(4.25):

$L_z\,\psi = m\hbar\,\psi.$

Now, there are 2 values of $m \to 1$and 0.

$L_z Y_{1,0} = m\hbar Y_{1,0} = 0$ with probability 1/3,

$L_z Y_{1,1} = (m+1)\hbar Y_{1,1} = \hbar$.

And a measurement of L_z yields ħ with probability 2/3.

c) What values would a measurement of S^2 yield, and with what probabilities?

With Eq.(5.14) and $s = \frac{1}{2}$:

$S^2\chi_\pm = s(s+1)\hbar^2\chi_\pm = \frac{3}{4}\hbar^2\chi_\pm$.

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 Eq.(5.6) :
$S_z\chi_\pm = \pm\frac{1}{2}\hbar\chi_\pm$.
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) *The Undergraduate Course*, Fp:
$J^2\,\psi = j(j+1)\,\hbar^2\psi$.
$j = l + s$,
$|l - s| \leq j \leq l + s$,(6.26).
So, $j = \frac{3}{2}$
$J^2\,\psi = j(j+1)\hbar^2\psi = \frac{15}{4}\hbar^2\psi$,
or, $j = \frac{1}{2}$
$J^2\,\psi = j(j+1)\hbar^2\psi = \frac{3}{4}\hbar^2\psi$.
A measurement of J^2 yield $\frac{3}{4}\hbar^2$ with probability 2/3 and $\frac{15}{4}\hbar^2$ with probability 1/3.

(f) What values would a measurement of J_z yield, and with what probabilities?
With Eq.(11.8) *The Undergraduate Course*, Fp:
$J_z\psi = m_j\hbar\psi$,
and
$m_j = m + m_s$.
In (C.6.E.28):
$m = 0$, $m_s = \frac{1}{2}$, and $m = 1$, $m_s = -\frac{1}{2} \rightarrow m_j = \frac{1}{2}$
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.6.E.28) :
$|\psi|^2 = |R_{2,1}|^2(\frac{1}{3}|Y_{1,0}|^2|\chi_+|^2 + \frac{2}{3}|Y_{1,1}|^2|\chi_-|^2 - \frac{2}{3}Y_{1,0}^*Y_{1,1}\chi_+^*\chi_- - \frac{2}{3}Y_{1,1}^*Y_{1,0}\chi_-^*\chi_+)$. (C.6.E.30)
Using normalization and orthogonalization (C.6.E.30) becomes:
$|\psi|^2 = |R_{2,1}|^2(\frac{1}{3}|Y_{1,0}|^2 + \frac{2}{3}|Y_{1,1}|^2)$. (C.6.E.31)
Now plug the expression for the spherical harmonics, Eqs. (8.92) and (8.91), *The Undergraduate Course*, Fp, into (C.6.E.31), then we have:
$|\psi|^2 = |R_{2,1}|^2$. Finally, this expression can be written with Eq.(9.67), as: *The Undergraduate Course*, Fp,
$|\psi|^2 = \frac{1}{96\pi a_0^3}(\frac{r}{a_0})^2 e^{-r/a_0}$. (C.6.E.32)
As we see, the probability density does not depend on θ, ϕ .

(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: $|R_{2,1}|^2(\frac{1}{3}|Y_{1,0}|^2|\chi_+|^2)$, given $Y_{1,0} = \sqrt{\frac{3}{4\pi}}$.
This results into the expression given in (C.6.E.32).

Exercise 6.4 Calculate the potential energy for a neutron-proton system

In a low energy neutron-proton system (with zero orbital angular momentum) the potential energy is given by

$$V(\boldsymbol{x}) = V_1(r) + V_2(r)\left(3\frac{(\boldsymbol{\sigma_n}\cdot\boldsymbol{x})(\boldsymbol{\sigma_p}\cdot\boldsymbol{x})}{r^2} - \boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p}\right) + V_3(r)\boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p}, \qquad \text{(C.6.E.33)}$$

where
$r = |\boldsymbol{x}|$, and
$\boldsymbol{\sigma_n}$ denotes the vector of the Pauli matrices of the neutron, and $\boldsymbol{\sigma_p}$ denotes the vector of the Pauli matrices of the proton.
(C.6.E. 33) represents a special potential energy. I have not seen such one before. Well, section 12.10 on the hyperfine structure of *The Undergraduate Course* shows an example, partially, of such a potential energy.

Calculate the potential energy for the neutron-proton system [Hint: Calculate the expectation value of $V(\boldsymbol{x})$ with respect to the overall spin state.]:
(a) in the spin singlet(i.e., spin zero) state:
Table for two spin one-half system, page 97, fourth column

$$|0,0\rangle = \frac{1}{\sqrt{2}}(|\tfrac{1}{2},-\tfrac{1}{2}\rangle - |-\tfrac{1}{2},\tfrac{1}{2}\rangle = \frac{1}{\sqrt{2}}[\binom{1}{0}\binom{0}{1} - \binom{0}{1}\binom{1}{0}] \to \frac{1}{\sqrt{2}}[\binom{1}{0}\otimes\binom{0}{1} - \binom{0}{1}\otimes\binom{1}{0} =$$

$$= \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}, \text{ the overall spin state, } |sing\rangle. \qquad \text{(C.6.E.34)}$$

(b) in the spin triplet(i.e., spin one) state, for comparison I choose the second column of the CGC's Table:

$$|1,0\rangle = \frac{1}{\sqrt{2}}(|\tfrac{1}{2},-\tfrac{1}{2}\rangle + |-\tfrac{1}{2},\tfrac{1}{2}\rangle) \to \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix}, \text{ the overall spin state, } |trip2\rangle.$$

Now, what I call the overall Pauli operators.
I start with $\boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p}$, and construct the tensor product of the Pauli matrices. I will include the unit vectors along the three axis:

$$\begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix} \otimes \begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Operate this 4×4 matrix on the singlet state:

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 2 & 0\\ 0 & 2 & -1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}0\\ 1\\ -1\\ 0\end{pmatrix} = -\frac{3}{\sqrt{2}}\begin{pmatrix}0\\ 1\\ -1\\ 0\end{pmatrix}.$$

Hence, the singlet state is an eigenvector of $\boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p}$. The eigenvalue is -3. This result is also found below with a bit more work.

Operate the 4×4 matrix on the triplet state:

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

Hence, the triplet state is an eigenvector of $\boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p}$. The eigenvalue is 1. This result is also found below with a bit more work.

The next for which I construct the overall operator is $(\boldsymbol{\sigma_n}\cdot\boldsymbol{x})(\boldsymbol{\sigma_p}\cdot\boldsymbol{x})$. I will suppress the unit vectors. So, keep in mind, products like $x\cdot y = 0$, etc.

$$\begin{pmatrix}z & x-iy\\ x+iy & -z\end{pmatrix}\otimes\begin{pmatrix}z & x-iy\\ x+iy & -z\end{pmatrix} = \begin{pmatrix}z^2 & 0 & 0 & x^2-y^2\\ 0 & -z^2 & x^2+y^2 & 0\\ 0 & x^2+y^2 & -z^2 & 0\\ x^2-y^2 & 0 & 0 & z^2\end{pmatrix}.$$

Now, I found the two overall operators for the overall spin states.

Finally, calculate $\langle V(\boldsymbol{x})\rangle$.

Again for comparison I choose the first column of the CGC's Table for the triplet state:

$$|trip1\rangle = \begin{pmatrix}1\\ 0\\ 0\\ 0\end{pmatrix}. \qquad \text{(C.6.E.34a)}$$

a) The spin singlet state.

$\langle V(\boldsymbol{x})\rangle = \langle sing|V(\boldsymbol{x})|sing\rangle$**,** and (C.6.E.34).

I calculate the expectation value for the various elements of $V(\boldsymbol{x})$ in (C.6.E.33).

- $V_1(r) \rightarrow \langle V_1(r)\rangle = V_1(r)$.

Next

- $[V_3(r)-V_2(r)]\,\boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p} \rightarrow [V_3(r)-V_2(r)]\,\langle sing|\boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p}|sing\rangle =$

$$= \frac{1}{2}[V_3(r)-V_2(r)](0,1,-1.0)\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 2 & 0\\ 0 & 2 & -1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}0\\ 1\\ -1\\ 0\end{pmatrix} = -3[V_3(r)-V_2(r)].$$

Finally

- $3V_2(r)\frac{(\boldsymbol{\sigma_n}\cdot\boldsymbol{x})(\boldsymbol{\sigma_p}\cdot\boldsymbol{x})}{r^2} \rightarrow \frac{3V_2(r)}{r^2}\langle sing|(\boldsymbol{\sigma_n}\cdot\boldsymbol{x})(\boldsymbol{\sigma_p}\cdot\boldsymbol{x})|sing\rangle =$

$$= \frac{3V_2(r)}{2r^2}(0,1,-1.0)\begin{pmatrix}z^2 & 0 & 0 & x^2-y^2\\ 0 & -z^2 & x^2+y^2 & 0\\ 0 & x^2+y^2 & -z^2 & 0\\ x^2-y^2 & 0 & 0 & z^2\end{pmatrix}\begin{pmatrix}0\\ 1\\ -1\\ 0\end{pmatrix}.$$

With $r^2 = x^2+y^2+z^2$, this contribution to the expectation value is $3V_2(r)$.

Combining the above results:

$\langle V(\boldsymbol{x})\rangle = V_1(r) - 3V_3(r).$ (C.6.E.35)

The same result as found below.

b)The spin triplet state.

$\langle V(\boldsymbol{x})\rangle = \langle trip1|V(\boldsymbol{x})|trip1\rangle$**,** and (C.6.E.34a).

I calculate the expectation value for the various elements of $V(\boldsymbol{x})$ in (C.6.E.33).

- $V_1(r) \rightarrow \langle V_1(r)\rangle = V_1(r)$.

Next

- $[V_3(r) - V_2(r)]\,\boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p} \rightarrow [V_3(r) - V_2(r)]\,\langle trip1|\boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p}|trip1\rangle =$

$$= [V_3(r) - V_2(r)](1,0,0.0)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = [V_3(r) - V_2(r)].$$

Finally

- $3V_2(r)\frac{(\boldsymbol{\sigma_n}\cdot\boldsymbol{x})(\boldsymbol{\sigma_p}\cdot\boldsymbol{x})}{r^2} \rightarrow \frac{3V_2(r)}{r^2}\langle trip1|(\boldsymbol{\sigma_n}\cdot\boldsymbol{x})(\boldsymbol{\sigma_p}\cdot\boldsymbol{x})|trip1\rangle =$

$$= \frac{3V_2(r)}{r^2}(1,0,0.0)\begin{pmatrix} z^2 & 0 & 0 & x^2-y^2 \\ 0 & -z^2 & x^2+y^2 & 0 \\ 0 & x^2+y^2 & -z^2 & 0 \\ x^2-y^2 & 0 & 0 & z^2 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \frac{3z^2V_2(r)}{r^2}.$$

Combining the results for the $|trip1\rangle$ state:

$$\langle V(\boldsymbol{x})\rangle = \langle trip1|V(\boldsymbol{x})|trip1\rangle = V_1(r) - V_2(r)\left[1 - \frac{3z^2}{r^2}\right] + V_3(r).$$

The same result as found below.

Just curious: what result is found for $|trip2\rangle$? Leaving out the details, the result is:

$$\langle V(\boldsymbol{x})\rangle = \langle trip2|V(\boldsymbol{x})|trip2\rangle = V_1(r) - V_2(r)\left[1 - \frac{6z^2}{r^2}\right] + V_3(r).$$

Without the details

$$\langle V(\boldsymbol{x})\rangle = \langle trip3|V(\boldsymbol{x})|trip3\rangle = V_1(r) - V_2(r)\left[1 - \frac{6z^2}{r^2}\right] + V_3(r)$$

For the triplet's I found a dependency on z^2.

Exercise 6.4 Summary and observations

-A single double ket → a singlet $j = 0, m = 0$.

-A triple of two single kets and one double ket → a triplet $j = 1, m = 1$.

$\left\langle sing\left|\left(3\frac{(\boldsymbol{\sigma_n}\cdot\boldsymbol{x})(\boldsymbol{\sigma_p}\cdot\boldsymbol{x})}{r^2} - \boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p}\right)\right|sing\right\rangle = 0$.

$\langle sing|\boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p}|sing\rangle = -3$.

$\langle trip1,3|(\boldsymbol{\sigma_n}\cdot\boldsymbol{x})(\boldsymbol{\sigma_p}\cdot\boldsymbol{x})|trip1,3\rangle = z^2$.

$\langle trip1,2,3|\boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p}|trip1,2,3\rangle = 1$.

$\langle trip2|(\boldsymbol{\sigma_n}\cdot\boldsymbol{x})(\boldsymbol{\sigma_p}\cdot\boldsymbol{x})|trip2\rangle = 2z^2$.

Below I reproduced the results of Exercise 2 Chapter 11 *The Undergraduate Course.*

I need to obtain: $\langle V(\boldsymbol{x})\rangle$

The vector of the Pauli matrices reads:

$\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$.

Consequently, the inner product of the matrices are:

$\boldsymbol{\sigma_n} \cdot \boldsymbol{\sigma_p} = \sigma_{nx}\sigma_{px} + \sigma_{ny}\sigma_{py} + \sigma_{nz}\sigma_{pz}$. (C.6.E.36)

When we operate $\boldsymbol{\sigma_n} \cdot \boldsymbol{\sigma_p}$ on the singlet state and the triplet state respectively, what will be the result?

Let us start with the singlet state:

$\frac{1}{\sqrt{2}}\left[\binom{0}{1}\binom{1}{0} - \binom{1}{0}\binom{0}{1}\right]$.

With (C.6.E.34):

$(\sigma_{nx}\sigma_{px} + \sigma_{ny}\sigma_{py} + \sigma_{nz}\sigma_{pz})\frac{1}{\sqrt{2}}[\binom{0}{1}\binom{1}{0} - \binom{1}{0}\binom{0}{1}]$.

σ_{nx} operates on the first column of the two column vectors between square brackets. σ_{px} on the second of the product of the two column vectors, etc. With the expressions for the Pauli matrices , the result is:

$\left(\sigma_{nx}\sigma_{px} + \sigma_{ny}\sigma_{py} + \sigma_{nz}\sigma_{pz}\right)\frac{1}{\sqrt{2}}\left[\binom{0}{1}\binom{1}{0} - \binom{1}{0}\binom{0}{1}\right] = -\frac{3}{\sqrt{2}}\left[\binom{0}{1}\binom{1}{0} - \binom{1}{0}\binom{0}{1}\right]$.

Hence, the singlet state is an eigenvector of $\boldsymbol{\sigma_n} \cdot \boldsymbol{\sigma_p}$. The eigenvalue is -3 .

Now with the triplet state. There are three triplet states. I choose one:

$\left(\sigma_{nx}\sigma_{px} + \sigma_{ny}\sigma_{py} + \sigma_{nz}\sigma_{pz}\right)\frac{1}{\sqrt{2}}\left[\binom{0}{1}\binom{1}{0} + \binom{1}{0}\binom{0}{1}\right]$.

With the expressions for the Pauli matrices:

$\left(\sigma_{nx}\sigma_{px} + \sigma_{ny}\sigma_{py} + \sigma_{nz}\sigma_{pz}\right)\frac{1}{\sqrt{2}}\left[\binom{0}{1}\binom{1}{0} + \binom{1}{0}\binom{0}{1}\right] =$

$=(1 + 1 - 1)\frac{1}{\sqrt{2}}[\binom{0}{1}\binom{1}{0} + \binom{1}{0}\binom{0}{1}]$.

Hence, the triplet state is an eigenvector of $\boldsymbol{\sigma_n} \cdot \boldsymbol{\sigma_p}$ **.** The eigenvalue is 1.

What about $\langle\frac{(\boldsymbol{\sigma_1}\cdot\boldsymbol{r})(\boldsymbol{\sigma_1}\cdot\boldsymbol{r})}{r^2}\rangle$?

$\boldsymbol{\sigma_n} \cdot \boldsymbol{x} = \sigma_{1x}x + \sigma_{1y}y + \sigma_{1z}z$. (C.6.E.37)

So,

$(\boldsymbol{\sigma_n} \cdot \boldsymbol{x})\left(\boldsymbol{\sigma_p} \cdot \boldsymbol{x}\right) = (\sigma_{nx}x + \sigma_{ny}y + \sigma_{nz}z)(\sigma_{px}x + \sigma_{py}y + \sigma_{pz}z)$. (C.6.E.38)

Now calculate $\langle V(\boldsymbol{x})\rangle$.

ad (a) The spin singlet state as given by Eq.(11.75), *The Undergraduate Course:*

Hence, in general we have to find out about:

$\chi^{\dagger}V(\boldsymbol{x})\chi$.

Now:

$\chi = \frac{1}{\sqrt{2}}[\binom{0}{1}\binom{1}{0} - \binom{1}{0}\binom{0}{1}]$, $\chi^{\dagger} = \frac{1}{\sqrt{2}}[\binom{0}{1}\binom{1}{0} - \binom{1}{0}\binom{0}{1}]^{\dagger}$,

and $V(\boldsymbol{x})$ is given by (C.6.E.33).

We already calculated:

$(\sigma_{nx}\sigma_{px} + \sigma_{ny}\sigma_{py} + \sigma_{nz}\sigma_{pz})\frac{1}{\sqrt{2}}\left[\binom{0}{1}\binom{1}{0} - \binom{1}{0}\binom{0}{1}\right] = -\frac{3}{\sqrt{2}}[\binom{0}{1}\binom{1}{0} - \binom{1}{0}\binom{0}{1}]$.

The easy part of the job:

$\langle V_1\rangle = V_1$,

and ,

$(-V_2 + V_3)\boldsymbol{\sigma_n} \cdot \boldsymbol{\sigma_p}\frac{1}{\sqrt{2}}\left[\binom{0}{1}\binom{1}{0} - \binom{1}{0}\binom{0}{1}\right] = -(-V_2 + V_3)\frac{3}{\sqrt{2}}[\binom{0}{1}\binom{1}{0} - \binom{1}{0}\binom{0}{1}]$.

For the expectation value of the easy part we find:

$$-3\,(-V_2+V_3)+V_1\,. \qquad \text{(C.6.E.39)}$$

In addition we must operate (C.6.E.38) on the singlet state. Instead of 3 , we have to find the result of 9 operators given in (C.6.E.38) 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:

$$\left[\binom{0}{1}\binom{1}{0}-\binom{1}{0}\binom{0}{1}\right]^{\dagger}(\sigma_{nx}x+\sigma_{ny}y+\sigma_{nz}z)(\sigma_{px}x+\sigma_{py}y+\sigma_{pz}z)\left[\binom{0}{1}\binom{1}{0}-\binom{1}{0}\binom{0}{1}\right]. \qquad \text{(C.6.E.40)}$$

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.6.E.39) gives us for the expectation value, including the factor $\frac{3V_2}{\sqrt{2}\sqrt{2}r^2}$, :

$\langle V(r)\rangle = V_1 - 3V_3\,.$

ad(b) I choose the spin triplet state as given by Eq.(11.74), *The Undergraduate Course*, the Pauli representation:

$\chi=\binom{1}{0}\binom{1}{0}$ and $\chi^{\dagger}=[\binom{1}{0}\binom{1}{0}]^{\dagger}$.

Again we have to calculate

$\chi^{\dagger}V(\boldsymbol{x})\chi\,.$

I start with, what I called the easy part of the job:

$\langle V_1\rangle = V_1\,,$

and

$(-V_2+V_3)\chi^{\dagger}\boldsymbol{\sigma_n}\cdot\boldsymbol{\sigma_p}\chi\,.$

Then

$$(-V_2+V_3)[\binom{1}{0}\binom{1}{0}]^{\dagger}\left(\sigma_{nx}\sigma_{px}+\sigma_{ny}\sigma_{py}+\sigma_{nz}\sigma_{pz}\right)\binom{1}{0}\binom{1}{0}=(-V_2+V_3)\,. \qquad \text{(C.6.E.41)}$$

So for the easy part of the job we find:

$$V_1-V_2+V_3\,. \qquad \text{(C.6.E.42)}$$

In addition we have to calculate:

$$[\binom{1}{0}\binom{1}{0}]^{\dagger}(\sigma_{nx}x+\sigma_{ny}y+\sigma_{nz}z)(\sigma_{px}x+\sigma_{py}y+\sigma_{pz}z)\binom{1}{0}\binom{1}{0}, \qquad \text{(C.6.E.43)}$$

where I neglected $\frac{3V_2}{r^2}$ in (C.6.E.41).

The result of (C.11.E.43) is, $\frac{3V_2}{r^2}$ included,

$$3V_2\frac{z^2}{r^2}\,. \qquad \text{(C.6.E.44)}$$

The expectation value of the potential energy for the triplet $\chi=\binom{1}{0}\binom{1}{0}$ is, combining (C.6.E.42) and (C.6.E.44):

$\langle V(\boldsymbol{x})\rangle = V_1 - V_2(1-\frac{3z^2}{r^2}) + V_3\,.$

Exercise 6.5 Consider two electrons in a spin singlet state, $|sing\rangle$, (i.e., spin zero) state

a) If a measurement of the spin of one(1) of the electrons show that it is in the state with $S_z \equiv S_{z1} = \frac{\hbar}{2}$, what is the probability that a measurement of the z-component of the spin of the other(2) electron yields $S_z \equiv S_{z2} = \frac{\hbar}{2}$?

Subscripts 1 and 2 are used for convenience.

$S_z = \frac{\hbar}{2}$ is short hand for the eigenvalue of the spin operator, $S_z = \frac{\hbar}{2}\sigma_z$, to be $\frac{\hbar}{2}$.

The spin singlet state $|j,m\rangle = |0,0\rangle$, table page 97:

$$|A\rangle = \frac{1}{\sqrt{2}}\left(|\tfrac{1}{2},-\tfrac{1}{2}\rangle - |-\tfrac{1}{2},\tfrac{1}{2}\rangle\right) = \frac{1}{\sqrt{2}}[\binom{1}{0}_1 \otimes \binom{0}{1}_2 - \binom{0}{1}_1 \otimes \binom{1}{0}_2]. \qquad \text{(C.6.E.45)}$$

This problem can be found in Chapter 11 Exercise 3 of *The Undergraduate Course, Fp.* There I had some trouble to deal with this problem.

Eq.(5.4):

$S_z|\tfrac{1}{2},\pm\tfrac{1}{2}\rangle = \pm\tfrac{1}{2}\hbar|\tfrac{1}{2},\pm\tfrac{1}{2}\rangle$.

Now use (5.4) with (C.6.E.45):

$$S_{z1}\frac{1}{\sqrt{2}}[\binom{1}{0}_1 \otimes \binom{0}{1}_2 - \binom{0}{1}_1 \otimes \binom{1}{0}_2] = \frac{\hbar}{2\sqrt{2}}[\binom{1}{0}_1 \otimes \binom{0}{1}_2 + \binom{0}{1}_1 \otimes \binom{1}{0}_2], \qquad \text{(C.6.E.46)}$$

and a triplet appears on the right hand side of (C.6.E.46).

Consequently, the conclusion is

$\langle A|S_{z1}|A\rangle = 0$.

Now I cite Susskind, page 174 and 175: "*If the expectation value of a component of the angular momentum operator is zero, it means that the experimental outcome is equally likely to be* $\frac{\hbar}{2}$ *or* $-\frac{\hbar}{2}$*. In other words, the outcome is completely uncertain. Even though we know the exact state vector,* $|sing\rangle$*, we know nothing at all about the outcome of any measurement of any component of either spin.*"

So, the probability that a measurement of the z-component of the spin of the other(2) electron yields $S_z \equiv S_{z2} = \frac{\hbar}{2}$ is ½ .

b) If a measurement of the spin of the spin of one(1) of the electrons show that it is in the state with $S_{y1} = \frac{\hbar}{2}$, what is the probability that a measurement of the x-component of the spin of the other(2) electron yields $S_{x2} = -\frac{\hbar}{2}$?

With the operator S_{y1} and (C.6.E.45):

$$S_{y1}|A\rangle = \frac{i\hbar}{2\sqrt{2}}[\binom{0}{1}_1 \otimes \binom{0}{1}_2 + \binom{1}{0}_1 \otimes \binom{1}{0}_2]. \qquad \text{(C.6.E.47)}$$

Again, the expectation value

$\langle A|S_{y1}|A\rangle = 0$.

So, the probability that a measurement of the x-component of the spin of the other(2) electron yields $S_x \equiv S_{x2} = -\frac{\hbar}{2}$ is ½ .

I could also have calculate the result of the composite operator, leaving out the details:

$\langle A|S_{x2}S_{y1}|A\rangle = 0$,
leading to the same conclusion.

c) Finally, if electron1 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?
Let's return to chapter 6 , section 5, *The Undergraduate Course*-Fp. 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:
$\psi = \frac{1}{\sqrt{2}}(\psi_1\psi_2 - \psi_2\psi_1)$. (C.6.E.48)
This resembles the singlet state (C.6.E.45).
Keep in mind: the products are tensor products.
Now I rephrase the question to be answered: what is the probability for I singlet to represent a triplet? Intuitively: the probability is 0.
Let's look into it.
$\psi_1 = \cos\alpha_1\,\chi_+ + \sin\alpha_1\,e^{i\beta_1}\chi_- \equiv a_1\chi_+ + b_1\chi_-$, (C.6.E.49)
and
$\psi_2 = \cos\alpha_2\,\chi_+ + \sin\alpha_2\,e^{i\beta_2}\chi_- \equiv a_2\chi_+ + b_2\chi_-$. (C.6.E.50)
With (C.6.E.48), (C.6.E.49) and (C.6.E.50) :
$\psi = \frac{(a_2b_1 - a_1b_2)}{\sqrt{2}}[\chi_- \otimes \chi_+ - \chi_+ \otimes \chi_-]$. (C.6.E.51)
Normalization of ψ gives us $|a_2b_1 - a_1b_2| = 1$.
(C.6.E.51) represents a singlet.
Hence, the probability is that the two spin state is a triplet is: 0.

Remarks on Tensor products

The singlet in (C.6.E.45) is a 4 vector:
$$\left[\binom{1}{0}_1 \otimes \binom{0}{1}_2 - \binom{0}{1}_1 \otimes \binom{1}{0}_2\right] = \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0. \end{pmatrix}. \quad \text{(C.6.E.52)}$$
How to deal with an operator like S_z being a 2×2 matrix and the effect on the first and second electron?
Well, for the first electron, the solution is, with $S_z \propto \sigma_z$:
$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \text{(C.6.E.53)}$$
the looked-for 4×4 matrix.
For the second electron:

$$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\otimes\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\end{pmatrix}. \qquad \text{(C.6.E.54)}$$

The analysis for the expectation values, etc, is straight forward.

7. Time-Independent Perturbation Theory

7.1 Introduction

In this chapter techniques are developed for finding approximate solutions.
See also *The Undergraduate Course Chapter 12*, Fp.
Fp introduced the Hamiltonian
$H = H_0 + H_1$, (7.1),
where
$H_1 \ll H_0$.

7.2 Two-State System

It is about time-independent perturbation theory.
Fp analysed a system in which there are two independent eigenkets of H_0 , represented by (7.2) and (7.3). These eigenkets are $|1\rangle$ and $|2\rangle$, mutually orthonormal and a complete set.
The next step is to solve the modified eigenvalue problem for H, given in (7.1).
Fp made the remark at the bottom of page 101 that the problem can be solved exactly.
How to find the matrix in (7.6)? Let's find out.
I use (7.2)-(7.5) and the definitions (7.7)-(7.9):
Multiply $\langle 1|$ into the left hand side of (7.4), use (7.2)-(7.3), (7.5) and of $\langle i|j\rangle = \delta_{ij}$ $\rightarrow$
$\rightarrow \langle 1|H_0 + H_1|E\rangle = \langle 1|E\rangle\langle 1|H_0 + H_1|1\rangle + \langle 2|E\rangle\langle 1|H_0 + H_1|2\rangle \rightarrow$
$\rightarrow \langle 1|E\rangle\langle 1|H_0|1\rangle + \langle 1|E\rangle\langle 1|H_1|1\rangle + \langle 2|E\rangle\langle 1|H_0|2\rangle + \langle 2|E\rangle\langle 1|H_1|2\rangle \rightarrow$
$\rightarrow \langle 1|E\rangle E_1 + \langle 1|E\rangle e_{11} + 0 + \langle 2|E\rangle e_{12}$. (C.7.1)
Multiply $\langle 2|$ into the left hand side of (7.4), use (7.2)-(7.3) and of $\langle i|j\rangle = \delta_{ij}$ $\rightarrow$
$\langle 2|H_0 + H_1|E\rangle = \langle 1|E\rangle\langle 2|H_0 + H_1|1\rangle + \langle 2|E\rangle\langle 2|H_0 + H_1|2\rangle \rightarrow$
$\rightarrow \langle 1|E\rangle\langle 2|H_0|1\rangle + \langle 1|E\rangle\langle 2|H_1|1\rangle + \langle 2|E\rangle\langle 2|H_0|2\rangle + \langle 2|E\rangle\langle 2|H_1|2\rangle \rightarrow$
$\rightarrow 0 + \langle 1|E\rangle e_{21} + \langle 2|E\rangle E_2 + \langle 2|E\rangle e_{22}$. (C.7.2)
Furthermore, with (7.4)
$\langle 1|H_0 + H_1|E\rangle = E\langle 1|E\rangle$, (C.7.3)
and
$\langle 2|H_0 + H_1|E\rangle = E\langle 2|E\rangle$. (C.7.4)
Equate the right hand side of (C.7.3) with right hand side of (C.7.1)
$E\langle 1|E\rangle = \langle 1|E\rangle E_1 + \langle 1|E\rangle e_{11} + 0 + \langle 2|E\rangle e_{12}$, (C.7.5)
and equate the right hand side of (C.7.4) with (C.7.2)
$E\langle 2|E\rangle = 0 + \langle 1|E\rangle e_{21} + \langle 2|E\rangle E_2 + \langle 2|E\rangle e_{22}$. (C.7.6)
Two equations, written in matrix form
$$\begin{pmatrix}E_1 - E + e_{11} & e_{12}\\ e_{21} & E_2 - E + e_{22}\end{pmatrix}\begin{pmatrix}\langle 1|E\rangle\\ \langle 2|E\rangle\end{pmatrix}=\begin{pmatrix}0\\ 0\end{pmatrix}. \qquad \text{(C.7.7)}$$
Since H_1 is Hermitian:
$e_{12} = {e_{21}}^*$,
and (C.7.7) is identical to (7.6), page 102.

For the special case $e_{11} = e_{22} = 0$, the determinant of this eigenvalue problem:

$$\begin{vmatrix} E_1 - E & e_{12} \\ {e_{12}}^* & E_2 - E \end{vmatrix} = 0, \quad \text{(C.7.8)}$$

a quadratic equation:

$$(E_1 - E)(E_2 - E) - |e_{12}|^2 = 0 \, . \quad \text{(C.7.9)}$$

The two eigenvalues of E , E_1' and E_2' , are given in (7.11),
or

$$E = \frac{1}{2}[(E_1 + E_2) \pm |E_1 - E_2| \sqrt{1 + 4\frac{|e_{12}|^2}{(E_1 - E_2)^2}}] \, . \quad \text{(C.7.10)}$$

Fp presented approximations for the eigen values presented in (C.7.10) considering
$\varepsilon = \frac{|e_{12}|}{|E_1 - E_2|}$, (7.12),
to be a small parameter. The expansion in the parameter ε is given in (7.13).
The eigenvalues E_1' and E_2' are given in (7.14) and (7.15).
Now, what about the coefficients
$\langle 1|E_i' \rangle$,
where $i = 1,2$?
With (C.7.7) and $e_{11} = e_{22} = 0$:

$$\begin{pmatrix} E_1 & e_{12} \\ {e_{12}}^* & E_2 \end{pmatrix} \begin{pmatrix} \langle 1|E_i' \rangle \\ \langle 2|E_i' \rangle \end{pmatrix} = E_i' \begin{pmatrix} \langle 1|E_i' \rangle \\ \langle 2|E_i' \rangle \end{pmatrix} . \quad \text{(C.7.11)}$$

For $i = 1$: two dependent equations, I obtained
$\langle 1|E_1' \rangle = -\frac{e_{12}}{E_1 - E_1'} \langle 2|E_1' \rangle$,
and
$\frac{e_{12}}{E_1 - E_1'} \to \infty$ for $\varepsilon \to 0$.
The other solution is

$$\langle 2|E_1' \rangle = \frac{{e_{12}}^*}{E_1' - E_2} \langle 1|E_1' \rangle \approx \frac{{e_{12}}^*}{E_1 - E_2} \langle 1|E_1' \rangle \, . \quad \text{(C.7.12)}$$

In column vector representation, (7.5), the eigenket is:

$$\langle 1|E_1' \rangle \begin{pmatrix} 1 \\ \frac{{e_{12}}^*}{E_1 - E_2} \end{pmatrix} . \quad \text{(C.7.13)}$$

With normalization, and (7.12) ,

$$|\langle 1|E_1' \rangle|^2 (1 + \varepsilon^2) = 1 \to \langle 1|E_1' \rangle \approx 1 - \frac{1}{2}\varepsilon^2 . \quad \text{(C.7.14)}$$

Then, with (7.5) and (C.7.12)

$$|1\rangle' = \langle 1|E_1' \rangle |1\rangle + \langle 1|E_1' \rangle \frac{{e_{12}}^*}{E_1 - E_2} |2\rangle + O(\varepsilon^2) \ldots \quad \text{(C.7.15)}$$

Now for $H_1 \to 0$ and $\varepsilon \to 0$ in (C.7.15) the expression reduces to
$|1\rangle' = |1\rangle$,
and $\langle 1|E_1' \rangle = 1$, as it should[See (C.7.14)].
Hence, (7.16) is found.
Completely similar, (7.17) is obtained.

7.2.1 *Intermezzo* Notation Style Guide

In chapter 1, Dirac notation,
a general operator: ξ,
the general eigenket: $|\xi\rangle$,

and
the general eigenvalue: ξ'.
In this section:
the energy operator: H,
the general eigenket: $|E\rangle$,
and
the general eigenvalue: E.
Now the two-state system and perturbation.
The unperturbed energy operator H_0 and the operator representing the perturbation H_1.
Now the indices conundrum starts.
(7.2): $H_0|1\rangle = E_1|1\rangle \rightarrow H_0|E_1\rangle = E_1|E_1\rangle$.
(7.5): $|E\rangle = \langle E_1|E\rangle|E_1\rangle + \langle E_2|E\rangle|E_2\rangle$.
(7.16): $|1\rangle' \equiv |E_1'\rangle = |E_1\rangle + \frac{{e_{12}}^*}{E_1 - E_2}|E_2\rangle + O(\varepsilon^2)$ …
End of Intermezzo.

7.3 Non-Degenerate perturbation Theory.

In this section systems with more than two energy eigenstates are analysed.
(7.19)-(7.21) are the basic equations.

Remark:
For example the three energy eigenstates. Leaving out the details. The matrix similar to the one in (C.7.7) becomes:

$$\begin{pmatrix} E_1 - E + e_{11} & e_{12} & e_{13} \\ e_{21} & E_2 - E + e_{22} & e_{23} \\ e_{31} & e_{32} & E_3 - E + e_{33} \end{pmatrix} \begin{pmatrix} \langle 1|E\rangle \\ \langle 2|E\rangle \\ \langle 3|E\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

and for a growing number of states, the matrix growth in proportion to say the least.
For that reason Fp searches for a modified version of the unperturbed energy eigenstates.

The eigenstates, $|n\rangle$, of the of the unperturbed Hamiltonian are assumed to be orthogonal:
$\langle m|n\rangle = \delta_{nm}$. (C.7.16)
To obtain (7.22) substitute (7.20) into (7.21):
$(H_0 + H_1)|E\rangle = \sum_k \langle k|E\rangle (H_0 + H_1)|k\rangle$. (C.7.17)
Now multiply (C.7.17) with the bra $\langle m|$:
$\langle m|(H_0 + H_1)|E\rangle = \sum_k \langle k|E\rangle \langle m|(H_0 + H_1)|E\rangle$. (C.7.18)
Select the m-term of (C.7.18):
with (7.19):
$\langle m|H_0|E\rangle = \langle m|E\rangle E_m$,
and with $e_{mk} = \langle m|H_1|k\rangle$, (7.23), and (7.21):
$\langle m|H_1|E\rangle = \langle m|E\rangle e_{mm}$,
and $\langle m|H_1|E\rangle = \sum_{k\neq m} e_{mk} \langle k|E\rangle$.
Then, collecting the results, plugging these into (C.7.18):
$\langle m|(H_0 + H_1)|E\rangle = \langle m|E\rangle E_m + \langle m|E\rangle e_{mm} + \sum_{k\neq m} e_{mk} \langle k|E\rangle$. (C.7.19)
Multiply (7.20) with the bra $\langle m|$:

$\langle m|(H_0 + H_1)|E\rangle = E\langle m|E\rangle$. (C.7.20)

Subtract (C.7.20) from (C.7.19) and (7.22) is found:

$(E_m + e_{mm} - E)\langle m|E\rangle + \sum_{k\neq m} e_{mk}\langle k|E\rangle = 0$, (7.22).

In (7.24) Fp presented the expansion parameter and introduced a modified version of the nth unperturbed eigenstate.

Then, (7.22) becomes to order ε^2 , with (7.25)-(7.26):

$[E_m - E_n + O(\varepsilon) + E_m \cdot O(\varepsilon)]\langle m|E\rangle + \sum_{k\neq m} e_{mk}\langle k|E\rangle = 0$. (C.7.24)

With

$\langle m|E\rangle = O(\varepsilon)$, in the summation of (C7.24), $\langle k|E\rangle = O(\varepsilon)$ except for $\langle n|E\rangle = 1$ and $e_{mk} = O(\varepsilon)\cdot(E_m - E_k)$,

(C.7.24) becomes up to $O(\varepsilon^2)$:

$(E_m - E_n)\langle m|E\rangle + e_{mn} \cong 0$, (7.29),

or

$\langle m|E\rangle \cong -\frac{e_{mn}}{E_m - E_n}$, (7.30).

Then Fp obtained (7.31) by substituting (7.30) into (7.22).

Caveat: e_{nn} given in (7.25) is still $O(\varepsilon)$ in (7.31). The latter equation gives the eigenvalue E_n' of the nth energy eigenstate.

Similar to the two-state system of the fore going section, with (7.30), the nth energy eigenstate is given by (7.33) using (7.27) and (C.7.17):

$|n\rangle' = \langle n|E\rangle|n\rangle + \sum_{k\neq n}\frac{e_{kn}}{E_n - E_k}|k\rangle \rightarrow$ (7.33), and (7.33) is properly normalized to $O(\varepsilon^2)$.

See also Mahan, 6.2.

For $n = 2$ the results of the two-state system is obtained.

7.4 Quadratic Stark Effect.

In this section an example of the perturbation theory is presented.

See also Chapter 12 of *The Undergraduate Course.*

A one-electron atom is subjected to a uniform electric field in the positive z-direction.

The unperturbed Hamiltonian is presented in (7.35), the perturbation is given in (7.36).

According to (7.32) of the foregoing section, 7.3, $\Delta E_{n,l,m}$ in (7.37) compares with

$e_{nn} + \sum_{k\neq n}\frac{|e_{kn}|^2}{E_n - E_k}$,(7.32).

In $\Delta E_{n,l,m}$ the indices represent the radial quantum number and the two angular quantum numbers.

Fp. Subsequently derived selection rules for the quantum numbers m and l.

(7.39), $[L_z, z] = 0$, with (7.38):

$[L_z, z] = xp_y z - yp_x z - zxp_y + zyp_x$. (C.7.25)

Furthermore:

$xz = zx, yz = zy$ .and $[p_i, x_j] = i\hbar\delta_{ij}$.

So, in (C.7.25):

$zx \rightarrow xz$,and $zy \rightarrow yz$.

Plug these results into (C.7.25), then

$[L_z, z] = x[p_y, z] + y[z, p_x]$.

With $[p_i, x_j] = i\hbar\delta_{ij}$:

$[L_z, z] = 0$.
Deriving of (7.42) use have been made of:
$[L_z^2, z] = 0$, and, a.o., $L_x[L_x z] = -i\hbar L_x y$.
In the last line of (7.42) the expressions for L_x and L_y have been used.
In the first line of (7.45) commutator brackets should be used, a typo.
To find (7.46) from (7.45) in the reduction process, use has been made of:
$L_z[z, L_z] = 0$.
Evaluating (7.50) keep in mind $|n, l. m\rangle$ is an eigenstate of L^2 with the eigenvalue:
$l(l+1)\hbar^2$.
(7.61) is obtained using: $\sum|i\rangle\langle i| = 1$ and $\langle z^2\rangle = \frac{1}{3}\langle r^2\rangle$.
For the Hydrogen atom with $n = 1$: $\langle r^2\rangle = 3a_0^2$, (9.72) *The Undergraduate Course.*

7.5 Degenerate Perturbation Theory.

In this section the unperturbed Hamiltonian with degenerate energy levels is investigated.
Fp starts with applying non-degenerate perturbation theory.
Besides the unperturbed Hamiltonian with degenerate energy levels, another Hermitian operator L is introduced:
$[H_0, L] = 0$.
On page 108 Fp writes: "In general, Equation (7.70) is not satisfied". How come? According to the selection rules $l = l'$ can happen. So, $\delta_{ll'} = 1$ and the singular terms in (7.67) and (7.68) do not disappear.
In (7.71) $\langle n, k|n, l^{(1)}\rangle$ are the weights of the new eigenstates in terms of the original eigenstates → (7.78).
Reminder: m is not included due to the selection rule $m = m'$.
(7.73) represents the definition of orthogonality.

7.6 Linear Stark Effect

In this section the effect of an electric field on the excited energy levels are examined.
Fp introduced the usual notation for the various states of a hydrogen atom.
The perturbing Hamiltonian is given by (7.36) and (7.81)
$H_1 = e|\boldsymbol{E}|z$.
$n = 2$ is examined.
There are four states to deal with:
$|2,0,0\rangle, |2, 1, 0\rangle, |2, 1, 1\rangle$ and $|2, 1, -1\rangle$. (C.7.26)
Then the perturbation matrix is a 4×4 matrix.
The elements contributing to the perturbation matrix are:
$\langle n, l, m|z|n', l', m'\rangle$.
In section 7.4 the *selection rules* to evaluate the matrix elements not being zero are given:
$m = m'$ and $l = l'$ or $l' = l \pm 1$.
Due to the selection rules only two off diagonal elements of the matrix remains, as shown in (7.83). The diagonal elements are taken to be zero(due to parity, Mahan).

Remark: the integrals of the diagonal elements of the matrix (Hydrogen atom: central potential) contain the product $\sin\theta\cos\theta$ giving zero.

The only matrix element to be evaluated is given by (7.84). For central potentials the integral to be evaluated is, $z = r\cos\theta$:

$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\langle 2,0,0|r\cos\theta|2,1,0\rangle r^2\sin\theta dr d\theta d\phi$,

and with

(8.91), (8.92), (9.66) and (9.67)

the integral→ $3a_0$.

The matrix (7.83) is a block matrix. Consequently, to find the eigenvalues λ_i , two determinants need to be evaluated:

$$\begin{vmatrix} 0-\lambda & 3a_0 \\ 3a_0 & 0-\lambda \end{vmatrix} = 0 ,$$

and

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

Resulting into four eigenvalues:

$\lambda_1 = 3a_0$, $\lambda_2 = -3a_0$, $\lambda_3 = 0$ and $\lambda_4 = 0$.

I did not include $e|\boldsymbol{E}|$ in the eigenvalues.

Now I need to obtain the eigenvectors.

To this end I analyse:

$$\begin{pmatrix} 0 & 3a_0 & 0 & 0 \\ 3a_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \lambda_i \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}. \qquad \text{(C.7.27)}$$

Using simplicity, normalization and orthogonality the eigenvectors given in (7.85)-(7.88) are obtained:

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}\right] \text{ and } \frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}\right] . \qquad \text{(C.7.28)}$$

The resulting four states are obtained with (7.71) and presented in (7.89)-(7.92).

So,

$$|1\rangle = \frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}\right], \qquad \text{(C.7.29)}$$

$$|2\rangle = \frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}\right], \qquad \text{(C.7.30)}$$

$$|3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{(C.7.31)}$$

and

$$|4\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \qquad \text{(C.7.32)}$$

Note: the summation in (7.71) should read $\sum_{k=0,N_n}\langle n,k,m|n,l^{(1)},m\rangle\,|n,k,m)\rangle$?

7.7 Fine Structure

The energy levels of hydrogen-like atoms are considered.
In 12.8 of the *Undergraduate Course* Fp presented the fine structure of Hydrogen. There, two examples are presented for the perturbation of the Hamiltonian: one based on the lowest-order relativistic correction of the kinetic energy and the other of the *spin-orbit coupling.*
In section 5.5, the magnetic moment of spin and orbital motion is presented, (5.44).
Here, in section 7.7, the perturbation is based on the interaction between spin and angular momenta of the outermost electron of a hydrogen-like atom.
The spin-orbit coupling, the perturbation, is presented in (7.100).
As explained by Fp, in the application of the perturbation theory in this section one half of the value given in (7.100) has to be taken.
In chapter 6, Addition of Angular Momentum, there are two groups of operators shown which can be used. This is illustrated by (6.12) –(6.19).
An important remark just above (7.102): *"We know, from section 7.6, that the application of perturbation theory to a degenerate system is greatly simplified if the basis eigenstates of the unperturbed Hamiltonian are also eigenstates of the perturbing Hamiltonian."* Remark: I think the statement relates to section 7.5. Top page 109.
So, the operators used here are given in (6.16)-(6.19), the second group.
The basic equation is presented in (6.22) and the Clebsch-Gordon coefficients are presented as $\sin\alpha$ and $\cos\alpha$, (7.103) and (7.104). These equations represent for a given l, two states: spin up and spin down.
I derive (7.103) and (7.104) applying (6.22) and use the constraint $m = m_1 + m_2$.
(6.22):
$|j,m\rangle = \sum_{m_1,m_2}\langle m_1,m_2|j,m\rangle m_1,m_2\rangle$.
With $j = l + s = l + \frac{1}{2}$, $j_1 = l$, $j_2 = s = \frac{1}{2}$, $m = m_j = m_l + m_s$, and $m_l = m_1$, $m_s = m_2$, $-l \le m_l \le l$ and $m_s = \pm\frac{1}{2}$,
spin up (7.103)
$$|l+\tfrac{1}{2},m\rangle = \langle m-\tfrac{1}{2},\tfrac{1}{2}|l+\tfrac{1}{2},m\rangle\,|m-\tfrac{1}{2},\tfrac{1}{2}\rangle + \langle m+\tfrac{1}{2},-\tfrac{1}{2}|l+\tfrac{1}{2},m\rangle\,|m+\tfrac{1}{2},-\tfrac{1}{2}\rangle.$$
Fp defined:
$\cos\alpha = \langle m-\frac{1}{2},\frac{1}{2}|l+\frac{1}{2},m\rangle$, (7.11),
and
$\sin\alpha = \langle m+\frac{1}{2},-\frac{1}{2}|l+\frac{1}{2},m\rangle$.
Note:
with $m_j = m = l + \frac{1}{2}$,

$m-\frac{1}{2}=l$.
Consequently,
$\cos\alpha=1=\left\langle l,\frac{1}{2}\middle|l+\frac{1}{2},l+\frac{1}{2}\right\rangle$ and $\sin\alpha=\left\langle l+1,-\frac{1}{2}\middle|l+\frac{1}{2},l+\frac{1}{2}\right\rangle=0$.

Using the definitions of $\sin\alpha$ and $\cos\alpha$:
$|l+\frac{1}{2},m\rangle=\cos\alpha\,|m-\frac{1}{2},\frac{1}{2}\rangle+\sin\alpha\,|m+\frac{1}{2},-\frac{1}{2}\rangle$.
What about spin down (7.104)?
$|l-\frac{1}{2},m\rangle=\left\langle m+\frac{1}{2},-\frac{1}{2}\middle|l-\frac{1}{2},m\right\rangle|m-\frac{1}{2},\frac{1}{2}\rangle+\left\langle m-\frac{1}{2},\frac{1}{2}\middle|l+\frac{1}{2},m\right\rangle|m+\frac{1}{2},-\frac{1}{2}\rangle\rightarrow$
$\rightarrow\ |l-\frac{1}{2},m\rangle=\left\langle m+\frac{1}{2},-\frac{1}{2}\middle|l-\frac{1}{2},m\right\rangle|m-\frac{1}{2},\frac{1}{2}\rangle+\cos\alpha\,|m+\frac{1}{2},-\frac{1}{2}\rangle$.
Now:
$\left\langle l+\frac{1}{2},m\middle|l-\frac{1}{2},m\right\rangle=0.$
This results into:
$\sin\alpha=-\left\langle m+\frac{1}{2},-\frac{1}{2}\middle|l-\frac{1}{2},m\right\rangle$.
So, (7.104):
$|l-\frac{1}{2},m\rangle=-\sin\alpha\,|m-\frac{1}{2},\frac{1}{2}\rangle+\cos\alpha\,|m+\frac{1}{2},-\frac{1}{2}\rangle$.
Application of the recursion relations in (6.32) to obtain $\cos\alpha$:
$j=l+s=l+\frac{1}{2}$, $j_1=l$, $j_2=s=\frac{1}{2}$, $m=m_j=m_l+m_s$, and $m_l=m_1$, $m_s=m_2$.

Remark: compare this with the text on pages 113 and 114. There, page 114, the maximum value of m is ½. I consider this to be a typo.

Then, $m_1=m-\frac{1}{2}$ and $m_2=\frac{1}{2}$ (lower sign, meaning the J^- operator I suppose).
In addition, before the application Fp writes: *"(lower sign)".* I assume this remark to apply to the use of (6.32).
Now, (6.32):
$\sqrt{[\left(l+\frac{1}{2}\right)\left(l+\frac{3}{2}\right)-m(m-1)]}\left\langle\left(m-\frac{1}{2}\right),\frac{1}{2}\middle|l+\frac{1}{2},m-1\right\rangle=$
$=\sqrt{[l(l+1)-(m-\frac{1}{2})(m+\frac{1}{2})]}\left\langle\left(m+\frac{1}{2}\right),\frac{1}{2}\middle|l+\frac{1}{2},m\right\rangle+$
$+\sqrt{[\frac{1}{2}\cdot\frac{3}{2}-\frac{1}{2}\cdot\frac{3}{2}]}\left\langle\left(m-\frac{1}{2}\right),\frac{1}{2}\middle|l+\frac{1}{2},m\right\rangle\rightarrow$
$\rightarrow\sqrt{[\left(l+\frac{1}{2}\right)\left(l+\frac{3}{2}\right)-m(m-1)]}\left\langle\left(m-\frac{1}{2}\right),\frac{1}{2}\middle|l+\frac{1}{2},m-1\right\rangle=$
$=\sqrt{[l(l+1)-(m-\frac{1}{2})(m+\frac{1}{2})]}\left\langle\left(m+\frac{1}{2}\right),\frac{1}{2}\middle|l+\frac{1}{2},m\right\rangle.$ (C.7.33)
The expression $\sqrt{[\left(l+\frac{1}{2}\right)\left(l+\frac{3}{2}\right)-m(m-1)]}\left\langle\left(m-\frac{1}{2}\right),\frac{1}{2}\middle|l+\frac{1}{2},m-1\right\rangle=$
$=\sqrt{[l(l+1)-(m-\frac{1}{2})(m+\frac{1}{2})]}\left\langle\left(m+\frac{1}{2}\right),\frac{1}{2}\middle|l+\frac{1}{2},m\right\rangle$, in (C.7.33) is no way near (7.106).

I keep struggling with the recursion relation. Why is that? I am lost in notation?
Let's use the following notation, *The Undergraduate Course*, in (6.32) and consequently in (C.7.33):

$j = l + s = l + \frac{1}{2}$, $j_1 = l$, $j_2 = s = \frac{1}{2}$, $m = m_j = m_l + m_s$, $m_l = m_1$, $m_l \leq |l|$, and $m_s = m_2 = \frac{1}{2}$.

$$\sqrt{[\left(l+\tfrac{1}{2}\right)\left(l+\tfrac{3}{2}\right) - m_j(m_j-1)]}\left\langle m_j - m_s, m_s \middle| l+\tfrac{1}{2}, m_j - 1\right\rangle =$$
$$= \sqrt{[l(l+1) - m_l(m_l+1)]}\left\langle (m_l+1), m_s \middle| l+\tfrac{1}{2}, m_j\right\rangle. \qquad \text{(C.7.33a)}$$

Now , replace m_j by $m_j - 1$ in (C.7.33a), then the "new" m_j becomes the "old" $m_j + 1$:

$$\sqrt{[\left(l+\tfrac{1}{2}\right)\left(l+\tfrac{3}{2}\right) - m_j(m_j+1)]}\left\langle m_j - m_s, m_s \middle| l+\tfrac{1}{2}, m_j\right\rangle =$$
$$= \sqrt{[l(l+1) - m_l(m_l+1)]}\left\langle (m_l+1), m_s \middle| l+\tfrac{1}{2}, m_j + 1\right\rangle. \qquad \text{(C.7.33b)}$$

The next step is to replace $m_l = m_1 = m_j - \frac{1}{2}$, m_j by m; and $m_s = \frac{1}{2}$ in (C.7.33b):

$$\sqrt{[\left(l+\tfrac{1}{2}\right)\left(l+\tfrac{3}{2}\right) - m(m+1)]}\left\langle m - \tfrac{1}{2}, \tfrac{1}{2} \middle| l+\tfrac{1}{2}, m\right\rangle =$$
$$= \sqrt{[l(l+1) - (m-1)(m+1)]}\left\langle \left(m+\tfrac{1}{2}\right), \tfrac{1}{2} \middle| l+\tfrac{1}{2}, m+1\right\rangle, \text{(7.106).}$$

I would have appreciated when Fp had used the notation Of the *Undergraduate Course.*
I continue with (7.106).
Now, (7.106) reduces to (7.107). I did not see that "at a glance".
However, $l(l+1) - \left(m-\frac{1}{2}\right)\left(m+\frac{1}{2}\right) = \left(l+\frac{1}{2}\right)^2 - m^2 = (l+m+\frac{1}{2})(l-m+\frac{1}{2})$.
Furthermore, $\left(l+\frac{1}{2}\right)\left(l+\frac{3}{2}\right) - m(m-1) = (l+1)^2 - \left(m+\frac{1}{2}\right)^2 =$
$= (l+m+\frac{3}{2})(l-m+\frac{1}{2})$,
$(l-m+\frac{1}{2})$ represent the common factor in (7.106)
(7.108) is found by increasing the value of $m_l \leq l$:

$$\left\langle \left(m+\tfrac{1}{2}\right), \tfrac{1}{2} \middle| l+\tfrac{1}{2}, m+1\right\rangle = \sqrt{\tfrac{l+m+3/2}{l+m+5/2}}\left\langle \left(m+\tfrac{3}{2}\right), \tfrac{1}{2} \middle| l+\tfrac{1}{2}, m+2\right\rangle, \qquad \text{(C.7.35)}$$

and substitute this expression into (7.107).
Next Fp considers, page 114, the situation where *" m_l and m both take their maximum values, l and ½, respectively".* The maximum value of m is ½? A typo.
(7.103) and (7.104): the kets on the left hand side are $|j, m_j\rangle \rightarrow m = m_j = m_l + m_s$.
So, I suppose the maximum value of m_s to be ½. So: *" m_l and m_s both take their maximum values, l and ½, respectively".* Note: the use of m_l .
Increasing the value of m_l, (C.7.35)
$m + 2 \rightarrow m + 3 \rightarrow \cdots \rightarrow l + \frac{1}{2} \rightarrow$ the maximum value of $m_j (= m)$.
For example, let $m + 2$, in the right hand side of (7.108), to be the maximum value of $m_j = l + \frac{1}{2}$: set $m + 2 = l + \frac{1}{2} \rightarrow l + m + \frac{5}{2} = l + (m+2) + \frac{1}{2} = 2l + 1$.
Then, with (7.108), in general:

$$\left\langle \left(m-\tfrac{1}{2}\right), \tfrac{1}{2} \middle| l+\tfrac{1}{2}, m\right\rangle = \sqrt{\tfrac{l+m+1/2}{l+m+3/2}}\tfrac{\sqrt{l+m+3/2}}{\sqrt{l+m+5/2}}\tfrac{\sqrt{l+m+5/2}}{\sqrt{\ldots\ldots\ldots\ldots}}\tfrac{\sqrt{\ldots\ldots\ldots\ldots}}{\sqrt{2l+1}}\left\langle l, \tfrac{1}{2} \middle| l+\tfrac{1}{2}, l+\tfrac{1}{2}\right\rangle,$$

and

$\left\langle \left(m-\frac{1}{2}\right),\frac{1}{2}\middle| l+\frac{1}{2},m\right\rangle = \sqrt{\frac{l+m+1/2}{2l+1}}\left\langle l,\frac{1}{2}\middle| l+\frac{1}{2},l+\frac{1}{2}\right\rangle$, (7.109).

Remark: by continuing increasing m_l, $\sqrt{l+m+\frac{1}{2}}$ does not change.

In the Intermezzo below, I demonstrated (7.110) to be the CGC for both the maximum value of m_j and m. The reasoning in the text between (7.109) and (7.110), I do not understand.

Plug (7.110) into (7.109):

$$\left\langle \left(m-\frac{1}{2}\right),\frac{1}{2}\middle| l+\frac{1}{2},m\right\rangle = \sqrt{\frac{l+m+1/2}{2l+1}}. \qquad \text{(C.7.36)}$$

Consequently, with (C.7.36) and (7.105), $\cos\alpha$ is obtained.

7.7.1 *Intermezzo*: The Recursion Relation (6.32) and the table for CGC's.

I had some trouble in deriving (7.106). This was related with notation.

$j = l+s = l+\frac{1}{2}$, $j_1 = l$, $j_2 = s = \frac{1}{2}$, $m = m_j = m_l + m_s$, and $m_l = m_1$, $m_s = m_2 = \frac{1}{2}$.

Now, I will start the construction of the table for CGC's. The CGC to start with is the state with the maximum values of m_1 and m_2, i.e., l and ½ respectively:

$$|l+\tfrac{1}{2},l+\tfrac{1}{2}\rangle = \left\langle l,\frac{1}{2}\middle| l+\frac{1}{2},l+\frac{1}{2}\right\rangle |l,\tfrac{1}{2}\rangle.$$

Since there is just one CGC, $\left\langle l,\frac{1}{2}\middle| l+\frac{1}{2},l+\frac{1}{2}\right\rangle$, in compliance with $m = m_j = m_l + m_s$, then with (6.28):

$$\left|\left\langle l,\frac{1}{2}\middle| l+\frac{1}{2},l+\frac{1}{2}\right\rangle\right|^2 = 1.$$

So,

$$\left\langle l,\frac{1}{2}\middle| l+\frac{1}{2},l+\frac{1}{2}\right\rangle = \pm 1.$$

I choose $+1$. The result presented in (7.110). The CGC$= -1$ differs just a phase factor.

Hence I start the table with:

$$|l+\tfrac{1}{2},l+\tfrac{1}{2}\rangle = \left\langle l,\frac{1}{2}\middle| l+\frac{1}{2},l+\frac{1}{2}\right\rangle |l,\tfrac{1}{2}\rangle = |l,\tfrac{1}{2}\rangle.$$

I will use (6.31).

The lowering operator J^- on $|l+\frac{1}{2},m_j\rangle$ and $m_j = l+\frac{1}{2}$:

$$J^-|l+\tfrac{1}{2},m_j\rangle = \sqrt{[j(j+1)-m_j(m_j-1)]}|j,m_j-1\rangle =$$

$$= \sqrt{[(l+\tfrac{1}{2})\left(l+\tfrac{3}{2}\right)-m_j(m_j-1)]}\,|(l+\tfrac{1}{2}),m_j-1\rangle =$$

$$= \sqrt{[(l+\tfrac{1}{2})\left(l+\tfrac{3}{2}\right)-(l+\tfrac{1}{2})\left((l-\tfrac{1}{2})\right)]}\,|(l+\tfrac{1}{2}),(l-\tfrac{1}{2})\rangle = \sqrt{2l+1}\,|(l+\tfrac{1}{2}),(l-\tfrac{1}{2})\rangle, \qquad \text{(C.7.37)}$$

The right hand side of (6.31), with $J^- = J_1^- + J_2^-$ on $|l,\frac{1}{2}\rangle$

$$\sqrt{l(l+1)-m_l(m_l-1)}|(m_l-1),m_s\rangle + \sqrt{s(s+1)-m_s(m_s-1)}|m_l,m_s-1\rangle =$$

$$= \sqrt{l(l+1)-l(l-1)}\left|\left(l-\tfrac{1}{2}\right),\tfrac{1}{2}\right\rangle + |l,-\tfrac{1}{2}\rangle = \sqrt{2l}\left|\left(l-\tfrac{1}{2}\right),\tfrac{1}{2}\right\rangle + |l,-\tfrac{1}{2}\rangle,$$

(C.7.38)

(C.7.37) , (C.7.38) ,

$$|l+\tfrac{1}{2},(l-\tfrac{1}{2})\rangle = \sqrt{\tfrac{2l}{2l+1}}\,|(l-1),\tfrac{1}{2}\rangle + \tfrac{1}{\sqrt{2l+1}}\,|l,-\tfrac{1}{2}\rangle. \qquad \text{(C.7.39)}$$

In this way I found the two CGC's for the second column in the table below.
Table(incomplete, ….) of CGC's:

m_1	m_2	1	2	3	4	5	6	7	8
l	1/2	1	0	0	0	0	0	0	0
$l-1$	1/2	0	$\cos\alpha_1$	0	0	0	$-\sin\alpha_1$	0	0
l	$-1/2$	0	$\sin\alpha_1$	0	0	0	$\cos\alpha_1$	0	0
$l-2$	1/2	0	0	$\cos\alpha_2$	0	0	0	$-\sin\alpha_2$	0
$l-1$	$-1/2$	0	0	$\sin\alpha_2$	0	0	0	$\cos\alpha_2$	0
….	….	….	….	….	….	….	….	….	….
….	….	0	0	0	….	0	….	….	….
….	….	0	0	0	….	0	0	0	….
$-l$	$-l-1/2$	0	0	0	0	1	0	0	….
$j_1=l$ $j_2=s$	$j=j_1\pm j_2$	$l+1/2$	$l+1/2$	$l+1/2$	$l+1/2$	$l+1/2$	$l-1/2$	$l-1/2$	$l-1/2$
	$m_j=m_1+m_2$	$l+1/2$	$l-1/2$	$l-3/2$	…..	$-l-1/2$	$l-1/2$	$l-3/2$	….

$$|l+\tfrac{1}{2},l-\tfrac{1}{2}\rangle = \cos\alpha_1\,|l-1,\tfrac{1}{2}\rangle + \sin\alpha_1\,|l,-\tfrac{1}{2}\rangle, \qquad \text{(C.7.40)}$$

where I denoted in (C.7.39) $\cos\alpha_1 = \sqrt{\tfrac{2l}{2l+1}}$ and $\sin\alpha_1 = \tfrac{1}{\sqrt{2l+1}}$. These coefficients are shown in the table above. Plug $m = l-\tfrac{1}{2}$ into (7.111)→ $\cos\alpha = \sqrt{\tfrac{2l}{2l+1}}$ and into (7.112)→ $\rightarrow \sin\alpha = \tfrac{1}{\sqrt{2l+1}}$. This demonstrates that the CGC's approach works.

Obviously: $\cos^2\alpha_1 + \sin^2\alpha_1 = 1$.

Next: $\cos\alpha_2$ and $\sin\alpha_2$:

Operate J^- on $|l+\tfrac{1}{2},l-\tfrac{1}{2}\rangle$:

$$J^-\,|l+\tfrac{1}{2},l-\tfrac{1}{2}\rangle = \sqrt{j(j+1)-m(m-1)}\,|l+\tfrac{1}{2},l-\tfrac{3}{2}\rangle =$$

$$= \sqrt{\left(l+\tfrac{1}{2}\right)\left(l+\tfrac{3}{2}\right)-(l-\tfrac{1}{2})(l-\tfrac{3}{2})}\,|l+\tfrac{1}{2},l-\tfrac{3}{2}\rangle = 2\sqrt{l}\,|l+\tfrac{1}{2},l-\tfrac{3}{2}\rangle. \qquad \text{(C.7.41)}$$

Then, with (C.7.40):

$$(J_1^- + J_2^-)\left(\cos\alpha_1\,|l-1,\tfrac{1}{2}\rangle + \sin\alpha_1\,|l,-\tfrac{1}{2}\rangle\right). \qquad \text{(C.7.42)}$$

I evaluate the operators in (C.7.42), resulting in 4 expressions:

$$J_1^-\cos\alpha_1\,|l-1,\tfrac{1}{2}\rangle = \cos\alpha_1\sqrt{l(l+1)-(l-1)(l-2)}\,|l-2,\tfrac{1}{2}\rangle =$$

$$\cos\alpha_1\sqrt{4l-2}\,|l-2,\tfrac{1}{2}\rangle.$$

$$J_2^-\cos\alpha_1\,|l-1,\tfrac{1}{2}\rangle = \cos\alpha_1\sqrt{s(s+1)-\tfrac{1}{2}(-\tfrac{1}{2})}\,|l-\tfrac{1}{2},\tfrac{1}{2}\rangle = \cos\alpha_1\,|l-1,-\tfrac{1}{2}\rangle.$$

$$J_1^-\sin\alpha_1\,|l,-\tfrac{1}{2}\rangle = \sin\alpha_1\sqrt{l(l+1)-l(l-1)}\,|l-1,-\tfrac{1}{2}\rangle = \sin\alpha_1\sqrt{2l}\,|l-1,-\tfrac{1}{2}\rangle.$$

$J_2^- \sin\alpha_1 \,|l,-\frac{1}{2}\rangle = \sin\alpha_1 \sqrt{s(s+1)-(-\frac{1}{2})(-\frac{1}{2}-1)}\,|l,-\frac{3}{2}\rangle = 0.$

So, collecting the results from (C.7.41) and the 4 expressions resulting from (C.7.42):

$$|l+\tfrac{1}{2},l-\tfrac{3}{2}\rangle = \sqrt{\tfrac{2l-1}{2l+1}}|l-2,\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{2l+1}}|l-1,-\tfrac{1}{2}\rangle, \qquad \text{(C.7.43)}$$

where use has been made of $\cos\alpha_1 = \sqrt{\frac{2l}{2l+1}}$ and $\sin\alpha_1 = \frac{1}{\sqrt{2l+1}}$.

Then $\cos\alpha_2 = \sqrt{\frac{2l-1}{2l+1}}$ and $\sin\alpha_2 = \sqrt{\frac{2}{2l+1}}$.

Now, plug $m = l - \frac{3}{2}$ into (7.111) and (7.112):

$\cos\alpha = \sqrt{\frac{2l-1}{2l+1}}$ and $\sin\alpha = \sqrt{\frac{2}{2l+1}}$.

Without the details[8], I found

$$|l+\tfrac{1}{2},l-\tfrac{5}{2}\rangle = \sqrt{\tfrac{2l-2}{2l+1}}|l-3,\tfrac{1}{2}\rangle + \sqrt{\tfrac{3}{2l+1}}|l-2,-\tfrac{1}{2}\rangle. \qquad \text{(C.7.44)}$$

Then, $\cos\alpha_3 = \sqrt{\frac{2l-2}{2l+1}}$ and $\sin\alpha_3 = \sqrt{\frac{3}{2l+1}}$.

I did not plug $\cos\alpha_3$ and $\sin\alpha_3$ into the table above.

Is there a pattern for $\cos\alpha_i$ and $\sin\alpha_i$? There is:

$$\cos\alpha_i = \sqrt{\tfrac{2l-i+1}{2l+1}}, \text{ and } \sin\alpha_i = \sqrt{\tfrac{i}{2l+1}}, \qquad \text{(C.7.45)}$$

where, $\cos\alpha_0 = 1$ and $\sin\alpha_0 = 0$. In this way the first CGC$= 1$, in the table above, is obtained.

There is more. What is the relation of (C.7.45) with $\cos\alpha$ and $\sin\alpha$ given in (7.113) and (7.112) respectively?

Well,

$$\cos\alpha_i = \sqrt{\tfrac{2l-i+1}{2l+1}} = \sqrt{\tfrac{l+l-i+1}{2l+1}} = \sqrt{\tfrac{l+l-i+\frac{1}{2}+\frac{1}{2}}{2l+1}},$$

and $l - i + \frac{1}{2} = m \;\rightarrow \cos\alpha_i = \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}} \rightarrow (7.111).$

$l - i + \frac{1}{2} = m \;\rightarrow i = l - m + \frac{1}{2}$.

Plug the latter result into $\sin\alpha_i$, (C.7.45):

$\sin\alpha_i = \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}} \rightarrow (7.112).$

As it should be.

Two sets of CGC's can be implemented in the table. See the text at the top of page 97. It is about the use of orthonormalization. Another one is for the minimum value of $m_j = -l - 1/2$ and $j = l + 1/2$: the CGC is 1.

The general value of the CGC's (7.111) and (7.112) are needed for the states:
$|l + 1/2, m\rangle$ and $|l - 1/2, m\rangle$,
where $m = m_j$.

[8] The details are presented in Appendix 1.

When completed the table given above, the CGC's can be collected from this table or calculated with (7.111) and (7.112) through substitution of the actual value of m_j.
I developed the table, since I felt insecure applying the recursion relation (6.32) to construct the table presented on page 97. Consequently, I used (6.31) in the exercises 6.1 and 6.2.
In Chapter 6, Fp presented two groups of operators with eigenkets in (6.12)-(6.19). Both are complete sets of eigenkets, spanning their own space of states. I interpreted

$$|l+\tfrac{1}{2}, l+\tfrac{1}{2}\rangle = |l, \tfrac{1}{2}\rangle,$$

the two states, which the two spaces of states (j, m_j) and (m_l, m_s), have in common.
End of Intermezzo.

7.7.2 *Intermezzo* on Lowering and Raising Operators

Some remarks:

$$J^- |l+\tfrac{1}{2}, l+\tfrac{1}{2}\rangle = \sqrt{2l+1}\, |l+\tfrac{1}{2}, l-\tfrac{1}{2}\rangle,$$

$$J^- |l+\tfrac{1}{2}, l-\tfrac{1}{2}\rangle = \sqrt{4l}\, |l+\tfrac{1}{2}, l-\tfrac{3}{2}\rangle,$$

$$J^- |l+\tfrac{1}{2}, l-\tfrac{3}{2}\rangle = \sqrt{6l-3}\, |l+\tfrac{1}{2}, l-\tfrac{5}{2}\rangle,$$

$$J^- |l+\tfrac{1}{2}, l-\tfrac{5}{2}\rangle = \sqrt{8l-8}\, |l+\tfrac{1}{2}, l-\tfrac{7}{2}\rangle.$$

So,

$$(J^-)^4 |l+\tfrac{1}{2}, l+\tfrac{1}{2}\rangle = \sqrt{2l+1}\cdot\sqrt{4l}\cdot\sqrt{6l-3}\cdot\sqrt{8l-8}\, |l+\tfrac{1}{2}, l-\tfrac{7}{2}\rangle.$$

A pattern?
The pattern could be:

$$(J^-)^n\ |l+\tfrac{1}{2}, l+\tfrac{1}{2}\rangle = \prod_{i=1}^{n}[\sqrt{i(2l+1)-i(i-1)}\,]\, |l+\tfrac{1}{2}, l+\tfrac{1}{2}-n\rangle. \qquad \text{(C.7.46)}$$

Let's demonstrate this for

$$J^- |l+\tfrac{1}{2}, l-\tfrac{7}{2}\rangle = \sqrt{\left(l+\tfrac{1}{2}\right)\left(l+\tfrac{3}{2}\right)-(l-\tfrac{7}{2})(l-\tfrac{9}{2})}\, |l+\tfrac{1}{2}, l-\tfrac{9}{2}\rangle =$$

$$= \sqrt{10l-15}\, |l+\tfrac{1}{2}, l+\tfrac{1}{2}-5\rangle = \sqrt{5(2l+1)-4\cdot 5}\, |l+\tfrac{1}{2}, l+\tfrac{1}{2}-5\rangle. \qquad \text{(C.7.47)}$$

So, for $i = 5$ in (C.7.47):

$$J^- |l+\tfrac{1}{2}, l-\tfrac{7}{2}\rangle = \sqrt{i(2l+1)-i(i-1)}\, |l+\tfrac{1}{2}, l+\tfrac{1}{2}-5\rangle.$$

The pattern has been demonstrated.
Note: $n \leq l$.
Now:

$$J^+ |l+\tfrac{1}{2}, -l-\tfrac{1}{2}\rangle = \sqrt{2l+1}\, |l+\tfrac{1}{2}, -l+\tfrac{1}{2}\rangle,$$

$$J^+ |l+\tfrac{1}{2}, -l+\tfrac{1}{2}\rangle = \sqrt{4l}\, |l+\tfrac{1}{2}, -l+\tfrac{3}{2}\rangle, \text{ etc.}$$

A similar pattern as given in (C.7.43) can be obtained for
$(J^+)^n$.
End of *Intermezzo*

Fp found the expression for $\cos\alpha$ using the maximum value of $m_l = l$. With the expression for $\cos\alpha$, Fp presented, in (7.112), $\sin^2\alpha$.

What about the sign of $\sin\alpha$? Fp: *"A careful examination of the recursion relation, Equation (6.32), shows that the plus sign is appropriate."* A careful examination?
Now, with the general expression for the CGC's or the table given above the spin angular functions can be derived.
Fp defines spin angular functions in (7.115). See also Section 11.3 of *The Undergraduate Course:* $\mathcal{Y}_{lm}^{j=l\pm1/2}$. The general wave function is written as:
$\psi_{nlm\pm} = R_{nl}(r)\mathcal{Y}_{lm}^{\pm}$, (7.116).
In (7.117): $\boldsymbol{L}\cdot\boldsymbol{S}$ operates on the ket $|j,m_j\rangle$.
This result is also shown in The Undergraduate Course Chapter 12 , (12.135).
Plug $j = l \pm \frac{1}{2}$ into (7.117)→ (7.118) and (7.119) respectively.
Now , the integral:
$\oint \sin\theta\, d\theta d\varphi (\mathcal{Y}_{lm}^{+})^{\dagger}\boldsymbol{L}\cdot\boldsymbol{S}\,\mathcal{Y}_{lm}^{+} = \oint \sin\theta\, d\theta d\varphi \frac{l\hbar^2}{2}\left\langle l+\frac{1}{2}, m_j \middle| l+\frac{1}{2}, m_j \right\rangle = \frac{l\hbar^2}{2}$,(7.120).
Likewise:
$\oint \sin\theta\, d\theta d\varphi (\mathcal{Y}_{lm}^{-})^{\dagger}\boldsymbol{L}\cdot\boldsymbol{S}\,\mathcal{Y}_{lm}^{-} = -\oint \sin\theta\, d\theta d\varphi \frac{(l+1)\hbar^2}{2}\left\langle l-\frac{1}{2}, m_j \middle| l-\frac{1}{2}, m_j \right\rangle = \frac{(l+1)\hbar^2}{2}$, ... ,(7.121).
Note: the integral in (7.121) comprises the factor $\frac{1}{4\pi}$.
Next, Fp applies degenerate perturbation theory to evaluate the shift in energy, of a state whose wavefunction is $\psi_{nlm\pm}$, due to the spin-orbit Hamiltonian, H_{LS}.
In (7.122) Fp presented the first order energy-shift:
$\Delta E_{nlm\pm} = \int dV (\psi_{nlm\pm})^{\dagger} H_{LS}\psi_{nlm\pm}$, (7.122),
the integral is over all space: $dV = \frac{1}{4\pi} r^2 dr \sin\theta\, d\theta d\varphi$,
and
$H_{LS} = \frac{1}{2m_e{}^2c^2}\frac{1}{r}\frac{dV}{dr}\,\boldsymbol{L}\cdot\boldsymbol{S}$, (7.100) divided by 2 and V is the potential.
$\boldsymbol{L}\cdot\boldsymbol{S}$ operates on the orbital an d spin part of the wave function. This results are presented in (7.123)-(7.125).
Fp applies the results to a sodium atom of which the ground state is written as:
$(1s)^2(2s)^2(2p)^6(3s)$, (7.126).
The superscript represents the number of electrons in a shell. The number in front of s, p, etc. equals the radial quantum number n.
Furthermore: $s \to l = 0, p \to l = 1$. $(3s)$ in (7.126) is given without superscript. I suppose this is about one electron for the $n = 3, l = 0 (m = 0)$ shell.

7.8 Zeeman Effect

Consider a hydrogen-like atom placed in a uniform z-directed field.
The Hamiltonian H_B and magnetic moment $\boldsymbol{\mu}$ are presented in (7.128)-(7.130).
Next Fp assumes
$H_B \ll H_0 + H_{LS}$,
where H_{LS} represents the Hamiltonian of the spin-orbital interaction.
See for this case The Undergraduate Course and my notes(Noordzij).
Fp considers the states with the quantum numbers $j(= l \pm \frac{1}{2})$ and $m(= m_j)$: $|j,m\rangle$.
Then, with (7.37), the first order energy shift is given in (7.131).

The eigenvalue of J_z:
$J_z|j,m\rangle = m\hbar|j,m\rangle$.
I will look into more details for deriving (7.136):
with (7.131) and (7.132)
$\Delta E_{nlm\pm} = \frac{eB}{2m_e}\langle l \pm \frac{1}{2}, m \,|\, J_z + S_z \,|\, l \pm \frac{1}{2}, m\rangle$. (C.7.49)
Then , with the eigenvalue of J_z:
$\Delta E_{nlm\pm} = \frac{eB}{2m_e}(m\hbar + \left\langle l \pm \frac{1}{2}, m\middle|S_z\middle|l \pm \frac{1}{2}, m\right\rangle)$, (7.133).
Next, for the ket $|l \pm \frac{1}{2}, m\rangle$, (7.113) and (7.114) are used, resulting into (7.134), and
$S_z\,|m \pm 1/2, \mp\frac{1}{2}\rangle = \mp\hbar\,|m \pm \frac{1}{2}, \mp\frac{1}{2}\rangle$:
$S_z\,|l \pm \frac{1}{2}, m\rangle = \frac{\hbar}{2}[\pm\sqrt{\frac{l\pm m+\frac{1}{2}}{2l+1}}|m-\frac{1}{2},\frac{1}{2}\rangle - \sqrt{\frac{l\mp m+\frac{1}{2}}{2l+1}}|m+\frac{1}{2},-\frac{1}{2}\rangle]$. (C.7.50)
So, with $\left\langle m \pm \frac{1}{2}, \mp\frac{1}{2}\middle|m \mp \frac{1}{2}, \pm\frac{1}{2}\right\rangle = 0$, (7.134)and (C.7.50):
$[\pm\sqrt{\frac{l\pm m+\frac{1}{2}}{2l+1}}\left\langle m-\frac{1}{2},\frac{1}{2}\right| + \sqrt{\frac{l\mp m+\frac{1}{2}}{2l+1}}\left\langle m+\frac{1}{2},-\frac{1}{2}\right|]\frac{\hbar}{2}\left[\pm\sqrt{\frac{l\pm m+\frac{1}{2}}{2l+1}}|m-\frac{1}{2},\frac{1}{2}\rangle - \sqrt{\frac{l\mp m+\frac{1}{2}}{2l+1}}|m+\frac{1}{2},-\frac{1}{2}\rangle\right] =$
$= \frac{\hbar}{2(2l+1)}\left[\left(l \pm m + \frac{1}{2}\right) - \left(l \mp m + \frac{1}{2}\right)\right] = \pm\frac{m\hbar}{2l+1}$, (7.135) {(12.146)-*Undergraduate*}.
Plug (7.135) into (7.133)→(7.136), the *Lande formula*.
See (12.147) *The Undergraduate Course.*

7.8.1 *Intermezzo* Eigenkets for addition of angular momentum.

Let us look back. *The Undergraduate Course*:
There, Fp formulated similar expressions in terms of wave functions instead of kets.
$\psi^{(2)}_{l+\frac{1}{2},m_l+\frac{1}{2}} = (\frac{l+m_l+1}{2l+1})^{1/2}\psi^{(1)}_{m_l,1/2} + (\frac{l-m_l}{2l+1})^{1/2}\psi^{(1)}_{m_l+1,-1/2}$, (11.47),
where m_l is the orbital quantum number, $-l \le m_l \le l$.
Replace in (11.47), $m_l = m_j - \frac{1}{2} \rightarrow$
$\psi^{(2)}_{l+\frac{1}{2},m_l+1/2} = (\frac{l+m_j+\frac{1}{2}}{2l+1})^{1/2}\psi^{(1)}_{m_j-\frac{1}{2},1/2} + (\frac{l-m_j+\frac{1}{2}}{2l+1})^{1/2}\psi^{(1)}_{m_j+\frac{1}{2},-1/2} \equiv$ in ket notattion
$\equiv |l+\frac{1}{2}, m_j\rangle = (\frac{l+m_j+\frac{1}{2}}{2l+1})^{1/2}\,|m_j-\frac{1}{2},\frac{1}{2}\rangle + (\frac{l-m_j+\frac{1}{2}}{2l+1})^{1/2}\,|m_j+\frac{1}{2},-\frac{1}{2}\rangle$, (7.134).
Keep in mind: in *The Graduate Course* $m = m_j$.
Note in addition, using (11.48):
$l = 1, j = \frac{1}{2} \rightarrow m_j = \pm\frac{1}{2}$, for $m_l = 1 \rightarrow \psi^{(2)}_{l-\frac{1}{2},m_l+1/2} = -\psi^{(1)}_{2,-1/2} \rightarrow 0$ since $l = 1$. Then
(11.47) and (12.144) produce the same eigenstates.
See also Noordzij(2): the table $\psi^{(2)}_{l,s;j,m_j}$.
End of Intermezzo.

The Fp applies this *Lande formula*(7.136) to the sodium atom and looks for the effects of the magnetic field. At the bottom of page 114 Fp presented the ground state of the sodium atom in chemist's notation. Then, it is about the excitation of the 11th electron from $3s$ to higher energy states. The closest (in energy) are the $3p$ states (Fp page 116): the doublet

$(3p_{\frac{1}{2}})$ and quadruplet states $(3p_{\frac{3}{2}})$.
Note: the spin-orbit interaction of this atom is analysed in Section 7.7.
- $(3p)_{3/2}$ state:
$n = 3, l = 1$. The subscript 3/2 : $j = l + s = \frac{3}{2}$.
$m = m_j = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$.
With (7.136), the $+$ sign, I construct the following table, a quadruplet of states:

$m = m_j$	$\Delta E_{nlm+} \cdot \frac{2m_e}{e\hbar B}$
$3/2$	2
$1/2$	$2/3$
$-1/2$	$-2/3$
$-3/2$	-2

- $(3p)_{1/2}$ state:
$n = 3, l = 1$. The subscript 1/2 : $j = l - \frac{1}{2} = \frac{1}{2}$.
$m = m_j = \frac{1}{2}, -\frac{1}{2}$.
With (7.136), the $-$ sign, I construct the following table, a doublet of states:

$m = m_j$	$\Delta E_{nlm-} \cdot \frac{2m_e}{e\hbar B}$
$1/2$	$1/3$
$-1/2$	$-1/3$

Next Fp considered the extreme limit in which the energy shift due to the magnetic field greatly exceeds the shift induced by the spin-orbit effects. The *Paschen-Back limit*.
The energy shift is presented in (7.137), where use have been made of (7.132):
$J_z|n, l, m_j, m_s\rangle = m_j\hbar|n, l, m_j, m_s\rangle$ and $S_z|n, l, m_j, m_s\rangle = m_s\hbar|n, l, m_j, m_s\rangle$.
Then F p applies this result to a sodium atom's six $3p$ states. As shown in Noordzij(2) section 12.8, there are two $3p_{1/2}$ – and four $3p_{3/2}$ states. States resulting from the addition of spin - and orbital angular momentum.
Fp applies an intense magnetic field, the *Paschen-Back* limit. With this intense magnetic field, the $3p$ states are split into five groups(definition?). This is obtained with:
$-\frac{1}{2} \leq m_j \leq \frac{1}{2}$, $-\frac{3}{2} \leq m_j \leq \frac{3}{2}$ and $-\frac{1}{2} \leq m_s \leq \frac{1}{2}$.
Plug this into (7.137), $(m_j + m_s)$, delete double counting and 5 values(groups?) result:
$m_j + m_s = 2, 1, 0, -1,$ and -2 .
Keep in mind: $m_j = m_l + m_s$. However, I suppose m_j no longer to be a constraint. The magnetic Hamiltonian commutes with (6.12)-(6.15) and does not commutes with (6.16)-(6.19). So, m_j is just a sum of $m_l + m_s$. This is due to the external magnetic field. The result: the total angular momentum of the system is no longer conserved?
Looking at the values of $m_j + m_s$, the energy shifts are equally spaced.

Next, Fp discussed the energy-shift induced by the spin-orbit Hamiltonian. It is again about the excitation of the from $3s$ to some higher energy states(Fp page 116): the doublet $(3p_{\frac{1}{2}})$ and quadruplet states $(3p_{\frac{3}{2}})$.

Use has been made of

$\boldsymbol{L}\cdot\boldsymbol{S}$,

given in (7.102) and derived in *The Undergraduate Course, Chapter 11 On the Addition of Angular Momentum.*

$\boldsymbol{L}\cdot\boldsymbol{S}$ can be written as:

$2\cdot\boldsymbol{L}\cdot\boldsymbol{S}=2L_zS_z+2L_xS_x+2L_yS_y=2L_zS_z+\big(L_x+iL_y\big)\big(S_x-iS_y\big)+$

$+\big(L_x-iL_y\big)\big(S_x+iS_y\big)=2L_zS_z+L^+S^-+L^-S^+.$

Now, (7.140) with (7.141):

$\langle\boldsymbol{L}\cdot\boldsymbol{S}\rangle=\langle n,l,m_l,m_s|L_zS_z+(L^+S^-+L^-S^+)/2|n,l,m_l,m_s\rangle=$

$=\langle n,l,m_l,m_s|L_zS_z)|n,l,m_l,m_s\rangle=\hbar^2m_lm_s$.

The energy shift due to spin-orbit interaction, using the expectation value of $\boldsymbol{L}\cdot\boldsymbol{S}$ is presented in (7.142).

Fp applies this result again to a sodium atom of the states just above ground state:

two $3p_{1/2}$ – and four $3p_{3/2}$ states.

The quantum numbers (m_l,m_s), presented by Fp just below (7.142), (1,1/2), (0,1/2), (1,-1/2) or(?) (-1,1/2), (0,-1/2) and (-1,-1/2).

The energy shift:

	$\Delta E_{nlm_lm_s}\propto m_lm_s$	
Highest shift	$1\cdot\frac{1}{2}=\frac{1}{2}$	quartlet
	$0\cdot\frac{1}{2}=0$	quartlet
	$1\cdot\left(-\frac{1}{2}\right)=-\frac{1}{2}$	doublet
	$-1\cdot\frac{1}{2}=-\frac{1}{2}$	doublet
	$0\cdot(-\frac{1}{2})=0$	quartlet
Lowest shift	$-1\cdot\left(-\frac{1}{2}\right)=\frac{1}{2}$	quartlet.

The result of including this interaction is, the energy shifts are no longer equally spaced.

7.9 Hyperfine Structure

It's about the proton of the hydrogen atom and the magnetic moment of the proton.

The magnetic moment of the proton $\ll$ than the magnetic moment of the electron:

$\frac{\mu_p}{\mu_e}\propto\frac{m_e}{m_p}$.

The perturbing Hamiltonian is obtained from the expressions (7.144)-(7.147).

First-order perturbation produces the energy-shift by the expectation value of the perturbing Hamiltonian H_1:

$\langle 0,0,0|H_1|0,0,0\rangle$.

See the first term on the right hand side of (7.37), and

$$|0,0,0\rangle = R_{1,0}Y_{0,0} = \frac{2}{\sqrt{4\pi}}\frac{1}{a_0^{3/2}}e^{-\frac{r}{a_0}} . \quad \text{(C.7.51)}$$

The expectation value is presented in (7.149).

In (7.149):

$$\langle\frac{3(\boldsymbol{S_p}\cdot\boldsymbol{e_r})(\boldsymbol{S_e}\cdot\boldsymbol{e_r})-\boldsymbol{S_p}\cdot\boldsymbol{S_e}}{r^3}\rangle = 0 , \quad \text{(C.7.52)}$$

due to symmetry in the ground state.

To prove this, I need to evaluate, see Exercise 11.3 and Section 12.10 of *The Undergraduate Course*:

$$(\frac{3z^2}{r^2}-1)\frac{1}{r^3} . \quad \text{(C.7.53),}$$

where I used

$$\boldsymbol{e_r} = (\frac{x}{|r|},\frac{y}{|r|},\frac{z}{|r|}) .$$

Set $z = r\cos\theta$ in (7.53). Then (7.52) can be written as:

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\frac{1}{r}(3\cos^2\theta-1)\sin\theta e^{-\frac{2r}{a_0}}\,drd\theta d\phi = 0 .$$

With (C.7.51):

$|\psi_{000}(r=0)|^2 = \frac{1}{\pi a_0^3}$, the energy shift ΔE_{000} (7.150) is obtained.

The results of addition of angular momentum, Chapter 6, for *Two Spin One-Half Particles*:

$s = \frac{1}{2}\pm\frac{1}{2}$, or $|s_p - s_e| \le s \le s_p + s_e$

so there are two states one with $s = 1$ and $m_s = -1,0,1$,

the other with $s = 0$ and $m_s = 0$.

The eigenvalues of S_e^2 and S_p^2 , Equation (5.7):

$$S_e^2\chi_{\pm} = S_p^2\chi_{\pm} = \frac{3}{4}\hbar^2\chi_{\pm}.$$

and $S_z\chi_{\pm} = \pm\frac{1}{2}\hbar\chi_{\pm}$, (5.6).

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_{000} in (7.150), I need to evaluate $\langle\boldsymbol{S_p}\cdot\boldsymbol{S_e}\rangle$.

With (7.152):

$$\langle\boldsymbol{S_p}\cdot\boldsymbol{S_e}\rangle = \frac{1}{2}(\langle S^2\rangle - \langle S_e^2\rangle - \langle S_p^2\rangle). \quad \text{(C.7.54)}$$

For the singlet state:

$$\langle\boldsymbol{S_p}\cdot\boldsymbol{S_e}\rangle = \frac{1}{2}\left(0-\frac{3}{4}\hbar^2-\frac{3}{4}\hbar^2\right) = -\frac{3}{4}\hbar^2, \text{ (7.153).}$$

For the triplet states:

$$\langle\boldsymbol{S_p}\cdot\boldsymbol{S_e}\rangle = \frac{1}{2}\left(2\hbar^2-\frac{3}{4}\hbar^2-\frac{3}{4}\hbar^2\right) = \frac{1}{4}\hbar^2, \text{ (7.154).}$$

For completeness I present the table of Glebsch-Gordon coefficients, see Table on page 97:

		1	2	3	4
m_{sp}	m_{se}	$trip$	$trip$	$trip$	$sing$
$1/2$	$1/2$	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
$s_p = 1/2$ $s_e = 1/2$	$s = s_p + s_e$	1	1	1	0
	$m_s = m_{sp} + m_{se}$	1	0	-1	0

Exercises

Exercise 7.1 The energy-shift for a harmonic oscillator.

Calculate the energy-shift in the ground state of the one-dimensional harmonic oscillator when the perturbation

$V = \lambda x^4$,

is added to the unperturbed Hamiltonian:

$H_0 = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2$.

The properly normalized ground-state wavefunction is:

$\psi(x) = (\frac{m\omega}{\pi\hbar})^{1/4}\exp\left(-\frac{m\omega^2 x^2}{2\hbar}\right)$.

To first order, the energy-shift is defined by (7.37):

$\Delta E = \langle n, l, m, n|H_1|n, l, m\rangle = \langle n, l, m|\lambda x^4|n, l, m\rangle$.

Since the wave function is a continuous function, the following integral needs to be evaluated:

$\Delta E = \int_{-\infty}^{\infty} \psi^* V\psi dx$.

Then, with integration by parts and $\int_{-\infty}^{\infty} e^{-y^2}dy = \sqrt{\pi}$, the result for the energy-shift ΔE:

$\Delta E = \frac{3}{4}\,\lambda(\frac{\hbar}{m\omega^2})^2\frac{1}{\sqrt{\omega}}$.

Note: the integral for ΔE is symmetrical. So, the perturbation produces a first order shift. With a perturbation: $V = \lambda x$, the first order contribution is zero.

Exercise 7.2 The energy-shifts due to the Stark effect.

Calculate the energy-shifts due to the first-order Stark effect in the $n = 3$ state of a hydrogen atom. The perturbing Hamiltonian:

$H_1 = e|\boldsymbol{E}|z = eEr\cos\theta$.

You do need to perform all of the integrals, but you should construct the correct linear combination of states.

Note: I worked on this problem(Noordzij(3), Exercise 6.7)

$n = 3$: there are 9 degenerate orbital states.

Let us sum them up; see Chapters 8 and 9 of *The Undergraduate Course* on orbital motion and central potentials.

I will use the notation $|nlm\rangle$.

$|300\rangle$, $l = 0, m_l = 0$

The radial eigenfunction R_{30}:

$$R_{30} = 2(\tfrac{1}{3})^{3/2} e^{-r/3a_0}\left[1 - \frac{2r}{3a_0} + \frac{2}{27}\left(\frac{r}{a_0}\right)^2\right]. \quad \text{(C.E.7.1)}$$

The spherical harmonic is: $Y_{00} = \frac{1}{\sqrt{4\pi}}$.

Hence the eigenstate $|300\rangle = \frac{1}{\sqrt{\pi}}(\frac{1}{3})^{3/2} e^{-r/3a_0}\left[1 - \frac{2r}{3a_0} + \frac{2}{27}\left(\frac{r}{a_0}\right)^2\right]$. (C.E.7.2)

$|310\rangle, l = 1, m_l = 0.$

The radial eigenfunction R_{31} is :

$$R_{31} = \frac{1}{3}\left(\frac{2}{3}\right)^{\frac{5}{2}} \frac{r}{a_0} e^{-\frac{r}{3a_0}}\left(1 - \frac{r}{6a_0}\right). \quad \text{(C.E.7.3)}$$

The spherical harmonic $Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$.

The eigenstate $|310\rangle = \frac{1}{3}\sqrt{\frac{3}{4\pi}}\left(\frac{2}{3}\right)^{\frac{5}{2}} \frac{r}{a_0} e^{-\frac{r}{3a_0}}\left(1 - \frac{r}{6a_0}\right)\cos\theta$. (C.E.7.4)

$|311\rangle, l = 1, m_l = 1.$

The radial eigenfunction R_{31}, (C.E.7.3).

The spherical harmonic $Y_{11} = \sqrt{\frac{3}{8\pi}}\sin\theta\ e^{i\phi}$.

The eigenstate $|311\rangle = \frac{1}{3}\sqrt{\frac{3}{8\pi}}\left(\frac{2}{3}\right)^{\frac{5}{2}} \frac{r}{a_0} e^{-\frac{r}{3a_0}}\left(1 - \frac{r}{6a_0}\right)\sin\theta\, e^{i\phi}$. (C.E.7.5)

$|31-1\rangle, l = 1, m_l = -1.$

The radial eigenfunction R_{31} , (C.E.7.3).

The spherical harmonic $Y_{1-1} = \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-i\phi}$.

The eigenstate $|31-1\rangle = \frac{1}{3}\sqrt{\frac{3}{8\pi}}\left(\frac{2}{3}\right)^{\frac{5}{2}} \frac{r}{a_0} e^{-\frac{r}{3a_0}}\left(1 - \frac{r}{6a_0}\right)\sin\theta\, e^{-i\phi}$. (C.E.7.6)

$|322\rangle, l = 2, m_l = 2.$

The radial eigenfunction R_{32} is:

$$R_{32} = \frac{1}{81}\sqrt{\frac{8}{15}}(\frac{r}{a_0})^2 e^{-\frac{r}{3a_0}}. \quad \text{(C.E.7.7)}$$

The spherical harmonic $Y_{22} = \frac{3}{4}\sqrt{\frac{5}{6\pi}}\sin^2\theta\, e^{2i\phi}$.

The eigenstate $|322\rangle = \frac{1}{54}\sqrt{\frac{1}{\pi}}(\frac{r}{a_0})^2 \sin^2\theta\, e^{-\frac{r}{3a_0}} e^{2i\phi}$. (C.E.7.8)

$|32-2\rangle, l = 2, m_l = -2.$

The radial eigenfunction is given in (C.E.7.7). The spherical harmonic equals the one given for the state $|322\rangle$, except for the sign of ϕ.

The eigenstate $|32-2\rangle = \frac{1}{54}\sqrt{\frac{1}{\pi}}(\frac{r}{a_0})^2 e^{-\frac{r}{3a_0}} \sin^2\theta\, e^{-2i\phi}$. (C.E.7.9)

$|321\rangle, l = 2, m_l = 1.$

The radial eigenfunction is given by (C.E.7.7).

The spherical harmonic $Y_{21} = 3\sqrt{\frac{5}{24\pi}}\sin\theta\cos\theta\, e^{i\phi}$.

The eigenstate $|321\rangle = \frac{1}{81}\sqrt{\frac{1}{\pi}}(\frac{r}{a_0})^2 e^{-\frac{r}{3a_0}} \sin\theta\cos\theta\, e^{i\phi}$. (C.E.7.10)

$|32-1\rangle, l=2, m_l=-1.$

The radial eigenfunction is given by (C.E.7.7). The spherical harmonic equals the one given for the state $|321\rangle$, except for the sign of ϕ.

The eigenstate $|32-1\rangle = \frac{1}{81}\sqrt{\frac{1}{\pi}}(\frac{r}{a_0})^2 e^{-\frac{r}{3a_0}} \sin\theta\cos\theta\, e^{-i\phi}$. (C.E.7.11)

$|320\rangle, l=2, m_l=0.$

The radial eigenfunction is given by (C.E.7.7).

The spherical harmonic $Y_{20} = \frac{1}{4}\sqrt{\frac{5}{\pi}}[3(\cos\theta)^2 - 1]$.

The eigenstate $|320\rangle = \frac{1}{162}\sqrt{\frac{2}{3\pi}}(\frac{r}{a_0})^2 e^{-\frac{r}{3a_0}}[3(\cos\theta)^2 - 1]$. (C.E.7.12)

So, the 9 degenerate eigenstates are obtained with the same eigenvalue $E_3 = -\frac{E_{Ry}}{9}$.

The next step to take to find out about the Stark effect on these degenerated states.

What does the matrix looks like?

Fp: *You do need to perform all of the integrals, but you should construct the correct linear combination of states.*

So, I need to find the matrix elements,(7.53):

$\langle n,l,m|z|n',l',m'\rangle$,

where

$z = r\cos\theta$.

Fp, page 106, (7.102): *The matrix elements vanish unless* $l = l' = 0$ *or* $l' = l \pm 1$. *The selection rule……It follows from (7.53) that the matrix elements vanishes by symmetry when* $l = l' = 0$. It is about integrating $\int_0^{\pi} \cos\theta d\theta = 0$. In addition, a lot of zero's results from $\int_0^{2\pi} e^{\pm ik\phi} = 0$, for $k \geq 1$ and $\{k \in \mathbb{N}\}$. Furthermore: $k = m + m'$.

These selection rules are the tools to construct the matrix as diagonalized as possible. So, it is about the arrangement of the basis vectors. However, some trial and error are involved (Mahan, page 169). It is about the choice of sequence of basis vectors (Styer, page 216).

Let us start with constructing the following Table E7.2, which resembles the character of the matrix→Block Matrix:

0	$\|300\rangle$	$\|310\rangle$	$\|320\rangle$	$\|311\rangle$	$\|321\rangle$	$\|31-1\rangle$	$\|32-1\rangle$	$\|322\rangle$	$\|32-2\rangle$
$\|300\rangle$	0	A							
$\|310\rangle$	A	0	B						
$\|320\rangle$		B	0						
$\|311\rangle$				0					
$\|321\rangle$					0	C			
$\|31-1\rangle$					C	0			
$\|32-1\rangle$							0		

$\|322\rangle$								0	
$\|32-2\rangle$									0

Table E7.2 The matrix elements for $n = 3$ of the Hydrogen atom.

The nonzero off diagonal elements are indicated by Capitals representing the integrals $\langle n, l, m|z|n', l', m'\rangle$ with use of (C.E.7.1)-(C.E.7.12).
The energy shifts are:
$A = \langle 300|eEr\cos\theta\,|310\rangle = 3\sqrt{6}eEa_0$,
$B = \langle 310|eEr\cos\theta\,|320\rangle = 3\sqrt{3}\,eEa_0$,
and
$C = \langle 32-1|eEr\cos\theta\,|31-1\rangle = \frac{9}{2}\,eEa_0$.
The table E7.2 shows the character of a Block Matrix of which the eigen values are:
$0, \pm 9eEa_0$ and $\pm\frac{9}{2}\,eEa_0$.

Exercise 7.3 The energy-shift due to relativistic mass increase.

The Hamiltonian of the valence electron in a hydrogen-like atom can be written as

$$H = \frac{p^2}{2m} + V(r) - \frac{p^4}{8m_e^3c^2}\,. \qquad \text{(C.E.7.13)}$$

Here, the final term on the right-hand side of (C.E.7.13) is the first-order correction in the Hamiltonian H_1 due to the electron's relativistic mass increase. Treating H_1 as a small perturbation, deduce that it causes an energy-shift in the energy eigenstate characterized by the standard quantum numbers n, l, m of

$$\Delta E_{nlm} = -\frac{1}{2m_ec^2}(E_n^2 - 2E_n\langle V\rangle + \langle V^2\rangle), \qquad \text{(C.E.7.14)}$$

where E_n is the unperturbed energy and α the fine structure constant.
Note(Nz): α does not show up explicitly in (C.E.7.14).

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$$

In *The Undergraduate Course* FP, according to special relativity, derived from the kinetic energy the lowest-order relativistic correction to this energy (12.115).
There Fp presented a result for a Coulomb potential.
In this exercise 7.3, $V(r)$ is not specified.
Now, I need to find the first order correction, completely similar to (12.117):

$$\Delta E_{nlm} = \langle n, l, m|H_1|n, l, m\rangle = -\frac{1}{8m_e^3c^2}\langle n, l, m|p^4|n, l, m\rangle =$$
$$= -\frac{1}{8m_e^3c^2}\langle n, l, m|p^2p^2|n, l, m\rangle. \qquad \text{(C.E.7.15)}$$

For the unperturbed hydrogen-like atom:

$$p^2|n, l, m\rangle = 2m_e(E_n - V)|n, l, m\rangle. \qquad \text{(C.E.7.16)}$$

Plug (C.E.7.16) into (C.E.7.15):

$$\Delta E_{nlm} = -\frac{1}{2m_ec^2}\langle n, l, m|E_n^2 - 2E_nV + V^2|n, l, m\rangle =$$
$$= -\frac{1}{2m_ec^2}(E_n^2 - 2E_n\langle V\rangle + \langle V^2\rangle), \text{(C.E.7.14)},$$

where $\langle n, l, m|n, l, m\rangle = 1$ has been used.

Exercise 7.4 Calculate the energy-shift due to spin-orbit coupling and the electron's relativistic mass increase for an energy eigenstate of the hydrogen atom.

Consider an energy eigenstate of the hydrogen atom characterized by the standard quantum numbers n, l, m. Show that if the energy-shift due to spin-orbit coupling (See Section 7.7) is added to that due to the electron's relativistic mass increase(Exercise 7.3) then the net fine structure energy-shift can be written as

$$\Delta E_{nlm} = \frac{\alpha^2 E_n}{n^2}\left(\frac{n}{j+\frac{l}{2}} - \frac{3}{4}\right). \qquad \text{(C.E.7.17)}$$

Here, E_n is the unperturbed energy, α the fine structure constant, and $j = l \pm 1/2$ the quantum number associated with the magnitude of the sum of the electron's orbital and spin angular momenta.

All of the work has been done by Fp and presented in Section 12.8 *The Fin Structure of Hydrogen* of *The Undergraduate Course*.

The first thing to do, is to plug into (C.E.7.14):

$\langle V\rangle = -\frac{e^2}{4\pi\epsilon_0 r} = -\frac{e^2}{4\pi\epsilon_0}\langle\frac{1}{r}\rangle$, the expectation value of the Coulomb potential. Then with (9.55), (9.57) and (9.5.8) of Section 9.9 *Hydrogen Atom , The Undergraduate Course*, the result for the energy-shift due relativistic effects is, (12.121):

$$\Delta E_{nlm} = \frac{\alpha^2 E_n}{n^2}\left(\frac{n}{l+\frac{l}{2}} - \frac{3}{4}\right), (12.121).$$

As mentioned before, Fp presented all the work in Section 12.8 *The Fine Structure of Hydrogen* of *The Undergraduate Course*.

So, I need the energy-shift due to spin-orbital coupling. The energy- shift due to this coupling is given by (12.137) *The Undergraduate Course*:

$$\Delta E_{nlm} = \frac{\alpha^2 E_n}{n^2}\left[\frac{n\left\{\frac{3}{4}+l(l+1)-j(j+1)\right\}}{2l\left(l+\frac{1}{2}\right)(l+1)}\right] ,(12.137).$$

FP: *A comparison of this expression with Eq.(12.121) reveals that the energy-shift due to spin-orbit coupling is of the same order of magnitude as due to the lowest-order relativistic correction to the Hamiltonian. We can add these two corrections together(linearity)(making use of the fact that* $j = l \pm \frac{1}{2}$ *for a hydrogen atom-see Section 11.3 of The Undergraduate Course) to obtain a net energy-shift of*

$$\Delta E_{nlm} = \frac{\alpha^2 E_n}{n^2}\left(\frac{n}{j+\frac{l}{2}} - \frac{3}{4}\right), (12.138) \rightarrow \text{(C.E.7.17)}.$$

Note: in the derivation above use has been made of $\langle\frac{1}{r^2}\rangle = \frac{1}{n^3(l+\frac{1}{2})a_0^2}$, and $\langle\frac{1}{r^3}\rangle = \frac{1}{n^3 l(l+\frac{1}{2})(l+1)a_0^3}$. The latter expectation value results from the correction to the Hamiltonian (12.127) due to spin-orbit correction.

8 Time-Dependent Perturbation Theory

8.1 Introduction

Now the perturbation Hamiltonian is considered to be time-dependent.

Fp: *A time-dependent perturbation allows the system to make transitions between its unperturbed eigenstates.*

That's the key issue of this chapter.

See also *The Undergraduate Course*, Chapter 13 with the same title. In this chapter, the notation is based on the "wave function" notation.
In (8.2), I suppose $|n\rangle$ to be a complete set of eigenstates of the unperturbed Hamiltonian H_0. Furthermore, I understood the Hamiltonian H to have a, different, complete set of eigenstates. That understanding is wrong. The small time-dependent perturbation "*allows the system to make transitions between the unperturbed eigenstates".*

8.2 General Analysis

Fp starts with a system at time t_0 in a state $|A\rangle$ which is some linear superposition of the unperturbed energy eigenstates:
$|A\rangle = \sum_n c_n |n\rangle$, (8.3).
Next, Fp calculated the time evolution of $|A\rangle$, (8.4).
This is based on the analysis of Section 4.12, *Stationary States*, *The Undergraduate Course*, *(4.158)*.
Note: From now on I present the numbers indicating equations of *The Undergraduate Course* in *Light Italic.*
(4.158):
$\psi_t(x,t,E_i) = \psi_i(x)e^{-iE_it/\hbar}$.
The result of calculating the probability of finding the system in state $|n\rangle \rightarrow P_n(t)$, (8.5):
$P_n(t) = |\langle n|A\rangle|^2$,
where use has been made of:
$\langle n|m\rangle = \delta_{nm}$.
Consequently, the state $|n\rangle$ is projected out.
At the top of page 124 Fp writes: *"Here we have carefully separated* ……". So, Fp assumed on beforehand the phase oscillations of the eigenkets $|n\rangle$ to be fast compared with the variations of the amplitudes $c_n(t)$.
Schrödinger's time evolution gives (8.7) and with differentiating (8.6) → (8.9).
Equating the right-hand side of (8.8) and (8.9) → (8.10).
Note: obviously, the operator H_1 does depend on $\frac{\partial}{\partial t}$.
Finally, a differential equation for the coefficient $c_n(t)$ is obtained.
The matrix elements → $H_{nm}(t) = \langle n|H_1(t)|m\rangle \neq 0$, (8.12).
For the differential equation (8.11) exact solutions cannot be found.

8.3 Two-State System

For a two-state system, (8.11) can be solved exactly.
Fp assumes the diagonal matrix elements of the interaction Hamiltonian to be zero.
The two first order differential equations resulting from (8.11) can be combined into a second order differential equation (8.20).
Fp looked for a solution of this differential equation for certain initial conditions.
The solutions are presented by (8.21) and (8.22). By plugging these solutions into the relevant equations, the solutions appear to be appropriate.
On the other hand, from a textbook on differential equations or with WolframAlpha and the initial conditions the general solution is obtained, with $c_2(t=0) = 0$, the general solution is:

$c_2 = d\exp[\frac{-i(\omega-\omega_{21})t}{2}]\sin(\Omega t)$, (C.8.3.1)

where

$\Omega = \sqrt{\gamma^2 + \frac{(\omega-\omega_{21})^2}{4}}$.

Plug (C.8.3.1) into (8.19) and set $c_1(t=0) = 1$, results into

$d = -\frac{i\gamma}{\Omega}$.

In (8.23) and (8.24), Fp presented the probability of finding the system in one of the two states, $P_2(t)$ and $P_1(t)$ respectively.

Having obtained the equations for the amplitudes and the probabilities, Fp analyzed the meaning of these results. He mentioned the results to exhibit all the features of classic resonance.

Remark on resonance: resonance means the frequency of the perturbation ω matches the frequency of ω_{21}. The latter frequency is of the order of magnitude of the fast phase oscillations of the eigenkets I suppose. ω is the frequency of $c_n(t)$. At the top of page 124: $\omega \ll \omega_{21}$. Well, that's my conclusion. Consequently, for the theory to be consistent, ω will not match ω_{21}? No resonance according to the theory? On the other hand: *"…..the time-dependent perturbation is only effective at causing transitions between state 1 and 2 if its frequency of oscillation lies in the approximate range* $\omega_{21} - \frac{2\gamma}{\hbar} \leq \omega \leq \omega_{21} + \frac{2\gamma}{\hbar}$*."* A contradiction with the premises of slow oscillations of the perturbation with respect to the fast phase oscillations of the eigenkets?

8.4 Spin Magnetic Resonance

A bound electron placed in a uniform z-directed magnetic field, and then subjected to a small time-dependent magnetic field rotating in the x-y plane. A bound electron: no orbital angular momentum.

So with (5.46), the magnetic moment expressed in the angular momentum spin operator:

$\boldsymbol{\mu} = -\left[\frac{eB_1}{m_e}\cos(\omega t)S_x, \frac{eB_1}{m_e}\sin(\omega t)S_y, \frac{eB_0}{m_e}S_z\right]$. (C.8.4.1)

Then with (C.8.4.1)→ (8.29) and (8.30).

So for the spin ½ particle the unperturbed Hamiltonian (8.31) is obtained.

With the raising and lowering operators (8.32) is found.

Rehearsal in order to derive (8.33):

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

Then Fp analyzed this system and with spin up and spin down, the system is a two-state system as analyzed in Section 3.1.

8.5 Dyson Series.

In this section Fp tries to find approximate solutions for the general system as presented in (8.11):

$i\hbar\frac{dc_n}{dt} = \sum_m H_{nm}(t)\exp[i\omega_{nm}(t-t_0)]c_m(t)$.

See also Chapter 3 on Quantum Dynamics and the sections on the time evolution operator $T(t)$.

Fp introduced in this section another time evolution operator:

$|A, t_0, t\rangle = U(t_0, t)|A\rangle$, (8.39).

In *The Undergraduate Course*, Section 13.5, the first order approximate solution of (8.11) has been derived without the use of the time evolution operator.
With (8.7), Schrödinger's time evolution, time dependent, equation, (8.39) can be written as:
$i\hbar\frac{\partial}{\partial t}|A,t_0,t\rangle = i\hbar\frac{\partial}{\partial t}U(t_0,t)|A\rangle = (H_0+H_1)U(t_0,t)|A\rangle$,
for any $|A\rangle$.
So, the differential equation for $U(t_0,t)$, (8.40), is found.
First, Fp derives the solution for the time evolution operator without external perturbation, (8.42). This solution is a phase factor.
With $U(t_0,t)$ given in (8.42):
$U(t_0,t) =$exp$[-\frac{iH_0(t-t_0)}{\hbar}]$,
the unitary character of the unperturbed time evolution operator of $U(t_0,t)$ is shown→
$\rightarrow U^{\dagger}(t_0,t)U(t_0,t)=1$.
Then, with this solution (8.42), Fp proposes a solution with the perturbation switched on.
Plug this proposed solution, (8.43), into (8.40) and (8.44) is obtained.

8.5.1 *Intermezzo Time Evolution Operator*

(8.44) can be solved ;
$U_1(t_0,t) =$exp$[-\frac{i}{\hbar}\int_{t_0}^{t}dt' H_l(t_0,t')]$. (C.8.5.1)
Caveat: H_l instead of H_1, (8.45).
Then, with (8.42):
$U(t_0,t) =$ exp$[-\frac{i}{\hbar}\int_{t_0}^{t}dt'\{H_0+H_l(t_0,t')\}]$. (C.8.5.2)
Furthermore for $c_n(t)=\langle n|U_1(t_0,t)|i\rangle$, (8.49), and with (C.8.5.1):
$c_n(t)=\left\langle n\left|\exp[-\frac{i}{\hbar}\int_{t_0}^{t}dt' H_l(t_0,t')]\right|i\right\rangle$. (C.8.5.3)
End of Intermezzo.

Just below (8.44) Fp writes: "*where*
$H_l(t_0,t) =$exp$[+\frac{iH_0(t-t_0)}{\hbar}]\,H_1exp[-\frac{iH_0(t-t_0)}{\hbar}]$, (8.45)".

In deriving (8.44), I show a "a step in between":
$i\hbar\exp\left[-\frac{iH_0(t-t_0)}{\hbar}\right]\frac{\partial U_1(t_0,t)}{\partial t}=H_1\exp\left[-\frac{iH_0(t-t_0)}{\hbar}\right]U_1(t_0,t)$. (C.8.5.4)
Multiply (C.8.5.1) with $\exp\left[+\frac{iH_0(t-t_0)}{\hbar}\right]\rightarrow$
$\rightarrow i\hbar\frac{\partial U_1(t_0,t)}{\partial t}=\exp\left[+\frac{iH_0(t-t_0)}{\hbar}\right]H_1\exp\left[-\frac{iH_0(t-t_0)}{\hbar}\right]U_1(t_0,t)$. (C.8.5.5)
Then with (8.45), (8.44) is obtained.
By definition, (8.39), the eigenstate at $t=t_0$ evolves with time as:
$|i,t_0,t\rangle = U(t_0,t)|i\rangle$.
Then, with (8.6), $|i,t_0,t\rangle$ is expressed as (8.47).

8.5.2 *Intermezzo Time Evolution and Eigenstates*

$|i\rangle$ is an eigenstate of H_0 and $|i,t_0,t\rangle$ is "some other eigenstate at a subsequent time" , Section 8.1 .Now, as mentioned before, I consider $|n\rangle$ to represent a complete set of eigenstates of the operator H_0 of which $|i\rangle$ an also an eigenstate. I just learned $|i,t_0,t\rangle$ is some other unperturbed

eigenstate of the operator H_0, Section 8.1.
Assume the completeness to be correct, how is it possible to express $|i, t_0, t\rangle$ in $|m\rangle$, where $|m\rangle$ is a member of the complete set of eigenstates of the operator H_0? Or do I consider
$c_m(t)\exp[-\frac{iE_m(t-t_0)}{\hbar}]|m\rangle$,
to be a new phase-shifted ket in the same space of ket states $|m\rangle$?
Then, the question remains: *"…a time-dependent perturbation allows the system to make transitions between its unperturbed energy eigenstates…. "*, what does that mean? For example: at $(t = t_0)$ $|i\rangle$ and $H_0|i\rangle = E_i|i\rangle$ and after $(t - t_0) \rightarrow H_0|k\rangle = E_k|k\rangle$?
End of Intermezzo.

Using (8.43), $|i, t_0, t\rangle$ can also be written as:
$|i, t_0, t\rangle = U(t_0, t)|i\rangle = \exp\left[-\frac{iH_0(t-t_0)}{\hbar}\right] U_1(t_0, t)|i\rangle$, (8.48).
Now, equate (8.47) and (8.48):
$\exp\left[-\frac{iH_0(t-t_0)}{\hbar}\right] U_1(t_0, t)|i\rangle = \sum_m c_m(t)\exp[-\frac{iE_m(t-t_0)}{\hbar}]|m\rangle$. (C.8.5.6)
Left multiplication of (C.8.5.6) by $|n\rangle$:
$\langle n|\exp\left[-\frac{iH_0(t-t_0)}{\hbar}\right] U_1(t_0, t)|i\rangle = \sum_m c_m(t)\langle n|\exp[-\frac{iE_m(t-t_0)}{\hbar}]|m\rangle$. (C.8.5.7)
Now,
$\langle n|\exp\left[-\frac{iH_0(t-t_0)}{\hbar}\right] = \exp[-\frac{iE_n(t-t_0)}{\hbar}]\langle n|$, (C.8.5.8)
where use has been made of Taylor series expansion of the exp-function.
Plug (C.8.5.8) into (C.8.5.7) and with
$\langle n|m\rangle = \delta_{nm}$, (8.49) is found.
Let's still pay some attention to (8.47):
I suppose $|i, t_0, t_0\rangle = |i\rangle$.
When I plug $t = t_0$ into (8.47) $\rightarrow |i, t_0, t_0\rangle = \sum_m c_m(t_0)\,|m\rangle$. (C.8.5.9)
So $\sum_m c_m(t_0)\,|m\rangle = |i\rangle$?
Well, the outer product operator helps:
$\sum_i \sum_m c_m(t_0)|i\rangle\langle i\,|m\rangle = \sum_i c_m(t_0)|i\rangle\,\delta_{im} = |i\rangle$,
since $|c_i|^2 = 1$, the probability to be in state $|i\rangle$.
At the top of page 129 represents the differential equation (8.44) by the integral equation in (8.51).
The approximate solution to (8.51) is found by iteration → (8.52), the Dyson series.
Note: Expanding (C.8.4.2) produces the first three terms in (8.52).

8.5.3 *Intermezzo Time Evolution and a small Time Step*

(8.52):
Set $t - t_0 = \Delta t$, a small time step.
Then, to first order in Δt:
$U_1(t_0, t_0 + \Delta t) \approx 1 - \frac{i}{\hbar}\int_{t_0}^{t_0+\Delta t} H_l dt \approx 1 - \frac{i}{\hbar} H_l \Delta t$.
With (8.42), to first order in Δt:
$U(t_0, t_0 + \Delta t) = \exp[-iH_0\Delta t/\hbar)]U_1(t_0, t_0 + \Delta t) \approx 1 - \frac{i}{\hbar}(H_0 + H_l)\Delta t.$ (C.8.5.10)
Since (C.8.5.10) has been expanded to first order in Δt, then the expansion of (8.45) can be truncated :
$H_l \approx H_1 \rightarrow H_0 + H_l \approx H_0 + H_1 = H.$
Now, with (8.39):
$|A, t_0, t_0 + \Delta t\rangle = U(t_0, t_0 + \Delta t)|A\rangle.$ (C.8.5.11)

(C.8.5.11) and (C.8.5.10):

$$|A, t_0, t_0 + \Delta t\rangle = |A\rangle - \frac{i}{\hbar} H|A\rangle \Delta t \rightarrow \frac{|A, t_0, t_0+\Delta t\rangle - |A\rangle}{\Delta t} = \frac{i}{\hbar} H|A\rangle \,. \qquad \text{(C.8.5.12)}$$

With the limit $\Delta t \rightarrow 0$, (C.8.5.12) gives:

$$\hbar \frac{\partial}{\partial t} |A\rangle = -i\, H|A\rangle \,. \qquad \text{(C.8.5.13)}$$

Well, that looks familiar, the *time-dependent* Schrödinger equation.
See also Susskind, pages 100-102.
End of intermezzo

With (8.11)-(8.13), (8.57)-(8.59) are found.
These expressions result from Section 8.2 *General Analysis* .
To simplify (8.56) use has been made of the outer product:
$\sum_m |m\rangle \langle m| = 1.$
So,
$\langle n|H_l(t_0, t')H_l(t_0, t'')|i\rangle = \sum_m \langle n|H_l(t_0, t')|m\rangle \langle m|H_l(t_0, t'')|i\rangle$ →(8.59).

Remark:
The simplification: Compare the integrals in (8.55) and (8.58).
Caveat once more: it's about H_l and not about H_1. May be, a subscript p instead of 1 could have been of some help.
For example to evaluate $c_n^{(1)}$ in (8.55):

$$\langle n|H_l(t_0, t'|i\rangle = \left\langle n\left|\exp\left[+\frac{iH_0(t'-t_0)}{\hbar}\right] H_1 \exp\left[-\frac{iH_0(t'-t_0)}{\hbar}\right]\right|i\right\rangle \,. \qquad \text{(C.8.5.14)}$$

With Taylor series expansions and:
$\langle n|H_0 = E_n\langle n|\,,\, H_0|i\rangle = E_i|i\rangle \rightarrow \langle n|H_l(t_0, t'|i\rangle = \exp[i\omega_{ni}(t' - t_0)]H_{ni}(t')$,
where ω_{ni} and H_{ni} are given in (8.60) and (8.61) respectively.

8.6 Sudden Perturbation

In this section a particular example of H_1 is analyzed. It's about a constant perturbation suddenly switched on. So, H_1 is a step function.
Fp calculates the first-order perturbation. Use has been made of (8.13).

8.6.1 *Intermezzo on Simplification*

(8.58):

$$c_n^{(1)}(t) = -\frac{i}{\hbar}\int_{t_0}^{t} \exp[i\omega_{ni}(t' - t_0)]H_{ni}(t')\, dt',$$

and $t_0 = 0$ with $H_{ni} = \langle n|H_1(t)|i\rangle = H_1\langle n|i\rangle = H_1\delta_{ni}$,
then, with (8.58)

$$c_n^{(1)}(t) = -\frac{i}{\hbar} H_{ni} \int_0^t \exp[i\omega_{ni}t']\, dt' = \frac{H_{ni}}{E_n - E_i}[1 - \exp(i\omega_{ni}t)], \text{ (8.65).}$$

So, t in the integrand of the first integral of (8.65) should be deleted, a typo.
However, what about $H_{ni} = H_1\delta_{ni}$, above? That is wrong, since the perturbation operator is generally a function of the position, momentum, and spin operators(Fp). So:
$\langle n|H_1(t)|i\rangle \neq H_1\langle n|i\rangle$.
End of Intermezzo.

In (8.66) and (8.67) the transition probability between the states $|i\rangle$ and $|n\rangle$ is presented.
In *The Undergraduate Course Section 13.6 Harmonic Perturbations* Fp also dealt with the non-conservation of energy.
In (8.68) the sinc(x) is defined; sinc$(0) = 1$.
Conservation of energy: $E_n = E_i$, Fp.
In (8.73) ,with (8.74):
$dx = \frac{tdE_n}{2\hbar}$.
At the bottom of page 131 Fp introduced the transition rate to be the transition probability per unit time, (8.77).
(8.78) and (8.79), I suppose:
$w_{i\to[n]} = \int w_{i\to n}\,\rho(E)dE$,
where the delta function "selects" $E_n \cong E_i$.
On page 132 Fp calculated the second order transition in the Dyson series.
In the first line of (8.80), the second integral is:

$$\int_0^{t'} dt''\exp(i\omega_{mi}t'') = \frac{1}{i\omega_{mi}}[\exp(i\omega_{mi}t') - 1]. \qquad \text{(C.8.6.1)}$$

Note: $\exp(i\omega_{mi}t'')$ instead of $\exp(i\omega_{mi}t)$, a typo.
Then, with (C.8.6.1):
$\int_0^t dt'\{\exp[it'(\omega_{nm} + \omega_{mi})] - \exp(i\omega_{nm}t')\}$,
has to be evaluated.
With (8.60):

$$\omega_{nm} + \omega_{mi} = \frac{E_n - E_m + E_m - E_i}{\hbar} = \frac{E_n - E_i}{\hbar} = \omega_{ni}. \qquad \text{(C.8.6.2)}$$

Use the factor $\frac{1}{i\omega_{mi}}$ in (C.8.6.1), with the definition in (8.60):

$$\frac{1}{i\omega_{mi}} = -\frac{i\hbar}{E_m - E_i}. \qquad \text{(C.8.6.3)}$$

In this way, the second line of (8.80) is found.
The integrals in the second line of (8.80) are similar to the integral presented in (C.8.6.1).
So, for example,

$$\frac{1}{i\omega_{mi}}[\exp(i\omega_{ni}t) - 1] = \mathrm{t}\cdot\exp\left(\frac{i\omega_{ni}t}{2}\right)\frac{\exp\left(\frac{i\omega_{ni}t}{2}\right) - \exp\left(-\frac{i\omega_{ni}t}{2}\right)}{\frac{2i\omega_{ni}t}{2}} =$$

$$= t\cdot\exp\left(\frac{i\omega_{ni}t}{2}\right)\mathrm{sinc}\frac{\omega_{ni}t}{2}. \qquad \text{(C.8.6.4)}$$

To obtain, $c_n^{(1)}(t)$, given in (8.65):

$$\frac{H_{ni}}{E_n - E_i}[1 - \exp(i\omega_{ni}t)] = \frac{H_{ni}}{E_n - E_i}\exp\left(\frac{i\omega_{ni}t}{2}\right)\left[\exp\left(-\frac{i\omega_{ni}t}{2}\right) - \exp\left(\frac{i\omega_{ni}t}{2}\right)\right]. \qquad \text{(C.8.6.5)}$$

Using (8.60), the definition of ω_{ni}, (C.8.6.5) can be written as:

$$\frac{H_{ni}}{\hbar}\exp\left(\frac{i\omega_{ni}t}{2}\right)\frac{\exp\left(-\frac{i\omega_{ni}t}{2}\right) - \exp\left(\frac{i\omega_{ni}t}{2}\right)}{\omega_{ni}} = it\frac{H_{ni}}{\hbar}\frac{\exp\left(-\frac{i\omega_{ni}t}{2}\right) - \exp\left(\frac{i\omega_{ni}t}{2}\right)}{\frac{2i\omega_{ni}t}{2}} = -\frac{it}{\hbar}\exp\left(\frac{i\omega_{ni}t}{2}\right)H_{ni}\mathrm{sinc}\frac{\omega_{ni}t}{2}, \qquad \text{(C.8.6.6)}$$

Fp found the expression for $c_n^{(1)}(t)$ in (8.81) with a + sign instead of a – sign as in (C.8.6.6). Does it matter?
With (8.62), the transition probability between states $|i\rangle$ and $|n\rangle$:

$$P_{i\to n} = [c_n^{(1)} + c_n^{(2)}]^2. \qquad \text{(C.8.6.7)}$$

Then, with the same reasoning for the average of $\mathrm{sinc}\frac{\omega_{nm}t}{2}$ in (8.81) to be zero, I find for the

transition rate

$$w_{i\to[n]} = \frac{2\pi}{\hbar}\overline{\left|-H_{ni} + \sum_m \frac{H_{nm}H_{mi}}{E_m - E_i}\right|^2}\,\rho(E_n), \qquad \text{(C.8.6.8)}$$

or

$$w_{i\to[n]} = \frac{2\pi}{\hbar}\overline{\left|H_{ni} - \sum_m \frac{H_{nm}H_{mi}}{E_m - E_i}\right|^2}\,\rho(E_n)\ .$$

So, this certainly differs from (8.82). From the reasoning at the bottom of page 132 and at the top of page 133 about *virtual transition*, I conclude the first-order energy conserving transition is of importance. Consequently, the – sign in (C.8.6.8) does not matter?
The total result with the + sign for the transition rate is presented in (8.82).

8.7 Energy-Shifts and Decay-Widths

In Section 8.6 Fp examined how a state $|n\rangle$ becomes populated. Next, Fp considers how $|i\rangle$, the initial state becomes depopulated.

Remark:
I thought, FP examined a group of final states $|n\rangle$, all possessing nearby the same energy as the energy of $|i\rangle$.

A perturbation Hamiltonian is gradually turned on, (8.83).
In (8.83) H_1 is denoted to be a constant. Meaning independent of the time t I suppose, since $H_{ni} = \langle n|H_1|i\rangle$.
To derive Fermi's Golden rule for the exponential perturbation, (8.83), Fp used the following representation of the Dirac-δ-function:

$$\delta(y) = \lim_{\beta\to 0} \frac{\beta}{\pi(\beta^2+y^2)},$$

Chisholm and Morris, page 604 on *Representations of the δ-function.*
Then, (8.88) is found.
Since Fp wants to find out about the depopulation of the initial state, $c_i(t)$ is calculated.
Now:
$c_i^{(0)}(t) = \delta_{ii} = 1$, (8.54) and (8.90).
(8.91) is obtained using:
$H_{ii} = \langle i|H_1|i\rangle$, and $\omega_{ii} = 0$, (8.61) and (8.60) respectively.
(8.92) with $\omega_{mi} + \omega_{im} = 0$, (8.60).
Then $c_i(t)$ to second order is presented in (8.93):

$$c_i(t) = c_i^{(0)}(t) + c_i^{(1)}(t) + c_i^{(2)}(t).$$

The next step is to consider $(dc_i/dt)/c_i$ in the limit $\eta \to 0$.
The result of this limit is presented in(8.94).
The nominator in the first line of (8.94) follows straightforward from differentiating $c_i(t)$ with respect to time. What about the denominator in the first line of (8.94)?
The denominator, a complex expression,

$$c_i(t) = 1 - \frac{i}{\hbar}\frac{H_{ii}}{\eta}\,. \qquad \text{(C.8.7.1)}$$

So, $(\frac{-i}{\hbar})^2 \frac{|H_{ii}|^2}{\eta^2} \ll 1$ with η to be small? In practice, what numbers to be used to find out?
What about the expectation value

$H_{ii} = \langle i|H_1|i\rangle$?
H_1 in (8.83) is denoted to be a constant. Meaning: not dependent on time? On the other hand, H_1 "*is generally a function of the position, momentum and spin operators*", Fp.
$|i\rangle$ is the state at $t \to -\infty$, the unperturbed state. So, could the conclusion be:
$H_{ii} = \langle i|H_1|i\rangle = 0$ at $t \to -\infty$?
For $\eta = 0$ in(8.83), there is a step function at $t \to -\infty$.
However, I cannot explain why $(\frac{-i}{\hbar})^2 \frac{|H_{ii}|^2}{\eta^2}$ has been deleted in the denominator of (8.94), unless $(\frac{-i}{\hbar})^2 \frac{|H_{ii}|^2}{\eta^2} \ll 1$.
The last term on the right hand side of (8.93) could also be written as:
$\frac{-i}{\hbar}\sum_{m\neq i} \frac{|H_{mi}|^2}{2\eta(E_i - E_m + i\hbar\eta)} \exp(2\eta t) = \frac{-i}{\hbar}\sum_{m\neq i} \frac{|H_{mi}|^2}{2\eta[(E_i - E_m)^2 + (\hbar\eta)^2]} \exp(2\eta t)(E_i - E_m) +$
$-\sum_{m\neq i} \frac{|H_{mi}|^2}{2[(E_i - E_m)^2 + (\hbar\eta)^2]} \exp(2\eta t).$ (C.8.7.2)
Jumping to the bottom of page 134, the last term in (C.8.7.2) with $\eta \to 0$ produces the principal value in (8.98).
I continue with missing some answers.
Just below (8.94) Fp writes: "*This result is formally correct to second order in perturbed quantities*". I suppose the perturbed quantities are the $c_i^{(k)}$'s.
On top of page 135 Fp presented the solution,(8.99), of the differential equation in (8.95).

Then , the next question arises.
Fp normalized this solution such that
$c_i(t = 0) = 1.$
At the beginning of this section Fp writes:
$c_i(t \to -\infty) = 1$, see also (8.90)-(8.92).
I assume, since Fp refers in the derivation of (8.90)-(8.92) to (8.57)-(8.59), the perturbation starts at $t = 0$? However, does that contradict gradually turning on the perturbation at $t = -\infty$? This looks like the perturbation Hamiltonian to be
$H_1(t) = [\exp(\eta t) - 1]H_1,$ (C.8.7.3)
with the perturbation turned on at $t = 0$.
With (8.57)-(8.59), I arrive at different expressions for the higher order perturbed coefficients, for example:
$c_i^{(1)}(t) = -\frac{i}{\hbar}H_{ii}[\frac{\exp(\eta t)-1}{\eta} - t].$ (C.8.7.4)
Just below (8.104), Fp writes: "…., *given that it (the system)is definitely in state* $|i\rangle$ *at time* $t = 0$, …….". So, the perturbation is turned on at $t = 0$.

The conservation of probability in (8.107) follows from (8.79) and (8.104).
To derive (8.111), Fp used the Fourier inversion Theorem.
So, with (8.110)
$F(t) = \frac{1}{\sqrt{2\pi}}\int dE e^{-\frac{iEt}{\hbar}} f(E),$
and
$f(E) = \frac{1}{\sqrt{2\pi}}\int dt\, e^{\frac{iEt}{\hbar}} F(t),$ (C.8.7.5)

where

$F(t)$ =exp$[-\frac{i(E_i+\Delta E_i)t}{\hbar}]exp(-\frac{\Gamma_i t}{2\hbar})$, see also section 8.2 , *General Analysis*.

ΔE_i is given in (8.103) and Γ_i in (8.106).

Plug $F(t)$ into (C.8.7.5):

$$f(E) \propto \int dt\, e^{\frac{iEt}{\hbar}} \exp[-\frac{i(E_i+\Delta E_i)t}{\hbar}]\exp(-\frac{\Gamma_i t}{2\hbar}). \qquad \text{(C.8.7.6)}$$

Now, with

$t' = [E - (E_i + \Delta E_i) + i\Gamma_i/2] \cdot t$,

(C.8.7.6) can be written as:

$$f(E) \propto \frac{1}{E-(E_i+\Delta E_i)+i\Gamma_i/2} \int e^{it'} dt'.$$

Then, with (8.103):

$$|f(E)|^2 \propto \frac{1}{(E-[E_i+\mathrm{Re}(\Delta_i)])^2+\Gamma_i^2/4} \int e^{it'} dt' \int e^{-it'} dt' \ . \qquad \text{(C.8.7.7)}$$

I suppose $\int e^{it'} dt' \int e^{-it'} dt'$ to be a number.

Just below (8.111) Fp writes: *"In the absence of the perturbation, $|f(E)|^2$ is basically a delta-function …… ".*

Without perturbation, $\eta \to 0$, (8.88) reduces into a delta-function:

$$\lim_{\eta\to 0} \frac{\eta}{\eta^2+\omega_{ni}^2} = \pi\delta(\omega_{ni}) \ .$$

However in the numerator of (8.111), I do not find η.

8.8 Harmonic perturbations

Now a perturbation is considered that oscillates sinusoidally in time. See also Section 13.6 of *The Undergraduate Course.*

The harmonic perturbation Hamiltonian is presented in (8.112). The perturbation is switched on at $t = 0$.

Recapitulation of Section 8.6 and Section 13.6(*The Undergraduate Course*).

(8.113) can be written as:

$$c_n^{(1)} = -\frac{it}{\hbar}(V_{ni}\exp[\frac{i(\omega_{ni}+\omega)t}{2}]\mathrm{sinc}\left[\frac{(\omega_{ni}+\omega)t}{2}\right] + V_{ni}^{\dagger}\exp[\frac{-i(\omega_{ni}-\omega)t}{2}]\mathrm{sinc}\left[\frac{(\omega_{ni}-\omega)t}{2}\right]) \ , \qquad \text{(C.8.8.1)}$$

Where use have been made of

$$\frac{e^{i\alpha}-1}{2i} = e^{i\alpha/2}\frac{e^{i\alpha/2}-e^{-i\alpha/2}}{2i} = \frac{\alpha}{2}e^{i\alpha/2}\mathrm{sinc}\frac{\alpha}{2} \ .$$

Now the first term of (C.8.8.1) is non-negligible for

$\omega_{ni} + \omega \leq \frac{2\pi}{t}$,

and the second term for

$\omega_{ni} - \omega \leq \frac{2\pi}{t}$.

So, in the limit $t \gg 2\pi/|\omega_{ni}|$ or $|\omega| \approx |\omega_{ni}|$,

$$P_{i\to n} = \frac{t^2}{\hbar^2}\left\{|V_{ni}|^2\,\mathrm{sinc}^2\left[\frac{(\omega_{ni}+\omega)t}{2}\right] + \left|V_{ni}^{\dagger}\right|^2\mathrm{sinc}^2\left[\frac{(\omega_{ni}-\omega)t}{2}\right]\right\} . \qquad \text{(C.8.8.2)}$$

To obtain (C.8.8.2), expressions like

$\mathrm{sinc}\frac{(\omega_{ni}+\omega)t}{2}\mathrm{sinc}\frac{(\omega_{ni}-\omega)t}{2}$, vanish.

The processes of stimulated emission and absorption are introduced:

$\omega_{ni} + \omega \approx 0$ →stimulated emission,

$\omega_{ni} - \omega \approx 0$ →absorption.

With (C.8.8.2) and (8.78), the rate for stimulated emission and the transition rate for absorption are calculated.
About *detailed balancing*:

$$\frac{w_{i\to[n]}}{\rho(E_n)|_{E_n\cong E_i-\hbar\omega}} = \frac{w'_{[i\to n]}}{\rho(E'_n)|_{E'_n\cong E'_i+\hbar\omega}}. \qquad \text{(C.8.8.3)}$$

Now the balancing:
On the right hand side of(C.8.8.3), the final state E'_n of absorption is larger than the initial state E'_i . The symmetry or detailed balancing means:
$E'_i = E_n$, $E'_n = E_i$, and $w'_{[i\to n]} = w_{n\to[i]} \to (8.123)$.

8.9 Absorption and Stimulated Emission of Radiation.

In this section the results of time-dependent perturbation are used to investigate the interaction of anatomic electron with classical electromagnetic radiation.
See also Section 13.7 on Electromagnetic Radiation, *The Undergraduate Course*, Fp.
In (8.125), a particle of charge q in the presence of an electromagnetic field:
$\boldsymbol{p} \to \boldsymbol{q} - q\boldsymbol{A}$,
and *(13.65)*
$\boldsymbol{p} \to \boldsymbol{q} + q\boldsymbol{A}$.
The Maxwell equations also work in quantum mechanics.
In (8.129), the Hamiltonian, $q = -e$.
In (8.132) I do expect the term $\frac{e\boldsymbol{A}\cdot\boldsymbol{p}}{m_e}$ in stead of $-\frac{e\boldsymbol{A}\cdot\boldsymbol{p}}{m_e}$.
Let's consider the absorption case, with (C.8.8.2):

$$P_{i\to n} = \frac{t^2}{\hbar^2}\left|V^{\dagger}_{ni}\right|^2 \operatorname{sinc}^2\left[\frac{(\omega_{ni}-\omega)t}{2}\right], \qquad \text{(C.8.9.1)}$$

where

$$V_{ni} = -\left\langle n\left|\frac{eA_0\boldsymbol{\epsilon}\cdot\boldsymbol{p}}{m_e}\exp[-i\left(\frac{\omega}{c}\right)\boldsymbol{n}\cdot\boldsymbol{x}]\right|i\right\rangle. \qquad \text{(C.8.9.2)}$$

With $\boldsymbol{\epsilon}$ and $\boldsymbol{n}$ are unit vectors. See top of page 139.
In (8.143) Fp specifies the relation between energy density $U$and the amplitude of the monochromatic wave A_0.
Then with the definition of the transition rate
$w_i = \frac{d}{dt}P_{i\to n}$,
and the results of the foregoing sections on *Sudden Perturbation* and *Harmonic Perturbations,* 8.6 and 8.7 respectively, (8.144) is found.
In addition, Fp analyzed the transition rate for a non-monochromatic incident wave.
The energy density becomes an integral over a range of frequencies:
$U = \int u(\omega)d\omega$.
Plug $\int u(\omega)d\omega$ into (8.146). Take into account the delta function $\delta[\hbar(\omega_{ni} - \omega)$ and (8.147), the transition rate for absorption, is found.

8.10 Electric Dipole Approximation

In this section the exponent in (8.147) is approximated by the electric dipole approximation.
(8.150) follows from the first term, 1 , in the expansion in (8.149).
Furthermore (8.151) for the one-dimensional case, with $p = -i\hbar\frac{\partial}{\partial x}$:

$[x, H_0] = x\frac{p^2}{2m_e} - \frac{p^2}{2m_e}x = -x\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2} + x\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{m_e}\frac{\partial}{\partial x} = i\hbar p/m_e$.

(8.152):

$\langle n|p|i\rangle = -i\frac{m_e}{\hbar}\langle n|[x, H_0]|i\rangle = -i\frac{m_e}{\hbar}\langle n|xH_0 - H_0x|i\rangle = -i\frac{m_e}{\hbar}\langle n|xE_n - E_ix|i\rangle =$

$= im_e\omega_{ni}\langle n|x|i\rangle.$

Now, with(8.155):

$\boldsymbol{\epsilon}\cdot\langle n|\boldsymbol{p}|i\rangle = im_e\omega_{ni}\boldsymbol{\epsilon}\cdot\langle n|\boldsymbol{x}|i\rangle = im_e\omega_{ni}\boldsymbol{\epsilon}\cdot\boldsymbol{f}_{ni}.$

Then, (8.147) for a range of frequencies $U = \int u(\omega)d\omega$ →(8.153).

Just above (8.156) Fp mentioned, referring to section 7.4: *"….. $\langle n|z|i\rangle = 0$ unless the initial and final states satisfy…. "* → (8.156) and (8.157). These expressions represent the selection rules (7.41) and (7.52). Well, (7.52) indicates an additional selection rule: $\Delta l = 0$.

Then Fp mentioned below (8.157): *"It is easily demonstrated that $\langle n|x|i\rangle$ and $\langle n|y|i\rangle$ are only non-zero if $\Delta l = \pm 1$ and $\Delta m = 0, \pm 1$."* In The Undergraduate Course this is demonstrated for a hydrogen atom, where the electric dipole moment is non-zero.

Furthermore,

$\boldsymbol{d}_{in} = \langle i|e\boldsymbol{x}|n\rangle = e\boldsymbol{f}_{ni}$, *(13.99)*, is the effective electric dipole.

So, when the probability of spontaneous emission is zero, the electric dipole is zero.

Then, to *"…make a spontaneous transition from an energy state corresponding to the quantum numbers n, l, m to corresponding quantum numbers n', l', m' the modulus squared of the associated electric dipole, (13.128) is non-zero."*

Let's pay attention to $\langle n|x|i\rangle$ and $\langle n|y|i\rangle$, use the analysis of sections 7.4 and (13.11) *The Undergraduate Course.*

$\langle n|x|i\rangle$:

$[L_z, x^+] = L_z(x + iy) - (x + iy)L_z = \big(xp_y - yp_x\big)(x + iy) - x^+L_z =$

$\hbar x^+ + x^+L_z - x^+L_z = \hbar x^+.$

Nota Bene:

$L_z(x + iy) = \big(xp_y - yp_x\big)(x + iy) = \hbar x^+ + x^+L_z.$

With this information *(13.131)* is obtained.

Similarly is *(13.132)* for the lowering operator x^-.

With

$x = (x^+ + x^-)/2,$

and

$y = -i(x^+ - x^-)/2,$

Fp arrived at the conclusion below *(13.132)* summarized in (8.160) and (8.1.61).

In *The Undergraduate Course* in section 13.11, the selection rules are derived by considering transitions between the different levels of a hydrogen atom. However, the analysis is still rather general. It is about one valence electron orbiting outside a closed, spherical symmetric, shell(Section 7.4).

Then Fp introduced magnetic dipole transition.

The first order term in (8.149):

$+i\frac{\omega}{c}\boldsymbol{n}\cdot\boldsymbol{x}$,

Yields quadrupole transitions with different selection rules.

8.11 Spontaneous Emission

Now, in the absence of any external radiation, a spontaneous jump is considered. A spontaneous jump into a state with lower energy→emission.
it starts with black-body radiation and Planck's formula, representing the energy spectrum $u(\omega)$, (8.162).
Use is made of the expressions for absorption and stimulated emission as derived in section 8.10 →(8.153) and (8.154).
Just below (8.162), Fp explained detailed balancing for thermal equilibrium.
In (8.163), there are two systems of emission: spontaneous and stimulated for the two energy levels $E_2 > E_1$.
Below (8.163), I suppose $w_{2\to1}^{arm}$ should read $w_{2\to1}^{stm}$, a typo.
In (8.166) Fp presented the transition rate for spontaneous emission. I expected two frequencies: ω_{21} and ω_{12} . However, ω_{21}, the "selected "frequency, is used→detailed balancing.
To obtain (8.167) isotropic radiation, Fp presented the relevant equations in The Undergraduate Course: *(13.100) -(13.104).*. Then, it's about evaluating *(13.104)* for the unit sphere:
$\langle|\boldsymbol{\epsilon}\cdot\boldsymbol{f}_{21}|^2\rangle_{av} = \frac{f_{21}^2}{4\pi}\int\int \sin^3\theta\cos^2\phi\, d\theta d\phi = \frac{f_{21}^2}{3}$, (8.167).
With (8.167),(8.166),(8.169) and substituting $\omega = \omega_{21}$ in (8.162), (8.170) is found.
To obtain (8.171) Fp used the dipole moment, matrix element $\boldsymbol{f}_{21} = \langle 2|\boldsymbol{x}|1\rangle$, to be of the order of magnitude of the Bohr radius.
In this way Fp shows, finally,
$w_{2\to1}^{spn} \ll \omega_{21}$.
This assumption has been made at the top of page 124 in the section 8.2 on General Analysis.

Exercises

Exercise 8.1 About the inner product of the vector potential $\boldsymbol{A}$ and the momentum operator $\boldsymbol{p}$

Demonstrate that $\boldsymbol{p}\cdot\boldsymbol{A} = \boldsymbol{A}\cdot\boldsymbol{p}$ when $\nabla\cdot\boldsymbol{A} = 0$, where $\boldsymbol{p}$ is the momentum operator, and $\boldsymbol{A}(\boldsymbol{x})$ is a real function of the position operator $\boldsymbol{x}$. Hence, show that the Hamiltonian (8.132) is Hermitian.
$\boldsymbol{p}\cdot\boldsymbol{A} = \boldsymbol{A}\cdot\boldsymbol{p}$:
$-i\hbar\left(\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial z}\right)\cdot\left(A_x,A_y,A_z\right) = -i\hbar\left(A_x,A_y,A_z\right)\cdot\left(\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial z}\right)$.
Let's operate the operators $\left(\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial z}\right)$ and $\left(A_x,A_y,A_z\right)$ on a wave vector or wavefunction ψ, say.
So,
$\boldsymbol{p}\cdot\boldsymbol{A}\,\psi$:
$\left(\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial z}\right)\cdot\left(A_x,A_y,A_z\right)\psi = \nabla\cdot\boldsymbol{A}\psi + \boldsymbol{A}\cdot\left(\frac{\partial\psi}{\partial x}\boldsymbol{e}_x + \frac{\partial\psi}{\partial y}\boldsymbol{e}_y + \frac{\partial\psi}{\partial z}\boldsymbol{e}_z\right) = \boldsymbol{A}\cdot\left(\frac{\partial\psi}{\partial x}\boldsymbol{e}_x + \frac{\partial\psi}{\partial y}\boldsymbol{e}_y + \frac{\partial\psi}{\partial z}\boldsymbol{e}_z\right)$,
where use has been made of $\nabla\cdot\boldsymbol{A} = 0$.
Now,

$-i\hbar \boldsymbol{A} \cdot \left(\frac{\partial \psi}{\partial x}\boldsymbol{e}_x + \frac{\partial \psi}{\partial y}\boldsymbol{e}_y + \frac{\partial \psi}{\partial z}\boldsymbol{e}_z\right) = \boldsymbol{A} \cdot \boldsymbol{p}\,\psi \rightarrow \boldsymbol{p} \cdot \boldsymbol{A} = \boldsymbol{A} \cdot \boldsymbol{p}$.

The Hamiltonian in (8.132):

$H = \frac{p^2}{2m_e} - \frac{e\boldsymbol{A}\cdot\boldsymbol{p}}{m_e} + \frac{e^2A^2}{2m_e} - e\phi + V_0(r).$

Is H Hermitian?

Then the question reduces into: is $\boldsymbol{A} \cdot \boldsymbol{p}$ Hermitian since the other quantities in (8.132) are real functions. Since $\boldsymbol{A}(\boldsymbol{x})$ is a real function of the position operator $\boldsymbol{x}$, the question reduces furthermore.

Is $\boldsymbol{p}$ an Hermitian operator? Well, it is.

So:

$\boldsymbol{A} \cdot \boldsymbol{p} = (\boldsymbol{A} \cdot \boldsymbol{p})^\dagger = \boldsymbol{A} \cdot (\boldsymbol{p})^\dagger = \boldsymbol{A} \cdot \boldsymbol{p}.$

Hence

$H = H^\dagger.$

Exercise 8.2 Selection rules for the matrix elements of a hydrogen-like atom

Find the selection rules for matrix elements $\langle n, l, m|x|n', l', m'\rangle$, $\langle n, l, m|y|n', l', m'\rangle$, and $\langle n, l, m|z|n', l', m'\rangle$ to be non-zero. Here, $|n.\,l.\,m\rangle$ denotes an energy eigenket of a hydrogen-like atom corresponding to the conventional quantum numbers, n, l, and m.

Let's start with the matrix element:

- $\langle n, l, m|z|n', l', m'\rangle$.

Fp did already all the work.

In section 7.4 ,pages 105-106, Fp derived the selection rules for l and m . These rules are summarized in section 8.10:

$m' = m \rightarrow \Delta m = 0,$

and

$l' = l \pm 1 \rightarrow \Delta l = \pm 1.$

For these selection rules the matrix element is non-zero.

In my remarks on section 8.10, I also presented the selection rule $l = \ l' = 0$. I presented this to be $\Delta l = 0$. This is rather inaccurate. Since I cannot conclude from $\Delta l = 0 : l = \ l' = 0$!

$l = \ l' = 0$ represents spherical symmetry.

Now the selection rule for l, and

$\langle n, l, m|x|n', l', m'\rangle$.

In section 13.11 of *The Undergraduate Course*, Fp presented the tools to find out about the matrix element. Fp: *"….. a hydrogen(like) atom can only make a spontaneous transition from an energy state corresponding to the quantum numbers n, l, m to one corresponding to the quantum numbers n', l', m' if the modulus squared of the associated dipole moment, (13.128) is non-zero."* In section 13.11, Fp also mentioned the proof for $\langle n, l, m|z|n', l', m'\rangle$ can, via a trivial modification, also be used for the other two matrix elements. Trivial?

I suppose trivial means the use of $[L^2, x]$ instead of $[L^2, z]$ to find out about the selection rules for the matrix element $\langle n, l, m|x|n', l', m'\rangle$.

$[L^2, x] = \left[L_y^2, x\right] + [L_z^2, x]$, (C.8.E.1)

since $[L_x^2, x] = 0$.

Now, it's about operators operating on the wave function.

(C.8.E.1):

$\left[L_y^2, x\right] + [L_z^2, x] = L_y\left[L_y, x\right] + \left[L_y, x\right]L_y + L_z[L_z, x] + [L_z, x]L_z$. (C.8.E.2)

$L_y\left[L_y, x\right]$:

$L_y\{(zp_x - xp_z)x - x(zp_x - xp_z)\} = -i\hbar L_y z$. (C.8.E.3)

$\left[L_y, x\right]L_y$:

$\{(zp_x - xp_z)x - x(zp_x - xp_z)\}L_y = -i\hbar z L_y$. (C.8.E.4)

$L_z[L_z, x]$:

$L_z\{(xp_y - yp_x)x - x(xp_y - yp_x)\} = i\hbar L_z y$. (C.8.E.5)

It comes as no surprise, from comparison with (7.42)→ cyclic permutation,

$[L_z, x]L_z$ to be $i\hbar y L_z$.

So, (C.8.E.1)

$[L^2, x] = i\hbar(-L_y z - zL_y + L_z y + yL_z)$. (C.8.E.6)

(C.8.E.6):

$i\hbar(-L_y z - zL_y + L_z y + yL_z) = i\hbar(-2L_y z + 2L_z y - zL_y + yL_z + L_y z - L_z y) =$

$= i\hbar(-2L_y z + 2L_z y + \left[L_y, z\right] - [L_z, y]) = 2i\hbar(L_z y - L_y z + i\hbar x)$. (C.8.E.7)

Then,

$[L^2, x] = 2i\hbar(L_z y - L_y z + i\hbar x)$. (C.8.E.8)

The next step to be taken:

$\left[L^2, [L^2, x]\right]$, with (C.8.E.8) using permutations:

$\left[L^2, [L^2, x]\right] = 2i\hbar\left[L^2, (L_z y - L_y z + i\hbar x)\right] = 2i\hbar(L_z[L^2, y] - L_y[L^2, z] + i\hbar[L^2, x])$,

or just recombine $\left[L^2, (L_z y - L_y z + i\hbar x)\right]$ into $(L_z[L^2, y] - L_y[L^2, z] + i\hbar[L^2, x])$.

Then, with (7.42) and (7.43), i.e., using the expressions for $[L^2, z]$ and $[L^2, y]$

$\left[L^2, [L^2, x]\right] = -4\hbar^2 L_z(zL_x - L_z x) + 4\hbar^2 L_y(L_y x - yL_x) - 2\hbar^2(L^2 x - xL^2)$. (C.8.E.9)

Compare (C.8.E.9) with (7.45) and the permutations are demonstrated.

(C.8.E.9):

$\left[L^2, [L^2, x]\right] = -\hbar^2\{4L_z z L_x - 4L_z^2 x - 4L_y^2 x + 4L_y y L_x + 2(L^2 x - xL^2)\}$. (C.8.E.10)

(C.8.E.10):

$\left[L^2, [L^2, x]\right] = -\hbar^2\{4(L_z z + L_y y)L_x - 4(L_z^2 + L_y^2)x + 2(L^2 x - xL^2)\}$. (C.8.E.11)

Now, $[L_x^2, x] = 0 \rightarrow L_x x L_x = x L_x^2 = L_x^2 x$.

Plug this into (C.8.E.11):

$\left[L^2, [L^2, x]\right] = -\hbar^2\{4(L_z z + L_y y + L_x x)L_x - 4(L_z^2 + L_y^2 + L_x^2)x + 2(L^2 x - xL^2)\}$, (C.8.E.12)

With (7.47): $L_z z + L_y y + L_x x = 0$, an operator,

$\left[L^2, [L^2, x]\right] = 2\hbar^2(L^2 x + xL^2)$. (C.8.E.13)

Consequently, with (7.49)-(7.52) and $z \rightarrow x$, the conclusion for the matrix element $\langle n, l, m|x|n', l', m'\rangle$ to be non-zero is

$l' = l \pm 1$, or $\Delta l = \pm 1$.

For the matrix element $\langle n, l, m|y|n', l', m'\rangle$ not to be zero is, with similar analyzes and using circular permutations, the conclusion is also:

$\Delta l = \pm 1$.

Next, the selection rule for m.

In section 12.5 of *The Undergraduate Course* and section 7.4 the selection rule for the matrix element $\langle n, l, m|z|n', l', m'\rangle$ is $\Delta m = 0$.

With $[L_z, z] = 0$, $\Delta m = 0$ is given in (7.41).
What about the matrix element $\langle n, l, m|x|n', l', m'\rangle$? There is no operator as $[L_x, x] = 0$. In section 13.11 of *The Undergraduate Course*, the raising and lowering operators are used:
$x^{\pm} = x \pm iy$, *(13.129).*
So:
$x = (x^+ + x^-)/2,$
and
$y = -i(x^+ - x^-)/2.$
$[L_z, x^+] = L_z(x + iy) - (x + iy)L_z = \big(xp_y - yp_x\big)(x + iy) - x^+L_z =$
$= \hbar x^+ + x^+L_z - x^+L_z = \hbar x^+.$
Nota Bene:
$L_z(x + iy) = \big(xp_y - yp_x\big)(x + iy) = \hbar x^+ + x^+L_z.$
So,
$[L_z, x^{\pm}] = \pm\hbar x^{\pm}$, *(13.130).*
Then:
$\langle n, l, m|[L_z, x^+] - \hbar x^+|n', l', m'\rangle = 0.$
Then:
$\langle n, l, m|L_z x^+ - x^+L_z - \hbar x^+|n', l', m'\rangle = \hbar\langle n, l, m|mx^+ - x^+m' - x^+|n', l', m'\rangle =$
$= \hbar(m - m' - 1)\langle n, l, m|x^+|n', l', m'\rangle = 0$, *(13.131).*
Simarlily,
$\langle n, l, m|L_z x^- - x^-L_z + \hbar x^-|n', l', m'\rangle = \hbar\langle n, l, m|mx^- - x^-m' + x^-|n', l', m'\rangle =$
$= \hbar(m - m' + 1)\langle n, l, m|x^-|n', l', m'\rangle = 0$, *(13.132).*
Just below *(13.132)*, Fp explained the matrix elements $\langle n, l, m|x|n', l', m'\rangle$ and $\langle n, l, m|y|n', l', m'\rangle$ to be non-zero if $m' = m \pm 1$, where us has been made of $x = (x^+ + x^-)/2$ and $y = -i(x^+ - x^-)/2$.
With the result of section 7.4 for the matrix element $\langle n, l, m|z|n', l', m'\rangle$ to be non-zero for $m' = m$, (8.160) and (8.161).

Exercise 8.3 About the dipole moment.

Demonstrate that
$\langle|\boldsymbol{\epsilon}\cdot\boldsymbol{f}_{21}|^2\rangle = \frac{f_{21}^2}{3}$,
where the average is taken over all directions of the incident radiation.
This result is presented in (8.167).
To obtain (8.167) isotropic radiation, Fp presented the relevant equations in To obtain (8.167) iso tropic radiation, Fp presented the relevant equations in *The Undergraduate Course*: *(13.100)-(13.104).*
Then, it's about evaluating *(13.104)* for the unit sphere:
$\langle|\boldsymbol{\epsilon}\cdot\boldsymbol{f}_{21}|^2\rangle_{av} = \frac{f_{21}^2}{4\pi}\int\int \sin^3\theta\cos^2\phi\, d\theta d\phi = \frac{f_{21}^2}{3}$, (8.167).
With (8.167),(8.166),(8.169) and substituting $\omega = \omega_{21}$ in (8.162), (8.170) is found.
To obtain (8.171) Fp used the dipole moment, matrix element $\boldsymbol{f}_{21} = \langle 2|\boldsymbol{x}|1\rangle$, to be of the order of magnitude of the Bohr radius: *(13.100)-(13.104).*
I shall recapitulate the analysis of page 187 of *The Undergraduate Course*:
It is about unpolarized isotropic radiation. "…… *we can define a set of Cartesian coordinates*

such that a wave vector $\boldsymbol{k}$*, which specifies the direction of wave propagation, points along the* z*-axis, and the vector* $\boldsymbol{f}_{21}$*, which specifies the direction of the atomic dipole moment, lies in the* x*-*z *plane. It follows that the vector* $\boldsymbol{\epsilon}$*, which specifies the direction of wave polarization, must lie in the* x*-*y *plane, since it has to be orthogonal to* $\boldsymbol{k}$*."*
So,
" $\boldsymbol{k} = (0,0,k)$*, (13.100)*
$\boldsymbol{f}_{21} = (f_{21}\ sin\,\theta\,, 0, f_{21}\,cos\,\theta), (13.101)$
$\boldsymbol{\epsilon} = (cos\,\phi\,, sin\,\phi), (13.102)$
which implies that "
$|\boldsymbol{\epsilon}\cdot\boldsymbol{f}_{21}|^2 = f_{21}^2\sin^2\theta\cos^2\phi$ *,(13.103).*
"We must average the above quantity ($|\boldsymbol{\epsilon}\cdot\boldsymbol{f}_{21}|^2$*) over all possible values of* θ *and* ϕ*. Thus,*
$\langle|\boldsymbol{\epsilon}\cdot\boldsymbol{f}_{21}|^2\rangle_{av} = \frac{f_{21}^2}{4\pi}\int\int sin^2\,\theta\,cos^2\phi\,d\Omega$ *, (13.104),*
where $d\Omega = sin\,\theta d\theta d\phi$*, and the integral is taken over all solid angle."*
Then,
$\langle|\boldsymbol{\epsilon}\cdot\boldsymbol{f}_{21}|^2\rangle_{av} = \frac{f_{21}^2}{4\pi}\int\int \sin^3\theta\cos^2\phi\,d\theta d\phi = \frac{f_{21}^2}{3}$, (8.167).
The modulus squared of the dipole moment d:
$d^2 = |ef_{21}|^2$, (8.167), (8.168) and *(13.128)*.

Exercise 8.4 About the spontaneous decay rate, the spectral line width, and the matrix elements

Demonstrate that the spontaneous decay rate (via an electric dipole transition) from any $2p$ state to a $1s$ state of a hydrogen atom is
$w_{2p\to1s} = (\frac{2}{3})^8\alpha^5\frac{m_ec^2}{\hbar} = 6.26\times10^8\text{s}^{-1}$,
where α is the fine structure constant.
Fp dealt with this problem in section 13.12 on $2P\to1S$ *Transitions in Hydrogen, The Undergraduate Course*.
I shall cite Fp: "*Let us calculate the rate of spontaneous emission between the first excited state (i.e.,* $n = 2$*) and the ground-state (i.e.,* $n' = 1$*) of a hydrogen atom. Now the ground-state is characterized by* $l' = m' = 0$*. Hence, in order to satisfy the selection rules(13.133) and (13.134), the excited state must have the quantum numbers* $l = 1$ *and* $m = 0, \pm1$*.*
The selection rules are:
$\Delta l = \pm1$, (8.160),
$\Delta m = 0, \pm1$, (8.161).
Note $l \geq 0 \to l = 1, m = 0, \pm1$.
The various matrix elements have to be calculated. To this end, the wave function of a hydrogen atom is needed:
$\psi_{n,l,m}(r,\theta,\phi) = R_{n,l}Y_{l,m}(\theta,\phi)$*, (13.135),*
where the radial functions $R_{n,l}$ *are given in Sect. 9.4 on Hydrogen Atom,(9.65)-(9.70), and the spherical harmonics* $Y_{l,m}$ *are given in Sect. 8.7 on spherical Harmonics, (8.91)-(8.96).*
Keep in mind: for the z-axis $\Delta m = 0$, and for the x- and y-axis $\Delta m = \pm1$.
To evaluate the integrals:
$x = r\sin\theta\cos\phi$,
$y = r\sin\theta\sin\phi$,

$z = r\cos\theta$.
For example, to obtain the matrix element $\langle 1,0,0|z|2,1,0\rangle$, the following integral has to be evaluated:

$$\langle 1,0,0|z|2,1,0\rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{1,0}Y_{0,0}(\theta,\phi)\ r\cos\theta\ [R_{2,1}Y_{1,0}(\theta,\phi)]^* r^2\sin\theta dr d\theta d\phi, \quad \text{(C.8.E.14)}$$

Then with *(9.65),(9.67),(8.91)* and *(8.92)*, the integral in (C.8.E.14) results into:

$\langle 1,0,0|z|2,1,0\rangle = \sqrt{2}\frac{2^7}{3^5}a_0$, *(13.138),*

after *"some straight-forward, but tedious integration".*

With the expressions for the radial wave function and the spherical harmonics, the matrix elements for the other coordinates are found:

$\langle 1,0,0|x|2,1,\pm 1\rangle = \pm\frac{2^7}{3^5}a_0$, *(13.136),*

and

$\langle 1,0,0|y|2,1,\pm 1\rangle = i\frac{2^7}{3^5}a_0$, *(13.137),*

where a_0 is the Bohr radius in Eq. (9.58).

Now, all the ingredients for calculating the spontaneous decay rate (via an electric dipole transition) are available.

To this end the modulus squared of the dipole moment is determined. For the $2P \to 1S$ transition the modulus squared of the dipole moment is the same for $m = 0,1,$ or -1.

The dipole moment d , (8.155), (8.168) and *(13.128)*:

$$e^2 f_{21}^2 = |\langle 1,0,0|ex|2,1,\pm 1\rangle|^2 + |\langle 1,0,0|ey|2,1,\pm 1\rangle|^2 + |\langle 1,0,0|ez|2,1,0\rangle|^2. \quad \text{(C.8.E.15)}$$

Plug into (C.8.E.15) the matrix elements.

Then:

$$d^2 = |ef_{21}|^2 = \frac{2^{15}}{3^{10}}(ea_0)^2\ . \quad \text{(C.8.E.16)}$$

To calculate the spontaneous rate of emission ω_{21} is needed, (8.170).

(8.60):

$\omega_{21} = \frac{E_2 - E_1}{\hbar}$.

Fp: *"Now, the energy of the eigenstates of the hydrogen atom characterized by the quantum numbers n, l, m is $E = E_0/n^2$, where the ground-state energy E_0 is specified in Eq. (9.57). Hence, the energy of the photon emitted during $2P \to 1S$ transmission is*

$\hbar\omega_{21} = \frac{E_0}{4} - E_0 = -\frac{3}{4}E_0$ *. (13.140).*

This corresponds to a wavelength of $1.215 \times 10^{-7} m$*."*

The rate of spontaneous transmission is given in (8.170) and *(13.141).*

$w_{2\to 1}^{spn} = \frac{{\omega_{21}}^3 e^2 f_{21}^2}{3\pi\epsilon_0\hbar c^3}$.

With (C.8.E.16), (13.140) and the given constants:

$w_{2\to 1}^{spn} = (\frac{2}{3})^8 \alpha^5 \frac{m_e c^2}{\hbar} = 6.27 \times 10^8\ s^{-1}$, *(13.143)*.

"*Here, $\alpha = 1/137$ is the fine-structure constant. Hence, the mean-life time of a hydrogen $2P$ state is*

$\tau_{2P} = (w_{2\to 1}^{spn})^{-1} = 1.6$ ns.

Incidentally, since the $2P$ only has a finite life-time, it follows from the energy-time uncertainty relation that the energy of this state is uncertain by an amount

$\Delta E_{2P} \sim \frac{\hbar}{\tau_{2P}} \sim 4 \times 10^{-7}$ eV, (13.144).
This uncertainty gives rise to a finite width of the spectral line associated with $2P \to 1S$ *transition. This natural line-width is of order*
$\frac{\Delta\lambda}{\lambda} \sim \frac{\Delta E_{2P}}{\hbar\omega_{21}} \sim 4 \times 10^{-8}$ *.(13.345) ".*

9 Scattering Theory

9.1 Introduction

The quantum theory of scattering is examined.
In Chapter 15 of *The Undergraduate Course*, Fp dealt with Scattering Theory.

9.2 Fundamental Equations

The Hamiltonian is introduced with a scattering potential.
(9.4), with (9.2) and (9.6):

$$H_0|\psi\rangle - E|\psi\rangle = -H_1|\psi\rangle \to -\frac{\hbar^2}{2m}\nabla^2|\psi\rangle - \frac{\hbar^2 k^2}{2m}|\psi\rangle = -H_1|\psi\rangle \to$$
$$\to -\langle \boldsymbol{x}|\frac{\hbar^2}{2m}\nabla^2|\psi\rangle - \frac{\hbar^2 k^2}{2m}\langle \boldsymbol{x}|\psi\rangle = -\langle \boldsymbol{x}|H_1|\psi\rangle. \qquad \text{(C.9.2.1)}$$

$\frac{\hbar^2 k^2}{2m}$ represents the free particle energy.
Then with (C.9.2.1) and $\nabla^2 \boldsymbol{x} = 0$, (9.5) is obtained.
To obtain (9.12), Fp used the outer product operator for continuous wave functions $|x''\rangle\langle x''|$.
(9.13)↔ (15.9), *The Undergraduate Course.*
The factor $1/(2\pi)^{3/2}$, results from normalization presented in (9.15).
(9.16), with the cosine rule, $r = |\boldsymbol{x}|$ and $r' = |\boldsymbol{x}'|$:

$$\lim_{r \gg r'} |\boldsymbol{x} - \boldsymbol{x}'| = \sqrt{x^2 + (x')^2 - 2\boldsymbol{x}\cdot\boldsymbol{x}'} \cong r\left(1 + \left(\frac{r'}{r}\right)^2 - \frac{\boldsymbol{x}\cdot\boldsymbol{x}'}{r}\right) \to r - \boldsymbol{e_r}\cdot\boldsymbol{x}' \ .$$

Then, the exponent in (9.13) can be written as a product of two exponents given in (9.19).
$\langle \boldsymbol{k}'|H_1|\psi\rangle$ can be considered as the Fourier transform of $\langle \boldsymbol{x}'|H_1|\psi\rangle$ in (9.22). Since, in (9.12), $\langle \boldsymbol{x}'|H_1|\psi\rangle = V(\boldsymbol{x}')\psi$.
The particle flux as presented in (9.23), can also be written as: $\boldsymbol{j} = \frac{i\hbar}{2m}(\psi\nabla\psi^* - \psi^*\nabla\psi)$.
With the incoming wave given in (9.24) the particle flux in (9.25) is found. Similarly, the particle flux associated with the scattered wave is obtained.

9.3 Born approximation

In this section further attention is given to (9.20).
The Born approximation is based on the assumption the scattering not to be particular strong. In that case the total wave function is set equal to the incident wave function. This could have been called the *Born identity*. However, *Born approximation* has been chosen.
This approximation is used to obtain an approximation for the scattering function $f(\boldsymbol{k}', \boldsymbol{k})$ in (9.22). In this way (9.32) is obtained.
(9.35) results from the isosceles triangle with $|k| = |k'|$, as explained by Fp just below (9.35).
(9.38) is found using integration by parts twice.

(9.39), the differential cross-section is obtained with (9.29), (9.35) and (9.37).
In (9.41): $E = \frac{(\hbar k)^2}{2m} = \frac{p^2}{2m}$.
On page 150, Fp considered low-and high energy approximations of the Yukawa potential. So, for the low energy approximation I expected the condition for bound states to be, with (9.37):
$\frac{2m}{\hbar^2}\frac{|V_0|}{\mu^3} \geq 2.7$, instead of $\frac{2m}{\hbar^2}\frac{|V_0|}{\mu^2} \geq 2.7$,
and for the high energy case, the high-k limit:
$\frac{2m}{\hbar^2}\frac{|V_0|}{\mu k^2} \ll 1$, instead of $\frac{2m}{\hbar^2}\frac{|V_0|}{\mu k} \ll 1$.

9.4 Partial Waves

Partial waves is about a series of spherical waves.
See also Chapters 8, 9 and section 15.4 of *The Undergraduate Course.*
For spherical harmonics and Legendre Polynomials see also Sections 4.4, 4.5.
(9.53) and (9.54), spherical Bessel functions and the Neumann function, are found in, i.e., Whittaker and Watson.
(9.57) is the generating function for spherical Bessel functions (Mahan, page 111).
Multiply (9.57) with $P_l(\cos\theta)$, use orthogonality (9.58), and (9.59) is found.
In (9.58) the expression for orthogonality is given. In §4.1 of Chapter 19, The orthogonality property, (9.58) has been derived (Chisholm and Morris).
Let's demonstrate the orthogonality property for $Y_{1,0}$ and $Y_{2,0}$.
First $Y_{1,0}$:
$\int_{-1}^{1}(\sqrt{\frac{4\pi}{3}}\sqrt{\frac{3}{4\pi}}\mu)^2\, d\mu = \frac{2}{3} = \frac{1}{1+1/2}$.
Next $Y_{2,0}$:
$\int_{-1}^{1}(\sqrt{\frac{4\pi}{5}}\sqrt{\frac{5}{16\pi}}[3\mu^2-1])^2 d\mu = \frac{2}{5} = \frac{1}{2+1/2}$,
and
$\int_{-1}^{1}\sqrt{\frac{4\pi}{3}}\sqrt{\frac{3}{4\pi}}\mu\sqrt{\frac{4\pi}{5}}\sqrt{\frac{5}{16\pi}}[3\mu^2-1]d\mu = 0$.
Note: no ϕ dependency → $m = 0$.
About (9.60), Fp: "It is well known ….." ,and the integral representation of the spherical Bessel function is presented. On page 214 of *The Undergraduate Course:"[see M. Abramowitz and I.A. Stegun, Handbook of mathematical functions, (Dover, New York NY, 1965), Eq.10.1.14]".*
I looked it up in my copy, page 438 (10.1.14):
$j_n(z) = \frac{1}{2}(-i)^n\int_0^\pi e^{iz\cos\theta}P_n(\cos\theta)\sin\theta\, d\theta.$
Now, substitute in this expression $\cos\theta = \mu$, then
$j_n(z) = -\frac{1}{2}(-i)^n\int_1^{-1} e^{iz\mu}\, P_n(\mu)d\mu = \frac{1}{2}(-i)^n\int_{-1}^{1} e^{iz\mu}\, P_n(\mu)d\mu.$
With $z = kr$ → (9.60).
The asymptotic behavior of the spherical Bessel functions and the Neuman function respectively, presented in (9.55) and (9.56) are plugged into (9.63)→ (9.64).
(9.65), FP: *"Note that $A_l = C_l\, cos\, \delta_l$ and $B_l = -C_l\, sin\, \delta_l$".*

The incident wave function, (9.47):
$\phi(\boldsymbol{x}) = \frac{1}{(2\pi)^{3/2}}\exp(ikr\cos\theta)$,
with (9.62)→ (9.67).
Comparing the coefficients in (9.66) and (9.67)→
→ $C_l = i^l(2l+1)\exp(i\delta_l) = \left(e^{\frac{i\pi}{2}}\right)^l (2l+1)\exp[i\left(\delta_l + \frac{l\pi}{2}\right)]$, (9.69).
(9.68):
$f(\theta) = (2\pi)^{3/2}\frac{r}{e^{ikr}}[\psi(\boldsymbol{x}) - \phi(\boldsymbol{x})]$.
With (9.66)-(9.68), $f(\theta)$ results into the expression presented in (9.70), the scattering amplitude.

9.5 Optical Theorem

In *The Undergraduate Course* the subject matter is part of section 15.4 on Partial Waves.
The differential scattering cross-section,(9.29):
$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$.
So, the total cross-section σ_{total} is found with the integral:
$\sigma_{\text{total}} = \oint d\Omega\,|f(\theta)|^2$.
There is a problem: $d\Omega$ is usually defined as the solid angle $r^2\sin\theta dr d\theta d\phi$.
Fp used $\sin\theta d\theta d\phi$ in (9.71). Actually Fp used $\sin\theta d\theta d\varphi$ →no r dependency.
To obtain (9.73), use has been made of:
$\mathrm{Im}[\exp(\mathrm{i}\delta_l)] = \sin\delta_l$.

9.6 Determination of Phase-Shifts

This section is about the evaluation of δ_l.
In (9.76) Fp presented the most general solution to the free space Schrödinger equation outside the range of the spherically symmetric potential. With no incoming spherical waves.
This compares with (9.63) and (9.69), given that
$A_l = C_l\cos\delta_l$,
and
$B_l = -C_l\sin\delta_l$.
Here, A_l and B_l are constants, where $A_l(r)$ in (9.76) is a combination of spherical Bessel functions and von Neumann functions.
Next, Fp derived the logarithmic derivative, β_{l+} of the lth radial wavefunction just outside the range of the potential: $r > a$.
Note: Mahan dealt with this problem in section 5.3.1 on Central Potentials in 3D. Mahan derives the tangent of the phase shift by matching the two solutions for $r < a$ and $r > a$ at $r = a$ by equating the eigenfunction and its first derivative. Then, divide the two equations.
So, it's equating of the logarithmic derivative at $r = a$, for $r < a$ and $r > a$.
Definition of the logarithmic derivative of a function is this derivative divided by the function. In this way β_{l+} in (9.78) is obtained.
Divide the right-hand side of (9.78) by $\cos\delta_l$ →an expression for δ_l , (9.79).
Next Fp derived a general solution for the Schrödinger equation for $r < a$ and a well-behaved solution at $r = 0$. Then, the general logarithmic derivative at $r = a$, β_{l-} ,(9.84), is

obtained. By equating $\beta_{l+} = \beta_{l-}$, both derivatives can be eliminated and the phase shift is found. The result is presented in (5.79), Mahan. There, the solution of the Schrödinger equation for $r < a$ is the spherical Bessel function.

9.7 Hard Sphere Scattering.

Hard sphere scattering means the potential is infinite for $r < a$ to be infinite.
Then, Fp:
$\beta_{l+} = \beta_{l-} = \infty \rightarrow$ (9.87).
On the other hand, at $r \downarrow a$,in (9.76) $\rightarrow \psi(a) \rightarrow 0$.
Consequently,
$\cos\delta_l\, j_l(ka) = \sin\delta_l \eta_l(ka) \rightarrow (9.87)$.
For $l = 0$, using equations (9.53) and (9.54) or (9.55) and (9.56), the phase-shift $\delta_0 = ka$, (9.89).
The radial wave function for $l = 0$, using equations (9.55), (9.56) and the phase-shift $\delta_0 = -ka$ (9.89), is presented in (9.90).
Then, Fp considers the low energy limit of $\tan\delta_l$. For the low energy case: $ka \ll 1$.
Well, $\tan x = x + \frac{1}{3}x^3 + \frac{2}{15}x^5 + \cdots$ for $-\pi/2 < x < \pi/2$.
Then,
$\tan\delta_0 \cong -ka$ and $\tan\delta_1 \cong -\frac{(ka)^3}{3}$.
So, $\delta_1 \ll \delta_0$.
In (9.95) Fp presented the differential cross-section as given in (9.29).
For $l = 0$:
$f(\theta) = \frac{e^{\delta_0}}{k}\sin\delta_0$,
since $P_0 = 1$,(9.51).
The high energy case. The total cross-section is given in (9.72)→(9.97).The result of the summation (9.97), an arithmetic series→(9.98).
In discussing the result given in (9.98), Fp mentioned the optical theorem about the so-called Poisson spot.

9.8 Low Energy Scattering

As mentioned in the fore going section, partial waves with $l > 0$ make a negligible contribution to the scattering cross-section.
Fp considered a finite potential well. So, $V_0 < 0$.
The external wavefunction $\rightarrow r > a$, and
the internal wavefunction $\rightarrow r < a$.
The solution for the latter case is derived from the differential equation (9.82). On the other hand for $r < a$ and $r \rightarrow 0$, the Neumann functions become singular. So the internal wave function is the spherical Bessel function for $l = 0$. Still, (9.82) defines k'.

Remark:
Let us match (9.99) and (9.100) at $r = a$ .Then,
$e^{i\delta_0}\sin(ka + \delta_0)\frac{1}{ka} = B\sin(k'a)\frac{1}{a} \rightarrow B = \frac{e^{i\delta_0}\sin(ka+\delta_0)}{k\sin(k'a)}$.

Fp, below (9.100): "*Here, B is a constant, …..*". To me, it looks to be a function of k, k' and δ_0.

(9.102) results from the Bessel function of imaginary argument i_l. This represents a decaying function for $l = 0$.
In (9.104) Fp presents the result for an attractive potential. (9.105) represents a repulsive potential.
For the attractive potential and (9.82):
$k'^2 = k^2 + \frac{2m}{\hbar^2}|V_0|$ → (9.109).

9.9 Resonance Scattering

This section is about a significant exception to the independence of the cross-section on energy.
In (9.111) it is shown the total cross-section to be dependent on $\frac{1}{k^2}$. so, the cross-section depends on the energy: $E = \frac{k^2\hbar^2}{2m}$.
The condition presented in (9.112) leads to: $k^2a^2 = 0$. Hence, $E = 0$ → a bound state at zero energy. This cannot be a stable situation.
In the subsequent analysis, Fp dealt with the phase shift $l \neq 0$.
Then, Fp obtained the *Breit-Wigner* formula → (9.118).

Exercises

Exercise 9.1 Application of the Born approximation

Consider a scattering potential 0f the form:
$V(r) = V_0 \exp(-\frac{r^2}{a^2})$.
Calculate the differential scattering cross-section, $d\sigma/d\Omega$, using the Born approximation.
The integral to be analyzed is given in (9.34):
$f(\theta) = -\frac{2m}{\hbar^2 q}\int_0^\infty rV(r)\sin(qr)dr$,
with
$q = 2k\sin(\frac{\theta}{2})$, (9.35).
Then,
$f(\theta) = -\frac{2mV_0}{\hbar^2 q}\int_0^\infty r\exp(-\frac{r^2}{a^2})\sin(qr)dr.$
Some work has to be done to evaluate the integral.
I used the WolframAlpha App.
The result is:
$f(\theta) = -\frac{mV_0}{2\hbar^2}\sqrt{\pi}a^3e^{-a^2q^2/4}$.
The differential scattering cross-section:
$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$,(9.29):
$\frac{d\sigma}{d\Omega} = (\frac{mV_0}{2\hbar^2})^2\pi a^6e^{-a^2q^2/2}$.

Exercise 9.2 Application of Partial Waves to obtain the total Cross-Section.

Consider a scattering potential that takes the constant value V_0 for $r < R$ and is zero for $r > R$, where V_0may be either positive of negative. Using the method of partial waves, show that for $|V_0| \ll E = \frac{k^2\hbar^2}{2m}$, and $kR \ll 1$, the differential cross-section is isotropic, and the total cross-section is:

$\sigma_{tot} = (\frac{16\pi}{9})\frac{m^2V_0^2R^6}{\hbar^4}$.

Definition of isotropic: Identical in all directions, invariant with respect to the direction. So, an isotropic differential cross-section is one of which the scattering probability into a unit element of a solid angle is independent of scattering angles.

The infinitesimal solid angle element is:

$d\Omega = \sin\theta d\theta d\phi$.

So,

$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \rightarrow$ constant C.

$\sigma_{tot} = C\oint \sin\theta d\theta d\phi = 4\pi C$.

What about C?

Assume the definition of isentropic scattering to be correct, I have to prove:

$\frac{d\sigma}{d\Omega} = (\frac{4}{9})\frac{m^2V_0^2R^6}{\hbar^4}$,

or

$f(\theta) = (\frac{2}{3})\frac{m|V_0|R^3}{\hbar^2}$, independent of θ (and ϕ).

The external wavefunction, $r > R$,(9.99):

$A_0(r) = e^{i\delta_0}\sin(kr + \delta_0)/kr$,

and

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

The internal wavefunction, $r < R$,(9.100):

$A_0(r) = B\sin(k'r)/r$,

and

$E - |V_0| = \frac{k'^2\hbar^2}{2m} \rightarrow k' \approx \sqrt{E}\sqrt{\frac{2m}{\hbar^2}}(1 - \frac{|V_0|}{2E}) \rightarrow \frac{k}{k'} \approx (1 + \frac{|V_0|}{2E})$. (C.9.E.1)

Now, I assume with $|V_0| \ll E$:

$k \cong k'$.

To find out about $\frac{d\sigma}{d\Omega}$, δ_0 has to be obtained. In section 9.8, Fp analyzed $k \ll k'$.

For $k \cong k'$, (9.105) can be used to obtain the phase shift:

$\tan(kR + \delta_0) = \frac{k}{k'}\tan(k'R)$.

Given is: $kR \ll 1$. Consequently, $k'R \ll 1$ and $\delta_0 \ll 1$.

Next, I use the series expansion for $\tan x = x + \frac{1}{3}x^3 + \frac{2}{15}x^5 + \cdots$.

Then, (9.105):

$kR + \delta_0 + \frac{1}{3}(kR)^3 + (kR)^2\delta_0 + kR\delta_0^2 + \delta_0^3 + \cdots = \frac{k}{k'}k'R + \frac{1}{3}\frac{k}{k'}(k'R)^3 + \cdots$, (C.9.E.2)

(C.9.E.2) becomes:

$$\delta_0\left(1+(kR)^2+kR\delta_0+\frac{1}{3}\delta_0^2+\cdots\right)=\frac{1}{3}[\frac{k}{k'}(k'R)^3-(kR)^3+\cdots]. \qquad \text{(C.9.E.3)}$$

With (C.9.E.1), (C.9.E.2) gives:

$$\delta_0=\frac{1}{3}[\left(1+\frac{|V_0|}{2E}\right)\left(1-\frac{3|V_0|}{2E}\right)(kR)^3-(kR)^3]\rightarrow\ -\frac{1}{3}\frac{|V_0|}{E}(kR)^3. \qquad \text{(C.9.E.4)}$$

Note: δ_0 a dimensionless number.

With E:

$$\delta_0=-\frac{2}{3}\frac{m|V_0|R^3}{\hbar^2}k\ . \qquad \text{(C.9.E.5)}$$

(9.70), $l=0$ and the approximation for $\sin\delta_0\approx\delta_0$:

$$f(\theta)=e^{i\delta_0}\sin(\delta_0)\frac{1}{k}=e^{i\delta_0}\delta_0/k.$$

Then with (C.9.E.5):

$$\frac{d\sigma}{d\Omega}=|f(\theta)|^2=(\frac{4}{9})\frac{m^2V_0^2R^6}{\hbar^4}\ .$$

Consequently, the differential cross-section is isotropic and the total cross-section is:

$$\sigma_{tot}=|f(\theta)|^2\oint\sin\theta d\theta d\phi=(\frac{16\pi}{9})\frac{m^2V_0^2R^6}{\hbar^4}\ . \qquad \text{(C.9.E.6)}$$

Suppose that the energy is slightly changed. Show that the angular distribution can be written as

$$\frac{d\sigma}{d\Omega}=A+B\cos\theta.$$

Suppose that the energy slightly changed? Meaning? Of the scattering potential? Well, that does not matter. Since, $|V_0|\ll E$, a slight change in V_0 produces again isotropic behavior of the differential cross-section.

So, I assume Fp meant in (9.70) the summation for the scattering amplitude is:

$$f(\theta)=e^{i\delta_0}\sin(\delta_0)\frac{1}{k}+3e^{i\delta_1}\sin(\delta_1)\sqrt{\frac{4\pi}{3}}Y_{1,0}(\theta)=$$

$$=e^{i\delta_0}\sin(\delta_0)\frac{1}{k}+3e^{i\delta_1}\sin(\delta_1)\frac{1}{k}\cos\theta\ . \qquad \text{(C.9.E.7)}$$

Now, with (C.9.E.7):

$$\frac{d\sigma}{d\Omega}=|f(\theta)|^2=\frac{1}{k^2}[e^{i\delta_0}\sin(\delta_0)+3e^{i\delta_1}\sin(\delta_1)\cos\theta]$$

$$=\frac{1}{k^2}[e^{i\delta_0}\sin(\delta_0)+3e^{i\delta_1}\sin(\delta_1)\cos\theta]\,[e^{-i\delta_0}\sin(\delta_0)+3e^{-i\delta_1}\sin(\delta_1)\cos\theta]=$$

$$=\frac{1}{k^2}[\sin^2(\delta_0)+9\sin^2(\delta_1)\cos^2\theta+6\sin(\delta_0)\sin(\delta_1)\cos(\delta_0-\delta_1)\cos\theta]\ , \qquad \text{(C.9.E.8)}$$

Compare (C.9.E.8) with $\frac{d\sigma}{d\Omega}=A+B\cos\theta$, what to conclude?

Remark: obviously I can write:

$f(\theta)=C+D\cos\theta$, where C and D are complex numbers.

When I am allowed to assume a priori $\sin^2(\delta_1)\ll\sin(\delta_0)\sin(\delta_1)\ll\sin^2(\delta_0)\rightarrow$

$$\rightarrow\frac{\sin(\delta_1)}{\sin(\delta_0)}\ll 1\ll\frac{\sin(\delta_0)}{\sin(\delta_1)},$$

(9.28) resembles $\frac{d\sigma}{d\Omega}=A+B\cos\theta$.

Hence,

$$\frac{d\sigma}{d\Omega}=\frac{1}{k^2}[\sin^2(\delta_0)+6\cdot\sin(\delta_0)\sin(\delta_1)\cos(\delta_0-\delta_1)\cos\theta]. \qquad \text{(C.9.E.9)}$$

An approximate expression for B/A, with (C.9.E.9):

$$\frac{B}{A}=\frac{6\cdot\sin(\delta_1)\cos(\delta_0-\delta_1)}{\sin(\delta_0)}\approx 6\frac{\sin(\delta_1)}{\sin(\delta_0)}.$$

Exercise 9.3 About scattering by a repulsive δ-shell potential

Consider scattering by a repulsive δ-shell potential:

$V(r) = \frac{\hbar^2}{2m}\gamma\delta(r-a)$,

where $\gamma > 0$.

Find the equation that determines the s-wave phase-shift, δ_0, as a function of k (where $E = \frac{k^2\hbar^2}{2m}$). Assume $\gamma \gg a^{-1}, k$.(Meaning: both a^{-1} and k ?)

Note , I will use a instead of R. R will be used for the radial wavefunction R_l.

The phase-shift needs to be determined. Consequently, the wave functions and their derivatives need to be matched at $r = a$. How to deal with this matching with a δ-shell potential involved when a discontinuity is involved? The wavefunctions can be matched, the derivatives ask for special attention.

I will use the method presented by Mahan on page 45. Mahan demonstrated this method for the one-dimensional case. To this end, the Schrödinger equation is written as:

$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}[E - V(x)]\psi(x).$ (C.9.E.10)

Integrate this equation, term by term, over the interval $a-\epsilon$ to $a+\epsilon$. Here, ϵ is small, and eventually $\epsilon \to 0$, with (C.E.9.10):

$\int_{a-\epsilon}^{a+\epsilon} dx\ \frac{d^2\psi(x)}{dx^2} = \left(\frac{d\psi}{dx}\right)_{a+\epsilon} - \left(\frac{d\psi}{dx}\right)_{a-\epsilon} = -\frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} dx\,[E - V(x)]\psi(x)$.(C.9.E.11)

In the integral on the right in (C.9.E.11), $-\frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} dx\,E$ vanishes.

For the integral with the delta-function potential:

$\frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} dx\,\frac{\hbar^2}{2m}\gamma\delta(x-a)\psi(x) \to \gamma\psi(a).$ (C.9.E.12)

Then, with (C.9.E.11):

$\left(\frac{d\psi}{dx}\right)_{a+\epsilon} - \left(\frac{d\psi}{dx}\right)_{a-\epsilon} = \gamma\psi(a).$ (C.9.E.13)

So, the tool for matching the derivates has been obtained.

Away from the singularity, $E = \frac{k^2\hbar^2}{2m}$ and $V = 0$.

$r > a$, and $l = 0$, the wavefunction is, (9.99):

$R_0(r) = e^{i\delta_0}\sin(kr + \delta_0)/kr$.

$r < a$, and $E \gg V$, since $\gamma\delta(r-a) \approx 0$, I assume. Though $\gamma \gg k$.

Then, (9.100), $E > 0$:

$R_0(r) = B\sin(kr)/r$.

At the singularity.

I use the notation for the wavefunction presented in (9.81) and (9.82), with (C.9.E.13):

$\left(\frac{du_0}{dr}\right)_{a+\epsilon} - \left(\frac{du_0}{dr}\right)_{a-\epsilon} = \gamma u_0(a),$ (C.9.E.14)

and

$u_0(r) = rR_0(r)$.

Matching the wave functions at $r = a$:

$e^{i\delta_0}\sin(ka + \delta_0)/k = B\sin(ka)$. (C.9.E.15)

The derivatives with (C.9.E.14) and $\epsilon \to 0$:

$e^{i\delta_0}\cos(ka + \delta_0) - Bk\cos(ka) = \gamma B\sin(ka)$. (C.9.E.16)

Combine (C.9.E.15) and (C.9.E.16):

$$\tan(ka+\delta_0)=\frac{k\sin(ka)}{\gamma\sin(ka)+k\cos(ka)}=\frac{\tan(ka)}{1+\frac{\gamma}{k}\tan(ka)}\,. \qquad \text{(C.9.E.17)}$$

Unless $\sin(ka)\ll\cos(ka)$ and with $\gamma\gg k$, (C.9.E.17)→

$$\tan(ka+\delta_0)=\frac{k}{\gamma}\,, \qquad \text{(C.9.E.18)}$$

→ δ_0 as a function of k ($\frac{k}{\gamma}$: a dimensionless number).

Obviously, also (C.9.E.17) gives δ_0 as a function of k.

Remark:

$$\tan(ka+\delta_0)=\frac{\tan(ka)+\tan\delta_0}{1-\tan(ka)\cdot\tan\delta_0}\,.$$

Then, with (C.9.E.17):

$$\tan\delta_0=-\frac{\frac{\gamma}{k}\tan^2(ka)}{1+\frac{\gamma}{k}\tan(ka)+\tan^2(ka)}\,. \qquad \text{(C.9.E.17a)}$$

Does (C.9.E.17) or (C.9.E.18) resembles the hard sphere result if $\tan(ka)$ is not close to zero?

The hard sphere phase-shift, (9.89):

$\delta_0=-ka.$

Well, with $\sin(ka)\sim\cos(ka)$ (or $\tan(ka)$ is not close to zero) and $\gamma\gg k\rightarrow\tan(ka+\delta_0)\approx 0\rightarrow\ \delta_0=-ka$, the hard sphere phase-shift. The same result is obtained from (C.9.E.17a)

About resonance.

Is resonance possible, when $\tan(ka)$ is close to zero? In other words, when $\cot\delta_0$ goes through zero from the positive side(?) as k increases.

$\tan(ka)\approx 0\rightarrow ka\approx 0$.

Furthermore, $\cot\delta_0\approx 0\rightarrow\delta_0\approx\frac{\pi}{2}$.

On page 158 Fp writes: *"We have seen that there is a resonant effect when the phase-shift of the s-waves takes the value $\pi/2$."*

Well, in the case of a repulsive δ-shell potential , $\cot\delta_0\approx 0\rightarrow\delta_0\approx\frac{\pi}{2}$. So, resonance behavior can occur.

Next, determine the approximate positions of the resonances. It do not know the definition of the position of the resonances. Are the resonances the resonant energies? Well, the resonant energies have to be compared in this exercise with the bound state energies for a particle confined within an infinite spherical well.

First, I will pay attention to the bound states for a particle confined within an infinite spherical well with radius a.

The radial wave function disappears at $r=a$.

$V(r)=0$ for $0<r<0$,

and

$V(r)=\infty$ for $a<r$.

The equations describing this potential are given in (9.53) and (9.54) with the above values for $V(r)$ or Eq. (5.16) with $V(r)=0$.

In the spherical well the solution is presented by (9.53), since the solution $y_l(kr)$ diverges at $r=0$.

So,

$R_l(kr) = C_1 j_l(kr)$, (C.9.E.19)

where, $k^2 = \frac{2mE}{\hbar^2}$.

$j_l(kr)$ must be forced to vanish at $r = a$. This will give us the eigenvalues. For some values of l these are given in the table below(Abramowitz and Stegun).

For $l = 0 : \rightarrow j_0(kr) = \frac{\sin kr}{kr}$

At $r = a : j_0(ka) = \frac{\sin ka}{ka}$,

consequently $k_n a = n\pi$. So $k_n = \frac{n\pi}{a}$.

The eigenvalues are: $E_n = \frac{\hbar^2}{2m}(\frac{n\pi}{a})^2$. So there is a bound state at zero energy: $n = 0$.

See the text below (9.112) in the section on Resonance Scattering.

To construct the table below, look up a table of zeros of spherical Bessel functions (Abramowitz and Stegun).

For $l = 0 : k_n a = n\pi$, $n = 1,2,3,4,5,6$.

And the six lowest eigenvalues are: $E_n = \frac{\hbar^2}{2m}(\frac{n\pi}{a})^2$, $n = 1,2,3,4,5,6$..

In addition, for $l = 1$ and $2 \rightarrow k_n a$, $n = 1,2,3,4,5,6$:

zeros	$l = 0$	$l = 1$	$l = 2$
$n =$	$k_n a =$	$k_n a =$	$k_n a =$
1	π	4.4934	5.7635
2	2π	7.7252	9.9050
3	3π	10.9041	12.3229
4	4π	14.0662	15.5146
5	5π	17.2208	18.6890
6	6π	20.3713	21.8539

And the eigenvalues are :

$E_n = \frac{\hbar^2}{2ma^2}(k_n a)^2$. (C.9.E.20)

These bound energies can be considered as resonance energies.

What about the resonance energies of the repulsive of the δ-shell potential?

I start with the determination of the phase-shifts for the repulsive δ-shell potential.

The general solution for the wave function at $r > a$, (9.76) and (9.77):

$\psi(\boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\sum_{l=0,\infty} i^l\,(2l+1)e^{i\delta_l}[\cos\delta_l\, j_l(kr) - \sin\delta_l \eta_l(kr)]$, (C.9.E.21)

and at $r < a$, (9.80) and (9.81):

$\psi(\boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\sum_{l=0,\infty} i^l\,(2l+1)\,\frac{u_l(r)}{kr}P_l(\cos\theta)$, (C.9.E.22)

where $u_l(r)$ satisfies the differential equation with $V(r) = 0$.

Then,

$u_l(r) = j_l(kr)$, (9.53) the spherical Bessel function.

Both wavefunctions are continuous at $r = a$, with (C.9.E.21) and (C.E.9.23):

$$\sum_{l=0,\infty} i^l\,(2l+1)\,\frac{u_l(a)}{a}P_l(\cos\theta) =$$

$$= \sum_{l=0,\infty} i^l\,(2l+1)e^{i\delta_l}[\cos\delta_l\, j_l(ka) - \sin\delta_l\eta_l(ka)]\,. \qquad \text{(C.9.E.23)}$$

In addition the matching condition presented in (C.9.E.13):

$$\left(\frac{d\psi}{dr}\right)_{a+\epsilon} - \left(\frac{d\psi}{dr}\right)_{a-\epsilon} = \gamma\psi(a). \qquad \text{(C.9.E.24)}$$

I assume to be allowed to analyze the equations (C.9.E.23) and (C.9.E.24), for a particular l.

Then, (C.9.E.23):

$$\frac{u_l(a)}{a}P_l(\cos\theta) = e^{i\delta_l}[\cos\delta_l\, j_l(ka) - \sin\delta_l\eta_l(ka)], \qquad \text{(C.9.E.25)}$$

and (C.9.E.21), (C.9.E.22), (C.9.E.24):

$$(e^{i\delta_l}[\cos\delta_l\frac{d}{dr}j_l(kr) - \sin\delta_l\frac{d}{dr}\eta_l(kr)])_{a+\epsilon} - \left(P_l(\cos\theta)\frac{d}{dr}\frac{j_l(kr)}{kr}\right)_{a-\epsilon} =$$

$$= \gamma\frac{u_l(a)}{a}P_l(\cos\theta). \qquad \text{(C.9.E.26)}$$

Now, the (C.9.E.25) and (C.9.E.26) determine the phase shift δ_l, similar to (9.79).

Divide (C.9.E.26) and ((C.9.E.25):

$$\frac{([\cos\delta_l\frac{d}{dr}j_l(kr) - \sin\delta_l\frac{d}{dr}\eta_l(kr)])_{a+\epsilon}}{[\cos\delta_l j_l(ka) - \sin\delta_l\eta_l(ka)]} = \frac{\left(\frac{d}{dr}\frac{j_l(kr)}{kr}\right)_{a-\epsilon} + \gamma\frac{u_l(a)}{ka}}{\frac{u_l(a)}{ka}}\,, \qquad \text{(C.9.E.27)}$$

and

$$u_l(a) = j_l(ka).$$

$$\frac{([\frac{d}{dr}j_l(kr) - \tan\delta_l\frac{d}{dr}\eta_l(kr)])_{r=a}}{[j_l(ka) - \tan\delta_l\eta_l(ka)]} = \frac{\left(\frac{d}{dr}\frac{j_l(kr)}{kr}\right)_{r=a} + \gamma\frac{j_l(ka)}{ka}}{\frac{j_l(ka)}{ka}}\,. \qquad \text{(C.9.E.28)}$$

$$([\frac{d}{dr}j_l(kr) - \tan\delta_l\frac{d}{dr}\eta_l(kr)])_{r=a}\cdot j_l(ka) =$$

$$= [j_l(ka) - \tan\delta_l\eta_l(ka)][ka\,\left(\frac{d}{dr}\frac{j_l(kr)}{kr}\right)_{r=a} + \gamma j_l(ka)]\,. \qquad \text{(C.9.E.29)}$$

Then

$$[\tan\delta_l\eta_l(ka)]\left[ka\,\left(\frac{d}{dr}\frac{j_l(kr)}{kr}\right)_{r=a} + \gamma j_l(ka)\right] - \left[\tan\delta_l\frac{d}{dr}\eta_l(kr)\right]_{r=a}\cdot j_l(ka) =$$

$$-\left[\frac{d}{dr}j_l(kr)\right]_{r=a}\cdot j_l(ka) + [j_l(ka)][ka\,\left(\frac{d}{dr}\frac{j_l(kr)}{kr}\right)_{r=a} + \gamma j_l(ka)]. \qquad \text{(C.9.E.30)}$$

Replace in(C.9.E.30)

$\frac{d}{dr} \to \frac{d}{dkr}$:

$$\tan\delta_l\left[\eta_l(ka)\left\{ka\left(\frac{d}{dkr}\frac{j_l(kr)}{kr}\right)_{r=a} + \frac{\gamma}{k}j_l(ka)\right\} - j_l(ka)\left(\frac{d}{dkr}\frac{\eta_l(kr)}{kr}\right)_{r=a}\right] =$$

$$= j_l(ka)[ka\,\left(\frac{d}{dkr}\frac{j_l(kr)}{kr}\right)_{r=a} + \frac{\gamma}{k}j_l(ka) - \left(\frac{d}{dkr}\frac{j_l(kr)}{kr}\right)_{r=a}]\,. \qquad \text{(C.9.E.31)}$$

In (C.9.E.31) all terms are dimensionless.

The expression for the phase-shift δ_l:

$$\tan\delta_l = \frac{j_l(ka)[ka\left(\frac{d}{dkr}\frac{j_l(kr)}{kr}\right)_{r=a} + \frac{\gamma}{k}j_l(ka) - \left(\frac{d}{dkr}\frac{j_l(kr)}{kr}\right)_{r=a}]}{\left[\eta_l(ka)\left\{ka\left(\frac{d}{dkr}\frac{j_l(kr)}{kr}\right)_{r=a} + \frac{\gamma}{k}j_l(ka)\right\} - j_l(ka)\left(\frac{d}{dkr}\frac{\eta_l(kr)}{kr}\right)_{r=a}\right]}\,. \qquad \text{(C.9.E.32)}$$

In the numerator and denominator $\frac{\gamma}{k} \gg 1$ and $\frac{\gamma}{a^{-1}} \gg 1$.

Now, a check, with $l = 0$ and ka =O(1), (C.9.E.32)→

$$\to \tan\delta_0 \approx \frac{(j_0(ka))^2}{\eta_0(ka)j_0(ka)} = -\tan ka \to \delta_0 = -ka\,.$$

$\delta_0 = -ka$, the hard sphere scattering.
Furthermore, with $\frac{\gamma}{k} \gg 1$, $\frac{\gamma}{a^{-1}} \gg 1$ and ka =O(1), (C.9.E.32)→
$$\rightarrow \tan\delta_l \approx \frac{j_l(ka)}{\eta_l(ka)}, \quad \text{(C.9.E.33)}$$
and
$$k = \sqrt{\frac{2m}{\hbar^2}E_r}\,.$$
I assume E_r to be the energy of the incident wave. In the text Fp used E_0 to denote the incident energy. Or, denotes subscript r resonance?
Resonances:
Resonance occurs for the maximum value of the differential scattering and consequently, the total cross-section.
(9.29), (9.51) and (9.70), the differential scattering:
$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = |\sum_{l=0,\infty}\sqrt{4\pi(2l+1)}\sin\delta_l Y_{l,0}(\theta,\varphi)|^2. \quad \text{(C.9.E.34)}$$
In (C.9.E.34) $\frac{d\sigma}{d\Omega}$ is at a maximum value for $n\pi/2$, where $\{n \in \mathbb{N} | n \text{ is odd }\}$.
Remark:
In the text Fp analyzed resonance for a spherical potential well in section 9.9. The resonance is about the instability of the bound state. In this exercise there is no well. No bound state. So, what does resonance mean physically? I do not know.

In the text, Fp derived the Brett-Wigner formula for $ka \ll 1$, and k is the wave number of the incident wave (9.99).
k' is the wave number of the internal wavefunction, (9.100) and (9.110).
From this I conclude, in the section on resonance scattering, (9.118) has been derived for $ka \ll 1$.
So, I will look into the case $ka \ll 1$.
With series expansion using $l = 0$, (C.9.E.32) can be approximated by:
$$\tan\delta_0 = -\frac{\gamma a \tan ka}{\gamma a+1}\,. \quad \text{(C.9.E.35)}$$
Given $\gamma \gg a^{-1}, k \rightarrow \gamma a \gg 1$.
Then, for $ka \ll 1 \rightarrow \tan\delta_0 = -\tan ka$, again the hard sphere scattering.
Now, I am in trouble. In this case the phase shift is nowhere near $\pi/2$: $\delta_0 \ll 1$.
First I will apply the expansion of $\cot(\delta_0)$ near resonance $E_r \rightarrow E$ and
$\tan\delta_0 = -\tan ka$, with (9.114)-(9.116):
$$\cot[\delta_0(E)] = \cot[\delta_0(E_r)] - \frac{1}{\sin^2[\delta_0(E_r)]}\frac{2}{\Gamma}(E-E_r). \quad \text{(C.9.E.36)}$$
With (9.75) the 0th partial cross-section is:
$$\sigma_0 = \frac{4\pi}{k^2}\sin^2[\delta_0(E)]\,. \quad \text{(C.9.E.37)}$$
Then,
$$\sigma_0 = \frac{4\pi}{k^2}\sin^2[\delta_0(E)] = \frac{4\pi}{k^2}\frac{1}{1+\cot^2[\delta_0(E)]}\,. \quad \text{(C.9.E.38)}$$
Plug (C.9.E.36) into (C.9.E.38):
$$\sigma_0 = \frac{4\pi}{k^2}\frac{1}{1+\{\cot[\delta_0(E_r)]-\frac{1}{\sin^2[\delta_0(E_r)]}\frac{2}{\Gamma}(E-E_r)\}^2} = \frac{4\pi}{k^2}\frac{\sin^4[\delta_0](\Gamma/2)^2}{\sin^4[\delta_0](\Gamma/2)^2+[\frac{\Gamma}{2}\sin\delta_0\cos\delta_0-(E-E_r)]^2}\,, \quad \text{(C.9.E.39)}$$

How to interpret (C.9.E.39) with $\delta_0 \ll 1$, near resonance with $E = E_r$?
With $E = E_r$ and $\delta_0 \ll 1$, (C.9.E.39)→ $\sigma_0 \approx {\delta_0}^2$.
Part of the exercise: Show that the resonances become extremely sharp as $\gamma \to \infty$.
To show this, I need an expression for the width of the resonance Γ.
I analyzed the case $ka \ll 1$ and obtained $\tan\delta_0 = -\tan ka$: hard sphere scattering.
No dependence on γ. Now what? I suppose a too rough an approximation.

Let us return to (C.9.E.17):
The resonance width for the phase-shift δ_0 is defined in (9.116)
With (C.9.E.17):

$$\cot(ka + \delta_0) = \frac{1+\frac{\gamma}{k}\tan(ka)}{\tan(ka)}. \qquad \text{(C.9.E.40)}$$

With $ka \ll \delta_0 \to \delta_0(E_r) = \frac{\pi}{2}$, (9.113).
Now, using (9.113), (9.114) and (9.115) :

$$\Gamma = -\frac{2}{\frac{d\cot(\delta_0)}{dE}}, \qquad \text{(C.9.E.41)}$$

for $E = E_r$.

$$\frac{d}{dE}\cot(\delta_0) = -\frac{1}{\sin^2\delta_0}\frac{d\delta_0}{dE} = \frac{d}{dE}\frac{1+\frac{\gamma}{k}\tan(ka)}{\tan(ka)}, \text{ at } E = E_r$$

Now,

$$k = \sqrt{\frac{2m}{\hbar^2}}\sqrt{E} \to \frac{dk}{dE} = \frac{1}{2}\sqrt{\frac{2m}{E\hbar^2}}. \qquad \text{(C.9.E.42)}$$

$$\frac{d}{dE}\tan(ka) = \frac{a}{\cos^2(ka)}\frac{dk}{dE}.$$

So,

$$\frac{d}{dE}\cot\delta_0 = \frac{d}{dE}\frac{1+\frac{\gamma}{k}\tan(ka)}{\tan(ka)} = -\frac{1}{2}\gamma\left(\frac{1+ka}{k^2}\right)\sqrt{\frac{2m}{E_r\hbar^2}}. \qquad \text{(C.9.E.43)}$$

With (C.9.E.37) $\gamma \to \infty$ and (C.9.E.41), the width $\Gamma \to 0$.
Consequently the resonances become extremely sharp.

Exercise 9.4 Elastic scattering of an electron by the ground state of a hydrogen atom.

Show that the differential cross-section for the elastic scattering of a fast electron by the ground-state of a hydrogen atom is:

$$\frac{d\sigma}{d\Omega} = \left(\frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q^2}\right)^2 \left(1 - \frac{16}{[4+(qa_0)^2]^2}\right), \qquad \text{(C.9.E.44)}$$

where $q = |\boldsymbol{k} - \boldsymbol{k}'|$, and a_0 is the Bohr radius.
Then,

$$|f(\theta)|^2 = \left(\frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q^2}\right)^2 \left(1 - \frac{16}{[4+(qa_0)^2]^2}\right).$$

$f(\theta)$ needs to be found.
Rewrite $|f(\theta)|^2$:

$$|f(\theta)|^2 = \left(\frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q^2}\right)^2 \frac{8(qa_0)^2+(qa_0)^4}{[4+(qa_0)^2]^2}.$$

So,

$$\{f(\theta)\}^* f(\theta) = \left(\frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q^2}\right)^2 \frac{2\sqrt{2}qa_0+i(qa_0)^2}{4+(qa_0)^2}\frac{2\sqrt{2}qa_0-i(qa_0)^2}{4+(qa_0)^2}, \qquad \text{(C.9.E.45a)}$$

and

$$f(\theta) = \pm\frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q^2}\frac{2\sqrt{2}qa_0 \pm i(qa_0)^2}{4+(qa_0)^2}\,. \qquad \text{(C.9.E.45b)}$$

Elastic scattering: $k = k'$. The prime represents the scattered wave.

$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$ and $E = \frac{\hbar^2 k^2}{2m}$. (C.9.E.45)

So, (C.9.E.44) can be written as:

$$\frac{d\sigma}{d\Omega} = \left(\frac{2}{a_0 q^2}\right)^2 (1 - \frac{16}{[4+(qa_0)^2]^2}), \qquad \text{(C.9.E.46)}$$

and the dimension of $\frac{d\sigma}{d\Omega}$ is m^2, (9,95).

A fast electron, I suppose, means the energy of the electron is larger than the coulomb potential of the ground-state of the hydrogen atom. So, Fp is not indicating at relativistic effects, e.g., relativistic mass increase.

The ground-state of a hydrogen atom, the wavefunction:

$$\psi_{n,0,0} = R_{n,0}(r)Y_{0,0}(\theta,\varphi)\,. \qquad \text{(C.9.E.47)}$$

The first question to answer is: how to model the scattering ground-state? Should I consider the scattering center as a one potential or as a proton plus an electron?

However, in that case the exercise is about a many particle system. I suppose this is not the intention here. What to do? I assume a simple model represented by the potential:

$$V = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}\,. \qquad \text{(C.9.E.48)}$$

So, (C.9.E.48) represents the scattering potential?

Remark:

The Coulomb potential V is proportional to the potential:

$\lim_{\tau\to 0}\frac{e^{-\tau}}{r}$.

This can be helpful to determine the Fourier transform of $-\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$.

The Fourier transform of this Coulomb potential is:

$$\tilde{V}(k) = -\frac{1}{\epsilon_0}\frac{e^2}{k^2},$$

where the z-axis is along the direction of k , $\boldsymbol{k}\cdot\boldsymbol{r} = kr\cos\theta$.

See also the evaluation of (C.9.E.52) below.

The ground-state energy of the hydrogen atom:

$E = E_0 = -\frac{m_e e^4}{2(4\pi\epsilon_0)^2\hbar^2}$, (9.57), *The Undergraduate Course.*

Next, the scattering $f(\theta)$ has to be obtained.

To this end Born approximation could be applied. However, in that case *the scattering is not particularly strong* (Fp). Fp did not indicate something about the strength of the scattering.

The scattering Hamiltonian is only a function of the position operator: (C.9.E.47).

The wave function of the scattering atom:

$$\psi_{1,0,0} = R_{1,0}(r)\cdot\frac{1}{\sqrt{4\pi}} = \frac{2}{\sqrt{4\pi}}\frac{1}{a_0^{3/2}}e^{-r/a_0}\,, \qquad \text{(C.9.E.49)}$$

see also chapters 8 and 9 of *The Undergraduate Course.*

I assume, a fast electron means weak interaction. Consequently, I will use the Born

Approximation.
In (C.9.E.48) the potential is the interaction potential between the incoming electron and the proton. So, to complete the picture of the potential the interaction with the bound electron must be included.
Then, the scattering potential for the incoming electron is:

$$V(\boldsymbol{r},\boldsymbol{r_b}) = \frac{e^2}{4\pi\epsilon_0}\left(-\frac{1}{r}+\frac{1}{|\boldsymbol{r}-\boldsymbol{r_b}|}\right), \qquad \text{(C.9.E.50)}$$

where the nucleus is at the origin. The fast electron is at $\boldsymbol{r}$ and the bound electron at $\boldsymbol{r_b}$.
For the ground-state, a most probable value for $|\boldsymbol{r_b}| = a_0$ and an expectation value for $|\boldsymbol{r_b}| = \frac{3a_0}{2}$.
See Chapter 9 *The Undergraduate Course*, Exercise 3e and 3f. I come back to these values later.
What I learned from Mahan (page 236) is, the bound electron usually to be averaged over its allowed positions. So, here the bound-state wave function comes into play.
In this way the potential becomes:

$$V(\boldsymbol{r},\boldsymbol{r_b}) = \frac{e^2}{4\pi\epsilon_0}\left(-\frac{1}{r}+\int r_b^2 dr_b \frac{{\psi_{1,0,0}}^2}{|\boldsymbol{r}-\boldsymbol{r_b}|}\sin\theta d\theta d\varphi\right). \qquad \text{(C.9.E.51)}$$

The average is actually the expectation value of position of the bound electron.
So, the integral as expectation value:

$$\int r_b^2 dr_b (\psi_{1,0,0})^* \frac{1}{|\boldsymbol{r}-\boldsymbol{r_b}|}\psi_{1,0,0}\sin\theta d\theta d\varphi \rightarrow \text{(C.9.E.51)}.$$

The scattering amplitude is proportional to the Fourier transform of the scattering potential $V(\boldsymbol{r},\boldsymbol{r_b})$ given by (C.9.E.51).
The first term in (C.9.E.51):

$$-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}.$$

Plug this term into (9.33)$\rightarrow (9.34)$. Then, this part of the potential, $-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$, contributes to the scattering amplitude, (9.34):

$$\frac{2m_e}{\hbar^2 q}\int_0^\infty dr'\, r'\frac{e^2}{4\pi\epsilon_0}\frac{1}{r'}\sin(qr') = \frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q}\int_0^\infty dr'\sin(qr'). \qquad \text{(C.9.E.52)}$$

In (C.9.E.52)

$$\int_0^\infty dr'\sin(qr') = \lim_{\gamma\to 0}\int_0^\infty e^{-\gamma r'}dr'\sin(qr') = \frac{1}{2i}\lim_{\gamma\to 0}\left(\frac{1}{\gamma-qi}-\frac{1}{\gamma+qi}\right) = \frac{1}{q}.$$

So, one part of scattering amplitude is, (C.9.E.52):

$$\frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q^2}. \qquad \text{(C.9.E.53)}$$

Now, what about the second term of the potential in (C.9.E.51):

$$\frac{e^2}{4\pi\epsilon_0}\int r_b^2 dr_b \frac{{\psi_{1,0,0}}^2}{|\boldsymbol{r}-\boldsymbol{r_b}|}\sin\theta d\theta d\varphi) \text{ ?} \qquad \text{(C.9.E.54)}$$

With (C.9.E.49), the integral in (C.9.E.54) becomes:

$$\frac{e^2}{4\pi\epsilon_0}\int r_b^2 dr_b \frac{1}{\pi}\frac{1}{a_0^3}\frac{e^{-2r_b/a_0}}{|\boldsymbol{r}-\boldsymbol{r_b}|}\sin\theta d\theta d\varphi). \qquad \text{(C.9.E.55)}$$

The expression in (C.9.E.56) represents the potential in (9.34).
Now, I use the following approximation:

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r_b}|} \cong \frac{1}{r}+\frac{\boldsymbol{r}\cdot\boldsymbol{r_b}}{r^3}.$$

I start with the first term of this approximation
Hence, (C.9.E.55):

$$\frac{e^2}{4\pi\epsilon_0}\int r_b^2 dr_b \frac{1}{\pi}\frac{1}{a_0^3}\frac{e^{-2r_b/a_0}}{r}\sin\theta d\theta d\varphi = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}. \qquad \text{(C.9.E.56)}$$

This contribution to the potential gives the second term for the scattering amplitude, (9.34):

$$-\frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q}\int_0^\infty dr' \sin(qr') = -\frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q^2}\ . \qquad \text{(C.9.E.57)}$$

For the scattering amplitude, (C.9.E.53) en (C.9.E.57):

$$f(\theta) = \frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q^2}(1-1) = 0. \qquad \text{(C.9.E.58)}$$

The differential cross-section:

$$\frac{d\sigma}{d\Omega} = 0. \qquad \text{(C.9.E.59)}$$

Not close to (C.9.E.44), to say the least. In this case the term $\frac{\boldsymbol{r}\cdot\boldsymbol{r_b}}{r^3}$ needs to be included.

However, then the exact expression is better used. See below.

Mahan derived the expression for the differential cross-section in section 7.6.3. There is the scattering cross-section as presented by Fp, found from combining Eqs. (7.122) and (7.125). The scattering cross-section is obtained from the Fourier transform of the potential given in Eq. (7.121). The scattering cross-section of Mahan is the differential cross-section of Fp. However, with Fp the scattering amplitude is (proportional to) the Fourier transform of the scattering potential with respect to the wave factor $q = |\boldsymbol{k} - \boldsymbol{k}'|$.

Now, I will use the most probable value of $|\boldsymbol{r_b}| = a_0$ in the expression of $\frac{1}{|\boldsymbol{r}-\boldsymbol{r_b}|}$.

Now, see, e.g., (10.62) and (10.63):

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r_b}|} = \frac{1}{r}(4\pi)^2.$$

Note: the right-hand side does not depend on r_b. A surprise? Well, draw a 2-dimensional picture, with various values of r_b and the result is demonstrated.

The scattering potential, (C.9.E.50):

$$V(\boldsymbol{r},\boldsymbol{r_b}) = \frac{e^2}{4\pi\epsilon_0}\left(-\frac{1}{r}+\frac{1}{|\boldsymbol{r}-\boldsymbol{r_b}|}\right) = \frac{e^2}{4\pi\epsilon_0}\left[-\frac{1}{r}+\frac{1}{r}(4\pi)^2\right] = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}[(4\pi)^2-1]\,. \qquad \text{(C.9.E.60)}$$

Plug this term into (9.33)→ (9.34):

$$f(\theta) = -\frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q^2}[(4\pi)^2-1]. \qquad \text{(C.9.E.61)}$$

The differential cross-section:

$$\frac{d\sigma}{d\Omega} = \left(\frac{2m_e e^2}{4\pi\epsilon_0\hbar^2 q^2}\right)^2[(4\pi)^2-1]^2. \qquad \text{(C.9.E.62)}$$

Again not close to (C.9.E.44).

I leave the exercise.

10 Identical Particles

10.1 Permutation symmetry.

A system of identical particles will be considered.

> Fp starts with two identical particles. The phenomenon of exchange degeneracy is introduced. This phenomenon creates a problem since a measurement does not uniquely determine the corresponding state ket.
>
> To deal with this problem, the permutation operator is introduced, and defined in (10.4), P_{12} *swaps the identities of particle 1 and 2*. I assume, applying the definition:
>
> $$P_{21}|k''\rangle|k'\rangle = |k'\rangle|k''\rangle\,. \qquad \text{(C.10.1)}$$

Then,
$P_{12}P_{21}|k''\rangle|k'\rangle = P_{12}|k'\rangle|k''\rangle = |k''\rangle|k'\rangle.$ (C.10.2)
Consequently,
$P_{12}P_{21} = 1.$ (C.10.3)
Fp writes, at the bottom of page 161: *"It is easily seen that*
$P_{21} = P_{12}$ *, (10.5),*
$P_{12}^2 = 1$*, (10.6)."*
Well, with (C.10.3) and (10.5), (10.6) is obtained.
On the other hand, $P_{12}P_{21} = 1$ and $P_{21}P_{12} = 1 \rightarrow P_{12}P_{21} = P_{21}P_{12} \rightarrow P_{21} = P_{12}$.
Is this the easy demonstration of (10.5)?
(10.5) in words: P_{12} *swaps the identities of particle 1 and 2, so does* P_{21}. What about the definition (10.4) and (10.5)? When (10.5) is correct, then:
$P_{12}|k''\rangle|k'\rangle = |k'\rangle|k''\rangle,$
is correct?
That is the meaning of P_{12} *swaps the identities of particle 1 and 2*? I suppose so.
What is precisely the meaning of swapping the identities of identical particles?
Nothing happens, I suppose?!

Remark: (10.5) is about operators. So,
$(P_{21} - P_{12}) \rightarrow |k'\rangle|k''\rangle = 0 \rightarrow P_{21}|k'\rangle|k''\rangle - P_{12}|k'\rangle|k''\rangle = 0 \rightarrow$
$\rightarrow P_{21}|k'\rangle|k''\rangle = |k''\rangle|k'\rangle.$
Hence , the permutation operator P_{21} operates in the same way as P_{12}.

In (10.7) Fp introduced the Hamiltonian of the two identical particle system.
(10.12): and (10.6)
$P_{12}HP_{12} = H \rightarrow P_{12}HP_{12} - P_{12}^2H = 0 \rightarrow P_{12}(HP_{12} - P_{12}H) = 0 \rightarrow [H, P_{12}] = 0,$
(10.13) with $P_{12} \neq 0$.
The eigenvalues of P_{12} are $+1$ and -1 :
$P_{12}^2|k'\rangle|k''\rangle = P_{12}|k''\rangle|k'\rangle = |k'\rangle|k''\rangle.$ (C.10.4)
So, the eigenvalue of P_{12}^2 is 1.
Hence, as mentioned by Fp, the eigenvalues of the permutation operator P_{12} are $+1$ and -1.
Then, $P_{12}|k'\rangle|k''\rangle = \pm|k'\rangle|k''\rangle$? Or, $P_{12}|k'\rangle|k''\rangle = \pm|k''\rangle|k'\rangle$?
Well, according to the definition of eigenvalue:
$P_{12}|k'\rangle|k''\rangle = \pm|k'\rangle|k''\rangle$.
However, according to the definition:
$P_{12}|k'\rangle|k''\rangle = |k''\rangle|k'\rangle.$
So, a question is: What is the meaning of this?
With (10.3), a general state can be written as:
$|k'k''\rangle = c_1|k'\rangle|k''\rangle + c_2|k''\rangle|k'\rangle$. (C.10.5)
Normalization of (C.10.5):
$\langle k'k''|k'k''\rangle = (c_1^*\langle k'|\langle k''| + c_2^*\langle k''|\langle k'|)(c_1|k'\rangle|k''\rangle + c_2|k''\rangle|k'\rangle).$ (C.10.6)
Then (C.10.6) with $\langle k'k''|k'k''\rangle = 1$ and $\langle k'|k''\rangle = \delta_{k'k''}$:
$c_1c_2^* + c_1^*c_2 = 1.$ (C.10.7)

Choose, on the basis of symmetry, $c_1 = c_2$, then, $c_2 = c_1 = \pm 1/\sqrt{2}$.
Remark: due to the chosen convention, i.e., the sequence of $|k'\rangle$ and $|k''\rangle$ in (C.10.6), I obtained (C.10.7). Choose a different sequence for the complex conjugate of the general state vector:
$c_1^*\langle k''|\langle k'| + c_2^*\langle k'|\langle k''|$.
I would have obtained:
$|c_1|^2 + |c_2|^2 = 1.$ (C.10.8)
I do prefer the latter sequence, not knowing which order Fp has chosen.

Next Fp considers a system of three identical particles. The overall state ket is presented in (10.18). with three identical particles there are three two-particle permutation operators as defined in (10.19)-(10.21). Again, Fp mentioned: "It is easily demonstrated….." and presented (10.22)-(10.24).
With the definitions of the permutation operators:
$P_{21}P_{12}|k'k''k'''\rangle = P_{21}|k''k'k'''\rangle = |k'k''k'''\rangle \rightarrow P_{21}P_{12} = 1.$
In the same way: $P_{12}P_{21} = 1$, (10.22).
With (10.22): $P_{21} = P_{12}$,
$P_{21}P_{12} = 1 \rightarrow P_{12}^2 = 1.$
There is still the question: What is precisely the meaning of swapping the identities of identical particles? Nothing happens, I suppose?!
(10.28)-(10.33) represents the six eigenvalue equations of the system:
3 particles→ 3! permutations.
(10.34) is found analogous to (10.13):
$P_{12}HP_{12} = H \rightarrow P_{12}HP_{12} - P_{12}^2H = 0 \rightarrow P_{12}(HP_{12} - P_{12}H) = 0 \rightarrow [H, P_{12}] = 0,$
(10.13) with $P_{12} \neq 0$.
In (10.35), a new operator is introduced: the cyclic permutation operator.
(10.36):
$P_{123}|k'k''k'''\rangle = P_{12}P_{31}|k'k''k'''\rangle = |k'''k'k''\rangle.$
With (10.28), (10.30) and (10.35):
$(HP_{123} - P_{123}H)|k'k''k'''\rangle = HP_{123}|k'k''k'''\rangle - P_{123}E|k'k''k'''\rangle =$
$= H|k'''k'k''\rangle - E|k'''k'k''\rangle = E(|k'''k'k''\rangle - |k'''k'k''\rangle) = 0 \rightarrow$ (10.37).
With 3 particles there are 3! Permutations.
Consequently, the normalization factor is: $\frac{1}{\sqrt{3!}}$.
The convention of the bra/ket for normalization, e.g.,:
$\langle k'''k''k'|k'k''k'''\rangle = |c_1|^2\langle k'''|\langle k''|\langle k'|k'\rangle|k''\rangle|k'''\rangle + \cdots + \cdots + \cdots$.
With symmetry, $|c_1|^2 = \frac{1}{3!}$.

10.2 Symmetrization Postulate

This postulate is about the totally symmetric ket and the totally anti-symmetric ket .
See also section 6.5 of The Undergraduate Course about bosons and fermions.
Replace in (10.44), on the left-hand side $|k'k''k'''\rangle$ by $|k'k'\,k'''\rangle$, and on the right-hand side $|k''\rangle$ by $|k'\rangle$. The kets on the right-hand side add up to $|0\rangle$.

10.3 Two-Electron System

See also section 6.4 of The Undergraduate Course.

The overall wave function is presented: (10.46), a product of the spatial wave function and the spinor.

The spatial probability distributions are presented in (10.53).

10.4 Helium Atom.

An example of a two-electron system is the helium atom.

First, Fp analyzed the case without the mutual interaction between the two electrons. The ground state energy is obtained. Apparently, a too rough estimate.

Next, Fp included the interaction and treated this interaction as a first order perturbation. A much better approximation of the ground state energy is obtained.

Finally, Fp discussed the situation in which one electron is in the ground state and the other is in indicated by the quantum numbers.

Exercises

Exercise 10.1 The particle interchange operator.

Demonstrate that the particle interchange operator, P_{12}, in a system of two identical particles is Hermitian.

An operator is Hermitian, section 1.8:

- When the eigenvalues of the operator are real.
- The eigenkets corresponding to different eigen values are orthogonal.
- The eigenvalues associated with the eigenket are the same as the eigenvalues associated with the eigenbra.

The eigenvalues of P_{12} are, (10.6): ± 1.

So, the eigenvalues are real.

Then, are $|k'k''\rangle_+$, (10.14), the eigenstate with eigenvalue $+1$ and $|k'k''\rangle_-$, (10.15), the eigenstates with eigenvalue -1 orthogonal?

$\langle k''k'|_-|k'k''\rangle_+ = \frac{1}{2}(\langle k''|\langle k'| - \langle k'|\langle k''|)((|k'\rangle|k''\rangle + |k''\rangle|k'\rangle) =$

$= \frac{1}{2}(\langle k''|\langle k'||k'\rangle|k''\rangle - \langle k'|\langle k''||k'\rangle|k''\rangle + \langle k''|\langle k'||k''\rangle|k'\rangle - \langle k'|\langle k''||k''\rangle|k'\rangle) =$

$= \frac{1}{2}(1 - 0 + 0 - 1) = 0.$

So, $|k'k''\rangle_+$ and $|k'k''\rangle$ are orthogonal.

Now,

$\langle k''|\langle k'|P_{12}$ →the complex conjugate: $(\langle k''|\langle k'|P_{12})^* = P_{12}|k'\rangle|k''\rangle = |k''\rangle|k'\rangle,$ (C.10.E.1)

The complex conjugate of

$(\langle k''|\langle k'|P_{12})^* \rightarrow [(\langle k''|\langle k'|P_{12})^*]^* = \langle k''|\langle k'|P_{12}$, (C.10.E.2)

and with (C.10.E.2), (C.10.E.2)→

$\rightarrow [(\langle k''|\langle k'|P_{12})^*]^* = \langle k''|\langle k'|P_{12} = \langle k'|\langle k''|.$

So, the eigenvalues associated with the eigenket are the same as the eigenvalues associated with the eigenbra.

Exercise 10.2 Two identical spin-1/2 particles in a box without interaction

Consider two identical spin-1/2 particles of mass m confined in a cubic box of dimension L. Find the possible energies and wave functions of this system in the case of no interaction between the particles.

Multiple-Particle Systems, The Undergraduate Course, page 87:

"*… , for the case of non-interacting particles, the multi-particle Hamiltonian of the system can be written as the sum of N independent single-particle Hamiltonians. ……., we expect their instantaneous positions to be completely uncorrelated with one other. This immediately implies that the multi-particle wavefunction, $\psi(x_1, x_2, \ldots, x_N, t)$ can be written as the product of N independent single-particle wavefunctions……".*

In section 7.3 of *The Undergraduate Course*, Fp dealt with the problem of a Particle in a Box without spin. The stationary wavefunction, the wave numbers, the energy and the quantum numbers are presented in Eqs. (7.32)-(7.39).

In this exercise, spin-1/2 particles are dealt with.

The spatial wave function for particle i in a box:

$$\omega(x_i, y_i, z_i) = (\frac{2}{L})^{3/2} \sin(k_{x_i} x_i) \sin(k_{y_i} y_i) \sin(k_{z_i} z_i), \quad \text{(C.10.E.3)}$$

where

$$k_{x_i} = \frac{l_{x_i}\pi}{L}, \quad \text{(C.10.E.4)}$$

$$k_{y_i} = \frac{l_{y_i}\pi}{L}, \quad \text{(C.10.E.5)}$$

$$k_{z_i} = \frac{l_{z_i}\pi}{L}. \quad \text{(C.10.E.6)}$$

l_{x_i}, l_{y_i} and l_{z_i} are positive integers.

With (5.9) of *The Undergraduate Course, One-Dimensional Potentials,* the energy is:

$$E_i = \frac{l_i^2 \pi^2 \hbar^2}{2mL^2}, \quad \text{(C.10.E.7)}$$

and

$$l_i^2 = {l_{x_i}}^2 + {l_{y_i}}^2 + {l_{z_i}}^2. \quad \text{(C.10.E.8)}$$

The overall wavefunction of the two spin-1/2 particles is given in (10.46):

$\psi(\boldsymbol{x}_1', \boldsymbol{x}_2'; s, m) = \phi(\boldsymbol{x}_1', \boldsymbol{x}_2')\chi(s, m)$.

$\chi(s, m)$ are given by (10.47)-(10.50).

In *The Undergraduate Course,* Fp gave two expressions for the overall wave function:

- $\psi_{E\ boson}(x_1, x_2)$, (6.41). This expression for the wavefunction *automatically satisfies the symmetry requirements on the wavefunction.* Symmetric, e.g., a photon.
- $\psi_{E\ fermion}(x_1, x_2)$, (6.42). This expression for the wavefunction *automatically satisfies the symmetry requirements on the wavefunction.* Anti-symmetric, e.g., an electron.

Now, back to The Graduate Course:

(10.51) the overall spatial wavefunction needs to be antisymmetric for the triplet state and symmetric for the singlet state. I do not know how to relate this result with the results of *The Undergraduate Course*.

So, there are two overall spatial wavefunctions for the two identical electrons: (10.51) and (10.52), with particle A and particle B:

the triplet T

$$\phi_T(\boldsymbol{x}_1', \boldsymbol{x}_2') = \frac{1}{\sqrt{2}}[\omega_A(x_1, y_1, z_1)\omega_B(x_2, y_2, z_2) - \omega_B(x_1, y_1, z_1)\omega_A(x_2, y_2, z_2)], \quad \text{(C.10.E.9)}$$

where the wave functions ω_A and ω_B are given by (C.10.E.3),
the singlet S

$$\phi_S(\boldsymbol{x}_1', \boldsymbol{x}_2') = \frac{1}{\sqrt{2}}[\omega_A(x_1, y_1, z_1)\omega_B(x_2, y_2, z_2) + \omega_B(x_1, y_1, z_1)\omega_A(x_2, y_2, z_2)] \,. \quad \text{(C.10.E.10)}$$

Note for the triplet, there are three overall wavefunction.
The possible energies with no interaction.
In this case we are dealing with the kinetic energy of the particles. The potential is one of the boundary conditions of a particle in a box: $V \to \infty$ at the walls of the box. Elsewhere inside the box $V = 0$.
So, the possible energies of the system are the sum of the kinetic energy of the particles A and B:

$$E = E_A + E_B = \frac{l_A^2 \pi^2 \hbar^2}{2mL^2} + \frac{l_B^2 \pi^2 \hbar^2}{2mL^2} \,, \quad \text{(C.10.E.11)}$$

with (C.10.E.8):
$l_A^2 = {l_{x_A}}^2 + {l_{y_A}}^2 + {l_{z_A}}^2$ and $l_B^2 = {l_{x_B}}^2 + {l_{y_B}}^2 + {l_{z_B}}^2$.
Then,

$$E = \frac{(l_A^2 + l_B^2)\pi^2 \hbar^2}{2mL^2} \,. \quad \text{(C.10.E.12)}$$

There are a couple of wave functions for this two particles in a box system: Three wave functions with triplet states and one wave function with a singlet state.
The overall wave functions with triplets:

$$\psi(\boldsymbol{x}_1', \boldsymbol{x}_2'; s, m) = \phi(\boldsymbol{x}_1', \boldsymbol{x}_2')\chi(s, m) = \phi(\boldsymbol{x}_1', \boldsymbol{x}_2')\chi_T =$$
$$= \frac{1}{\sqrt{2}}[\omega_A(x_1, y_1, z_1)\omega_B(x_2, y_2, z_2) - \omega_B(x_1, y_1, z_1)\omega_A(x_2, y_2, z_2)]\chi_T \,, \quad \text{(C.10.E.13)}$$

where χ_T is represented by (10.47)-(10.49).
The overall wave function with singlet:

$$\psi(\boldsymbol{x}_1', \boldsymbol{x}_2'; s, m) = \phi(\boldsymbol{x}_1', \boldsymbol{x}_2')\chi(s, m) = \phi(\boldsymbol{x}_1', \boldsymbol{x}_2')\chi_S =$$
$$= \frac{1}{\sqrt{2}}[\omega_A(x_1, y_1, z_1)\omega_B(x_2, y_2, z_2) + \omega_B(x_1, y_1, z_1)\omega_A(x_2, y_2, z_2)]\chi_S, \quad \text{(C.10.E.14)}$$

where χ_S is represented by (10.50).
The spatial wave function:

$$\omega_A(x_1, y_1, z_1) = \omega_A(x_A, y_A, z_A) = (\frac{2}{L})^{\frac{3}{2}} \sin(k_{x_A} x_A) \sin(k_{y_A} y_A) \sin(k_{z_A} z_A),$$
$$\omega_B(x_2, y_2, z_2) = \omega_B(x_B, y_B, z_B) = (\frac{2}{L})^{3/2} \sin(k_{x_B} x_B) \sin(k_{y_B} y_B) \sin(k_{z_B} z_B),$$
$$\omega_A(x_2, y_2, z_2) = \omega_A(x_B, y_B, z_B) = (\frac{2}{L})^{3/2} \sin(k_{x_B} x_B) \sin(k_{y_B} y_B) \sin(k_{z_B} z_B),$$

and

$$\omega_B(x_1, y_1, z_1) = \omega_B(x_A, y_A, z_A) = (\frac{2}{L})^{\frac{3}{2}} \sin(k_{x_A} x_A) \sin(k_{y_A} y_A) \sin(k_{z_A} z_A). \quad \text{(C.10.E.15)}$$

Plug (C.10.E.15) into (C.10.E.13) and (C.10.E.14). The result is a singlet wave function:

$$\phi(\boldsymbol{x}_1', \boldsymbol{x}_2')\chi_S =$$
$$= 2(\frac{2}{L})^3 \sin(k_{x_A} x_A) \sin(k_{y_A} y_A) \sin(k_{z_A} z_A) \sin(k_{x_B} x_B) \sin(k_{y_B} y_B) \sin(k_{z_B} z_B) \chi(0,0).$$

Exercise 10.3 Two spin-1 particles with no orbital angular momentum

Consider a system two spin-1 particles with no orbital angular momentum (i.e., both particles in the s-states). What are the possible eigenvalues of the total spin angular momentum of the system, as well as the projection along the z-direction, in the cases in which the particles are no-identical and identical?
The total spin angular momentum.

For the total spin angular momentum operator :

$S = S_1 + S_2$. (C.10.E.16)

The subscript of the operators indicates the two particles.

I look first into the results of a single spin. See chapter 5.

The simultaneous eigenstates of S_z and S^2 are $|s, s_z\rangle$.

$S_z|s, s_z\rangle = s_z\hbar|s, s_z\rangle$, (5.4),

$S^2|s, s_z\rangle = s(s+1)\hbar^2|s, s_z\rangle$, (5.5).

Or in the notation of the *Undergraduate Course*:

$S_z\chi_{s,m_s} = m_s\hbar\chi_{s,m_s}$, (10.16),

$S^2\chi_{s,m_s} = s(s+1)\hbar^2\chi_{s,m_s}$,(10.17).

Now for a spin-1 particle:

$s = 1$ and $s_z/\, m_s = 1,0,-1$.

Next, let's consider two spin-1 particles.

Then, see chapter 6 on Addition of Angular Momentum:

$J_z\chi_{s_1,s_2;m_1,m_2} = \left(S_{z_1} + S_{z_2}\right)\chi_{s_1,s_2;m_1,m_2} = (m_1 + m_2)\hbar\chi_{s_1,s_2;m_1,m_2}$, (C.10.E.17)

see also (11.23) *The Undergraduate Course.*

Two spin-1 particles.

In Exercise 6.2 I dealt with the Clebsch-Gordon coefficients for adding spin one to spin one. I present here the table of that exercise:

m	m_1	m_2	1	2	3	4	5	6	7	8	9
2	1	1	1	0	0	0	0	0	0	0	0
1	1	0	0	$1/\sqrt{2}$	0	0	0	$-1/\sqrt{2}$	0	0	0
0	1	-1	0	0	$1/\sqrt{6}$	0	0	0	$1/\sqrt{2}$	0	$1/\sqrt{3}$
1	0	1	0	$1/\sqrt{2}$	0	0	0	$1/\sqrt{2}$	0	0	0
0	0	0	0	0	$2/\sqrt{6}$	0	0	0	0	0	$-1/\sqrt{3}$
-1	0	-1	0	0	0	$1/\sqrt{2}$	0	0	0	$-1/\sqrt{2}$	0
0	-1	1	0	0	$1/\sqrt{6}$	0	0	0	$-1/\sqrt{2}$	0	$1/\sqrt{3}$
-1	-1	0	0	0	0	$1/\sqrt{2}$	0	0	0	$1/\sqrt{2}$	0
-2	-1	-1	0	0	0	0	1	0	0	0	0
	$s_1 = 1$ $s_2 = 1$	$S_{max} = 2$ $S_{min} = 0$	2	2	2	2	2	1	1	1	0
		m	2	1	0	-1	-2	1	0	-1	0

Now, which row represents identical particles? What are identical particles anyhow? When are spin one particles non-identical?

Identical particles are $m_1 = m_2$? Or as defined on page 161: interchange of $m_1$and m_2 does not alter the system?

Let us look into the various states.

The first column(1)[9]:

$\chi_{2,2} = \chi_{1,1}$,

the second

$\chi_{2,1} = \frac{1}{\sqrt{2}}\,\chi_{1,0} + \frac{1}{\sqrt{2}}\,\chi_{0,1}$,

the third

$\chi_{2,0} = \frac{1}{\sqrt{6}}\,\chi_{1,-1} + \frac{2}{\sqrt{6}}\,\chi_{0,0} + \frac{1}{\sqrt{6}}\,\chi_{-1,1}$,

the fourth

$\chi_{2,-1} = \frac{1}{\sqrt{2}}\,\chi_{0,-1} + \frac{1}{\sqrt{2}}\,\chi_{-1,0}$,

[9] The numbers of columns are indicated in the first row of the table.

the fifth
$\chi_{2,-2} = \chi_{-1,-1}$,
the sixth
$\chi_{1,1} = -\frac{1}{\sqrt{2}}\chi_{1,0} + \frac{1}{\sqrt{2}}\chi_{0,1}$,
the seventh
$\chi_{1,0} = \frac{1}{\sqrt{2}}\chi_{1,-1} - \frac{1}{\sqrt{2}}\chi_{-1,1}$,
the eight
$\chi_{1,-1} = -\frac{1}{\sqrt{2}}\chi_{0,-1} + \frac{1}{\sqrt{2}}\chi_{-1,0}$,
and
the nineth
$\chi_{0,0} = \frac{1}{\sqrt{3}}\chi_{1,-1} - \frac{1}{\sqrt{3}}\chi_{0,0} + \frac{1}{\sqrt{3}}\chi_{-1,1}$.
So, there are nine states:
four symmetric,
three antisymmetric,
and
two no-symmetric.
Am I allowed to indicate 7 to be identical and 2 to be non-identical?
Now, the eigenvalues.
$S^2 = s(s+1)\hbar^2 \rightarrow 6\hbar^2, 2\hbar^2$ and 0, and $s = 2,1,0$,
$S_z = (m_1 + m_2)\hbar \rightarrow 2\hbar, \hbar, 0, -\hbar, -2\hbar$.
For the non-identical particles as defined above (with '?'):
$S^2 = 0$ and $S_z = 0$.

11 Relativistic Electron Theory

11.1 Introduction

It is about electron dynamics and special relativity. The notation is presented.
The space-time 4-vector is introduced.
Reading the pages 171 and 172, I read also chapter 66 of Dirac: *Relativistic treatment of a particle*.
Where Fp denoted a^μ the contravariant components of the vector a, Dirac denoted these the covariant components of the vector a. Fp denoted a_μ the covariant components, and, as to be expected, Dirac denoted these the contravariant components. The Lorentz invariant scalar product is presented in (11.5) together with the Einstein summation convention.
The important fundamental tensor, $g_{\mu\nu}$ (Dirac $g^{\mu\nu}$) is defined in (11.6)-(11.9).
With the metric tensor, the connection between covariant components is given in (11.10).
This follows from (11.1)-(11.4).

11.2 Dirac Equation

The motion of an electron in the absence of an electromagnetic field is considered.

Dirac: "*I have an equation*".
It is a coincidence, chapter 11 in Dirac's book is titled: "*Relativistic theory of the electron*".
I cite from section 66 on *Relativistic Treatment of a Particle*:
"Let us see how the basic ideas of quantum theory can be adapted to the relativistic point of view that the four dimensions of space-times should be treated on the same footing. The

general principle of superposition of states, as given in Chapter I ,is a relativistic principle, since it applies to 'states' with the relativistic space-time meaning. However, the general concept of an observable does not fit in since an observable may involve physical things as widely separated points at one instant of time. In consequence, if one works with a general representation referring to any complete set of commuting observables, the theory cannot display the symmetry between space and time required by relativity. In relativistic quantum mechanics one must be content with having one representation which displays this symmetry. One then has the freedom to transform to another representation referring to a special Lorentz frame of reference if it is useful for a particular calculation.
For the problem of a single particle, in order to display the symmetry between space and time we must use the Schrödinger representation….".

First Fp introduced the quantum mechanical equivalent of the relation between energy and momentum, (11.16).
After presenting this equation Fp explained the insufficiency of (11.16) and "*We must therefore look for a new(wave, Dirac) equation"*.
Then, (11.17) is proposed. For completeness, I write (11.17) as:
$\left(p^{\mu}p_{\mu} + m_e^2c^2\right)\psi = 0.$ (C.11.1)
I expected the $m_e^2c^2$ with a minus sign as Dirac showed in Eq.(6) page 255.
The next step is to linearize (11.17) on the basis of the general laws or principles of quantum mechanics. This suggests a wave equation like the one given in (11.18). Dirac included m_ec in the factor β [Dirac, (7)].
It is instructive to execute the multiplication of (11.18) by the operator as given just above (11.19).
This multiplication results into (11.19). Use is made of the anti-commutator. May be it is a bit trivial, but expressions like:
$\alpha_1(p^1p^0 - p^0p^1) \rightarrow 0$, since the order of differentiation is irrelevant.
Fp writes: "Equations (11.20) -11.22) can then be shown to reduce to, (11.25):
$\{\gamma^{\mu}, \gamma^{\nu}\} = 2g^{\mu\nu}$, (11.25),
where $g^{\mu\nu}$ is the metric tensor.
The metric tensor:

$$g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

Now, with (11.25), let's find out about (11.20).
$\{\alpha_i, \alpha_j\} = 2\delta_{ij}$, (11.20).
Use (11,24):
$\alpha_i = \gamma^0\gamma^i.$
Then, (11.20):
$\alpha_i\alpha_j + \alpha_j\alpha_j = 2\delta_{ij}.$
With (11.22), (11.23) and (11.24):
$\alpha_i\alpha_j + \alpha_j\alpha_j = \gamma^0\gamma^i\gamma^0\gamma^j + \gamma^0\gamma^j\gamma^0\gamma^i = \beta\gamma^i\beta\gamma^j + \beta\gamma^j\beta\gamma^i = \beta^2\left(\gamma^i\gamma^j + \gamma^j\gamma^i\right) =$
$\{\gamma^i, \gamma^j\} = 2\delta_{ij}.$
Am I allowed to write, with (11.25):

$\{\gamma^i, \gamma^j\} = 2g^{ij}$?

On page 174, Fp writes: *"One way of satisfying the above anti-commutation relations is to represent the operators γ^μ as matrices. However, it turns out that the smallest dimension in which γ^μ can be realized is four."*

Dirac, page 256: *"We can easily obtain a representation of the four α's. They have similar algebraic properties to the σ's introduced in* § 37. *…".*

And Dirac explained why 4×4 matrices are needed.

Then, γ^0 , (11.26):

$\gamma^0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$, (11.26). Note: γ^0 represents also the tensor product: $\sigma_z \otimes I$

γ^1 , (11.27) and (5.70):

$\gamma^1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$, (11.27).

γ^2 , (11.27) and (5.71):

$\gamma^2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}$, (11.27).

γ^3 , (11.27) and (5.72):

$\gamma^3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$,(11.27)

Now, Fp mentioned: *"It is easily verified that these 4×4 matrices, satisfy the appropriate anti-commutation relations."*

So, with (11.25):

$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} \rightarrow \gamma^0\gamma^0 = g^{00}$?

We know $g^{00} = 1$, the first diagonal element of the metric tensor.

$\gamma^0\gamma^0$ is a product of 4×4 matrices. This results into 4×4 unity matrix. The unit matrix equals the number 1?

Another one:

$\{\gamma^0, \gamma^1\} = 2g^{01} \rightarrow \gamma^0\gamma^1 + \gamma^1\gamma^0 = 2g^{01}$?

$2g^{01} = 0$,

and

$$\gamma^0\gamma^1 + \gamma^1\gamma^0 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{pmatrix}.$$

$\{\gamma^0, \gamma^1\}$ is a product of 4×4 matrices. This results into a 4×4 zero matrix. The zero matrix equals the number 0?

With $\{\gamma^1, \gamma^1\} = 2g^{11} \rightarrow \gamma^1\gamma^1 + \gamma^1\gamma^1 = 2g^{11}$?

$2g^{11} = -2$,

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

In this way 4×4 matrices satisfy the appropriate anti-commutation relations.
With (11.29), (11.20) is obtained?
I choose as an example σ_x and σ_z , respectively.
Then,
$\sigma_x\sigma_z + \sigma_z\sigma_x = 2\delta_{xz}$?

$$\sigma_x\sigma_z + \sigma_z\sigma_x = \begin{pmatrix} \sigma_x\sigma_z + \sigma_z\sigma_x & 0 \\ 0 & \sigma_z\sigma_x + \sigma_x\sigma_z \end{pmatrix}.$$

With (5.70) and (5.72)

$$\begin{pmatrix} \sigma_x\sigma_z + \sigma_z\sigma_x & 0 \\ 0 & \sigma_z\sigma_x + \sigma_x\sigma_z \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = 2\delta_{xz}.$$

Next, FP, *"it is easily demonstrated* $\gamma^{\mu\dagger} = \gamma^0\gamma^\mu\gamma^0$ *for* $\mu = 0,3$. "
As an example I choose $\mu = 1$:
$\gamma^{1\dagger} = \gamma^0\gamma^1\gamma^0$?

$$\gamma^{1\dagger} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

and

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

Then

$$\gamma^0\gamma^1\gamma^0 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = \gamma^{1\dagger}.$$

Next (11.18) is written as (11.31).
Then, (11.32):
Dirac writes: *"As Hamiltonian we must take the expression as equal to* cp_0 *when we put the operator on* ψ *in (10) equal to zero, i.e. ….".*
Dirac's (10) is Fp's (11.18). In this way the time dependent wave equation is obtained and the expression between brackets on the right-hand side in (11.32) represents the Hamiltonian operator.
On page 256, as mentioned before, Dirac explained the 4×4 matrices. Dirac related the dimension of the matrices to the dimensions of the anti-commutating quantities.
Fp related the dimension to the negative energy states. Well, Dirac mentioned the negative energy state on page 256. "*For the present we shall consider only the positive-energy solutions and shall leave the negative-energy ones to §73",* Dirac. Still, Dirac needed the 4×4 matrices.
In (11.33) and (11.34), $\Phi_0 \to A_0(\phi)$ the scalar potential.
Then, (11.35) is obtained.

With (11.39)

$\psi^\dagger\gamma^0\gamma^\mu i\hbar\partial_\mu\psi - \psi^\dagger\gamma^0\gamma^\mu\frac{e}{c}\Phi_\mu\psi - \psi^\dagger\gamma^0 m_e c\psi = 0$. (C.11.2)

The Hermitian conjugate of (C.11.2):

$\psi^\dagger(-i\hbar\partial_\mu)\gamma^0\gamma^\mu\psi - \psi^\dagger\frac{e}{c}\Phi_\mu\gamma^0\gamma^\mu\psi - \psi^\dagger m_e c\gamma^0\psi = 0.$ (C.11.3)

Reminder: in (C.11.3), $(-i\hbar\partial_\mu)$ operates on $\psi^\dagger$.

Fp took the difference between (C.11.2) and (C.11.3):

$\psi^\dagger\gamma^0\gamma^\mu i\hbar\partial_\mu\psi + \psi^\dagger\big(i\hbar\partial_\mu\big)\gamma^0\gamma^\mu\psi = 0 \rightarrow \psi^\dagger\gamma^0\gamma^\mu\partial_\mu\psi + \partial_\mu\psi^\dagger\gamma^0\gamma^\mu\psi = 0.$ (C.11.4)

Then, Fp introduced the relativistic probability current $\boldsymbol{j}(\mathrm{x}, t)$ into (C.11.4):

$\partial_\mu j^\mu = 0$, (11.41),

where, (11.42),

$j^\mu = c\psi^\dagger\gamma^0\gamma^\mu\psi$.

This results finally into (11.44), while Fp also introduced the relativistic probability density, (11.43).

Fp mentioned on page 176, $\partial_\mu j^\mu = 0$, (11.41), to be Lorentz invariant. When this is so, the wave function is properly normalized in all inertial frames.

11.3 Lorentz Invariance of Dirac Equation

Two inertial frames are considered with their space-time coordinates. The relation between these coordinates are presented in (11.48).

(11.50):

$x^{\mu'}x_{\mu'} = x^\mu x_\mu.$

With (11.49):

$x^{\mu'}x_{\mu'} = x^{\mu'}a^\nu_\mu x_\nu.$

Using (11.48):

$x^{\mu'}a^\nu_\mu x_\nu = a^\mu_\nu x^\nu a^\nu_\mu x_\nu,$ (C.11.15)

Remark: Fp:"…*where the* a^μ_ν *are real numerical coefficients* …".

So, a^μ_ν are no vectors and /or tensors. Then, what is the meaning of the suffixes? Since, in (C.11.15), the suffix ν appears 4 times, I supposed something to be wrong.

Just below (11.11), shows g^λ_ν to be real numerical coefficients. There is no relation with (11.10), (11.11) and (11.51)?

(11.48) and (C.11.15):

$x^\mu x_\mu = a^\mu_\nu x^\nu a^\nu_\mu x_\nu \rightarrow a^\mu_\nu a^\lambda_\mu = g^\lambda_\nu$, (11.51).

(11.52) and (11.53):

I suppose, with (11.48),

$x^{\nu'} = a^\nu_\mu x^\mu$.

Then,

$a^\mu_\nu x^{\nu'} = a^\mu_\nu a^\nu_\mu x^\mu = x^\mu$, (11.52). (Three equal indices is wrong in this case?

(11.53) is obtained similarly.

In (11.56), Fp presented the Dirac equation in the S frame:

$\left[\gamma^{\mu}\left(p_{\mu}-\frac{e}{c}\Phi_{\mu}\right)-m_{e}c\right]\psi=0,$

whereas Fp presented the Dirac equation in (11.34) as:

$\left[\gamma^{\mu}\left(p_{\mu}-\frac{e}{c}\Phi_{\mu}\right)-m_{e}c\right]\psi=0$.

To transform the wave function, Fp used a 4×4 matrix A independent of x^{μ}.

Multiply (11.56) with A :

$\left[A\gamma^{\mu}\left(p_{\mu}-\frac{e}{c}\Phi_{\mu}\right)-Am_{e}c\right]\psi=A\gamma^{\mu}\left(p_{\mu}-\frac{e}{c}\Phi_{\mu}\right)\psi-m_{e}c\psi'=0$. (C.11.16)

Now,

$A\gamma^{\mu}\left(p_{\mu}-\frac{e}{c}\Phi_{\mu}\right)A^{-1}A\psi-m_{e}c\psi'\rightarrow\left[A\gamma^{\mu}\left(p_{\mu}-\frac{e}{c}\Phi_{\mu}\right)A^{-1}-m_{e}c\right]\psi'=0.$ (C.11.17)

What about $p_{\mu}A^{-1}$ and $\Phi_{\mu}A^{-1}$?

We have A to commute with p_{μ} and Φ_{μ}. Furthermore $AA^{-1}=I$.

Then,

$Ap_{\mu}=p_{\mu}A\rightarrow Ap_{\mu}A^{-1}=p_{\mu}AA^{-1}=p_{\mu}\rightarrow A^{-1}Ap_{\mu}A^{-1}=A^{-1}p_{\mu}\rightarrow p_{\mu}A^{-1}=A^{-1}p_{\mu}.$

Hence A^{-1} commutes with p_{μ} and consequently with Φ_{μ}.

So, (C.11.17) becomes:

$\left[A\gamma^{\mu}A^{-1}\left(p_{\mu}-\frac{e}{c}\Phi_{\mu}\right)-m_{e}c\right]\psi'=0$, (11.58).

Reminder: A a 4×4 transformation matrix. Then, $AA^{-1}=A^{-1}A=I$.

With covariant representation of (11.55):

$p_{\mu}=a_{\mu}^{\nu}p_{\nu'}$,

and

$\Phi_{\mu}=a_{\mu}^{\nu}\Phi_{\nu'}$, (11.59) is obtained.

Now, use (11.60):

$A\gamma^{\mu}A^{-1}a_{\mu}^{\nu}=\gamma^{\nu}.$

Reminder A to be a 4×4 transformation matrix and γ^{μ} to be matrices presented in (11.26) and (11.27).

Furthermore, I assume A to be Hermitian. Then, with (11.60):

$A\gamma^{\mu}A^{-1}a_{\mu}^{\nu}=\gamma^{\nu}\rightarrow\gamma^{\mu}AA^{-1}a_{\mu}^{\nu}=\gamma^{\nu}\rightarrow\gamma^{\mu}a_{\mu}^{\nu}=\gamma^{\nu}\rightarrow$ (11.61).

Remark: just below (11.61) Fp writes *"(since they are just numbers)"*. They?

With (11.61), (11.62) is obtained and Fp proved the Dirac equation to be Lorentz invariant.

Next is about the transformation matrix A.

Since $A^{-1}A=1$, (11.66) follows by inspection.

(11.67), with (11.64):

Plug $\Delta\omega^{\nu\mu}=-\Delta\omega^{\mu\nu}$ into (11.65).

Then,

$A=1-\frac{i}{4}\sigma_{\mu\nu}\Delta\omega^{\mu\nu}=1+\frac{i}{4}\sigma_{\mu\nu}\Delta\omega^{\nu\mu}$.

So, with the summation convention:

$A=1+\frac{i}{4}\sigma_{\nu\mu}\Delta\omega^{\nu\mu}$.

Consequently: $\sigma_{\mu\nu}=-\sigma_{\mu\nu}$,(11.67).

To obtain (11.68), the following expression,(11.61), needs to be evaluated:

$\left(1+\frac{i}{4}\sigma_{\mu\nu}\Delta\omega^{\mu\nu}\right)\gamma^{\nu}\left(1-\frac{i}{4}\sigma_{\mu\nu}\Delta\omega^{\mu\nu}\right)=\left(g_{\mu}^{\nu}+\Delta\omega_{\mu}^{\nu}\right)\gamma^{\mu}$. (C.11.18)

Now, (C.11.18) up to order $(\Delta\omega^{\mu\nu})^2$:

$\gamma^\nu + \frac{i}{4}\Delta\omega^{\mu\nu}\left(\sigma_{\mu\nu}\gamma^\nu - \gamma^\nu\sigma_{\mu\nu}\right) = g_\mu^\nu\gamma^\mu + \Delta\omega_\mu^\nu\gamma^\mu = \gamma^\nu + \Delta\omega_\mu^\nu\gamma^\mu,$ (C.11.19)

since $g_\mu^\nu = 1$, for $\mu = \nu$ and $g_\mu^\nu = 0$, for $\mu \neq \nu$.

To make the summation convention more explicit, (C.11.19):

$\Delta\omega_\beta^\nu\gamma^\beta = -\frac{i}{4}\Delta\omega^{\alpha\beta}\left(\gamma^\nu\sigma_{\alpha\beta} - \sigma_{\alpha\beta}\gamma^\nu\right)$, (11.68).

Having obtained (11.70), Fp writes it can be shown (11.71) is a suitable solution of (11.70). Let's find out.

I will make use of the inverse γ's: $\gamma^\nu = -\gamma_\nu$ for $\nu = 1,2,3$ and $g_\mu^\nu = 1$, for $\mu = \nu$ and $g_\mu^\nu = 0$, for $\mu \neq \nu$.

In addition, (11.25),

$\mu \neq \nu \rightarrow \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 0$,

and

$\mu = \nu \rightarrow \gamma^\nu\gamma^\nu = -2I$, contraction, i.e, the summation convention.

The inverse of γ^ν:

$\gamma^\nu = g^{\mu\nu}\gamma_\mu.$

Then,

$\gamma^0 = \gamma_0$, (C.11.20)

and $\nu = 1,2,3$

$\gamma^\nu = -\gamma_\nu$. (C.11.21)

So, $\gamma_\nu\gamma^\nu = 2I$.

Multiply (11.70) to the left with γ_ν:

$2i(\gamma_\nu g_\alpha^\nu\gamma_\beta - \gamma_\nu g_\beta^\nu\gamma_\alpha) = \gamma_\nu\gamma^\nu\sigma_{\alpha\beta} - \gamma_\nu\sigma_{\alpha\beta}\gamma^\nu = 2\sigma_{\alpha\beta} - \gamma_\nu\sigma_{\alpha\beta}\gamma^\nu.$ (C.11.22)

Now, evaluate $\gamma_\nu g_\alpha^\nu$:

$\alpha = 0 \rightarrow \gamma_0 g_0^0 + \gamma_1 g_0^1 + \gamma_2 g_0^2 + \gamma_3 g_0^3 = \gamma_0,$

$\alpha = 1 \rightarrow \gamma_0 g_1^0 + \gamma_1 g_1^1 + \gamma_2 g_1^2 + \gamma_3 g_1^3 = \gamma_1,$

$\alpha = 2 \rightarrow \gamma_0 g_2^0 + \gamma_1 g_2^1 + \gamma_2 g_2^2 + \gamma_3 g_2^3 = \gamma_2,$

and

$\alpha = 3 \rightarrow \gamma_0 g_3^0 + \gamma_1 g_3^1 + \gamma_2 g_3^2 + \gamma_3 g_3^3 = \gamma_3.$

So, for $\alpha = 0,3 \rightarrow \gamma_\nu g_\alpha^\nu = \gamma_\alpha$,

where use have been made of the values of g_α^ν given just below (11.11).

Similarly:

for $\beta = 0,3 \rightarrow \gamma_\nu g_\beta^\nu = \gamma_\beta.$

Next, in (C.11.22), evaluate $\gamma_\nu\gamma^\nu$, with (C.11.20) and (C.11.21):

for $\nu = 0,3 \rightarrow \quad \gamma_\nu\gamma^\nu = 2I.$

So, I found for (C.11.22):

$2i\left(\gamma_\alpha\gamma_\beta - \gamma_\beta\gamma_\alpha\right) = 2\sigma_{\alpha\beta} - \gamma_\nu\sigma_{\alpha\beta}\gamma^\nu,$

or

$2i\left[\gamma_\alpha, \gamma_\beta\right] = 2\sigma_{\alpha\beta} - \gamma_\nu\sigma_{\alpha\beta}\gamma^\nu$. (C.11.23)

What about $\gamma_\nu\sigma_{\alpha\beta}\gamma^\nu$ in (C.11.23)?

Well, contraction produces:

$\gamma_\nu\sigma_{\alpha\beta}\gamma^\nu = -2\sigma_{\alpha\beta}$. (C.11.24)

(11.74) is about evaluating $A^\dagger$ in (11.72), with (11.26) and (11.30):

$[\gamma_\mu, \gamma_\nu]^\dagger \rightarrow (\gamma_\nu^\dagger \gamma_\mu^\dagger - \gamma_\mu^\dagger \gamma_\nu^\dagger) \rightarrow (\gamma^0\gamma_\nu\gamma^0\gamma^0\gamma_\mu\gamma^0 - \gamma^0\gamma_\mu\gamma^0\gamma^0\gamma_\nu\gamma^0) \rightarrow$
$\rightarrow (\gamma^0\gamma_\nu\gamma_\mu\gamma^0 - \gamma^0\gamma_\mu\gamma_\nu\gamma^0) \rightarrow \gamma^0(\gamma_\nu\gamma_\mu - \gamma_\mu\gamma_\nu)\gamma^0 \rightarrow -\gamma^0[\gamma_\mu, \gamma_\nu]\gamma^0 \rightarrow (11.74),$
where $\Delta\omega^{\mu\nu}$ is a number.
(11.74):
$A^\dagger = \gamma^0 A^{-1}\gamma^0$.
Multiply this expression to the right by $\gamma^0\gamma^\mu A$:
$A^\dagger\gamma^0\gamma^\mu A = \gamma^0 A^{-1}\gamma^0\gamma^0\gamma^\mu A \rightarrow A^\dagger\gamma^0\gamma^\mu A = \gamma^0 A^{-1}\gamma^\mu A.$ (C.11.25)
With (11.61) rewritten as:
$A^{-1}\gamma^\mu A = a_\nu^\mu \gamma^\nu$,
(C.11.25) becomes
$A^\dagger\gamma^0\gamma^\mu A = a_\nu^\mu \gamma^0\gamma^\nu$,(11.75).
Keep in mind: a_ν^μ to be a real numerical coefficient.
Multiply (11.75) to the right and to the left with ψ' and ψ giving (11.76).
Then , use (11.57), (11.770 is obtained.
With the definition of the relativistic probability current j^μ ,(11.42), (11.78) shows the transformation of the current as the contravariant components of a 4-vector.

11.4 Free Electron Motion

In (11.79) the Hamiltonian of a free electron is presented. See (11.32), the right-hand side. Then, Fp used the Heisenberg picture to investigate the motion of the relativistic free electron. The formalism presented in (11.80) is given by (3.25) in section (3.2) on The Heisenberg equation of motion.
The commutator in (11.80) and using $p_1 = -i\hbar\frac{\partial}{\partial x}$:
$[x, H] = xH - Hx = x(c\boldsymbol{\alpha}\cdot\boldsymbol{p}) + x\beta m_e c^2 - (c\boldsymbol{\alpha}\cdot\boldsymbol{p})x - \beta m_e c^2 x =$
$= x(c\boldsymbol{\alpha}\cdot\boldsymbol{p}) - (c\boldsymbol{\alpha}\cdot\boldsymbol{p})x = i\hbar c\alpha_1,$
where $\boldsymbol{\alpha}$ does not operate on x and Fp writes: "…*where use has been made of the standard commutation relations between position and momentum operators*".
So, $x(c\boldsymbol{\alpha}\cdot\boldsymbol{p}) - (c\boldsymbol{\alpha}\cdot\boldsymbol{p})x = c\alpha_1 x p_1 - c\alpha_1 p_1 x = c\alpha_1 x p_1 + i\hbar c\alpha_1 - c\alpha_1 x p_1 = i\hbar c\alpha_1.$
Eq. (11.80) is Eq. 24 in Dirac's section 69 on *The motion of a free electron*.
Then, Fp follows the text of Dirac.
The connection with the probability current, as presented in (11.44) is mentioned:
$j_i = \psi^\dagger c\alpha_i\psi$, (11.44).
The operator $\dot{x}$ has eigenvalues $\pm c$, since $\alpha_1 = \gamma^0\gamma^1 = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix}$ has eigenvalues ± 1.
See Dirac top page 262. The same result is obtained when a field is present. According to Dirac and Fp, this is easily demonstrated.
Well, I think to this end the Hamiltonian in (11.37) is needed:
$H = -e\phi + c\boldsymbol{\alpha}\cdot(\boldsymbol{p} + e\boldsymbol{A}) + \beta m_e c^2$. (C.11.26)
Then,
$[x, H] = -xe\phi + cx\boldsymbol{\alpha}\cdot(\boldsymbol{p} + e\boldsymbol{A}) + x\beta m_e c^2 + e\phi x - c\boldsymbol{\alpha}\cdot(\boldsymbol{p} + e\boldsymbol{A})x - \beta m_e c^2 x =$
$= x(c\boldsymbol{\alpha}\cdot\boldsymbol{p}) - (c\boldsymbol{\alpha}\cdot\boldsymbol{p})x = c\alpha_1 x p_1 - c\alpha_1 p_1 x = c\alpha_1 x p_1 + i\hbar c\alpha_1 - c\alpha_1 x p_1 = i\hbar c\alpha_1.$
Furthermore Fp explained the eigenvalue c of the electron. This velocity is considered to be the velocity *at one instance in time*. The Heisenberg uncertainty relations and measurement

plays decisive role. To this end Fp examine how the electron velocity varies in time.
The formalism of chapter 3 ,(3.25), is applied to α_1, giving (11.81).
Just above (11.82): α_1 *anti- commutes with all terms in* H *except* $c\alpha_1 p^1$:

$$\alpha_1 H + H\alpha_1 =$$
$$= -e\alpha_1\phi + c\alpha_1\boldsymbol{\alpha}\cdot(\boldsymbol{p}+e\boldsymbol{A}) + \alpha_1\beta m_e c^2 - e\phi\alpha_1 + c\boldsymbol{\alpha}\cdot(\boldsymbol{p}+e\boldsymbol{A})\alpha_1 + \beta m_e c^2\alpha_1, \quad \text{(C.11.27)}$$

In (C.11.27), first,
$m_e c^2(\alpha_1\beta + \beta\alpha_1) = 0$, (11.21) and Dirac page 257.
Then,
$e\alpha_1(\phi, c\boldsymbol{\alpha}\cdot\boldsymbol{A}) + e(\phi, c\boldsymbol{\alpha}\cdot\boldsymbol{A})\alpha_1 = 0?$ (C.11.28)

Or, is still the case considered, as mentioned just below (11.18):"…, *because we are considering the case of no electromagnetic field,…"*? Then, we have the Hamiltonian as presented in (11.79).
I suppose so. Consequently, I can leave (C.11.28). With (11.27):
$\alpha_1 H + H\alpha_1 = 2cp^1$, (11.82), $\rightarrow\ H\alpha_1 = -\alpha_1 H + 2cp^1$. Plug the expression for $H\alpha_1$ into (11.81)→(11.83).
With (11.83):
$\alpha_1 = \frac{i\hbar}{2}\dot{\alpha}_1 H^{-1} + cp^1 H^{-1}.$ (C.11.29)
Plug $\dot{\alpha}_1$,(11.85) into (C.11.29)→(11.86) using $p^1 = p_x$.
Finally integrate (11.86)→(11.87).

11.5 Electron Spin.

Now Fp returns to the Hamiltonian of an electron in an electromagnetic field.
Now, the Hamiltonian presented in the foregoing section, (C.11.26) and (11.88), is applied.
With (11.21) the cross product in (11.89) is zero and with (11.22) $\beta^2 = 1$.
For convenience I present (5.92):
$(\boldsymbol{\sigma}\cdot\boldsymbol{a})(\boldsymbol{\sigma}\cdot\boldsymbol{b}) = \boldsymbol{a}\cdot\boldsymbol{b} + i\boldsymbol{\sigma}\cdot(\boldsymbol{a}\times\boldsymbol{b}) \rightarrow (11.95).$
Then, (11.98) is obtained.
(11.05):
$[L_x, r] = 0.$
With (11.03) and keeping in mind the commutator $[L_x, r]$ operates on a wavefunction, ψ say,
$i\hbar(z\frac{\partial r}{\partial y} - y\frac{\partial r}{\partial z})$ has to be evaluated.
Well, with $r = \sqrt{x^2+y^2+z^2}$,
$z\frac{\partial r}{\partial y} - y\frac{\partial r}{\partial z} = 0$, and (11.05) is obtained.
Next, (11.106),
$[L_x, p_x] = 0.$
The evaluation is about expressions like: $\frac{\partial}{\partial x}z\frac{\partial}{\partial y}\psi$
After applying the chain rule we have:

$z\frac{\partial^2}{\partial y\partial x} - z\frac{\partial^2}{\partial x\partial y} - y\frac{\partial^2}{\partial z\partial x} + y\frac{\partial^2}{\partial x\partial z} \to 0$.

Then, (11.107),

$[L_x, p_y] = i\hbar p_z.$

By using the chain rule, the result is:

$[L_x, p_y] = \hbar^2 \frac{\partial}{\partial z} \to i\hbar p_z.$

In the same way (11.108) is obtained.

$$[L_x, H] = i\hbar c\gamma^5 \left\{\left(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right)\boldsymbol{\Sigma}\cdot\boldsymbol{p} - \boldsymbol{\Sigma}\cdot\boldsymbol{p}\left(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right)\right\}. \qquad \text{(C.11.30)}$$

With

$\boldsymbol{\Sigma}\cdot\boldsymbol{p} = \Sigma_x p_x + \Sigma_y p_y + \Sigma_z p_z,$

the terms contributing to (C.11.30) are:

$$\Sigma_y p_z \text{ , and } -\Sigma_z p_y \to \Sigma_2 p_z - \Sigma_3 p_y, \qquad \text{(C.11.31)}$$

this expression results from

$\Sigma_z p_z z\frac{\partial}{\partial y}$, and $\Sigma_y p_y y\frac{\partial}{\partial z}$

Plug (C.11.31) into (C.11.30):

$[L_x, H] == i\hbar c\gamma^5(\Sigma_2 p_z - \Sigma_3 p_y)$, (11.109) .

Then, with the Heisenberg formalism, (3.25), and, (11.104), (11.110) is found.

Next the Heisenberg formalism is applied to $\dot{\Sigma}_1$ →(11.111).

(11.112):

$$\begin{pmatrix}\sigma_1 & 0\\ 0 & \sigma_1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} - \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\sigma_1 & 0\\ 0 & \sigma_1\end{pmatrix} = 0.$$

(11.113):

Σ_1 commute with itself.

(11.114):

$$[\Sigma_1, \Sigma_2] = \begin{pmatrix}\sigma_1\sigma_2 - \sigma_2\sigma_1 & 0\\ 0 & \sigma_1\sigma_2 - \sigma_2\sigma_1\end{pmatrix} = 2i\begin{pmatrix}\sigma_i & 0\\ 0 & \sigma_i\end{pmatrix} = 2i\Sigma_3.$$

Simarlily, (11.115) is obtained.

Then, using (11.112)-(11.115) and (11.102):

$[\Sigma_1, H] = [\Sigma_1, c\gamma^5\boldsymbol{\Sigma}\cdot\boldsymbol{p}] \to c\gamma^5\{\Sigma_1\boldsymbol{\Sigma}\cdot\boldsymbol{p} - \boldsymbol{\Sigma}\cdot\boldsymbol{p}\Sigma_1\} =$

$= c\gamma^5\{\Sigma_1\Sigma_2 p_2 - \Sigma_2 p_2\Sigma_1 - \Sigma_1\Sigma_3 p_3 + \Sigma_3 p_3\Sigma_1\}$ →(11.116).

With (11.111), (11.117) is obtained.

Then, (11.110) and (11.117)→ (11.118).

In (11.119), Fp presented the relation between the gyromagnetic moment and the spin operator. There the gyromagnetic ratio g appears. Now , we know with

$\boldsymbol{\Sigma} = 2\boldsymbol{S}/\hbar$, just below (11.118), and (11.101),

$g = 2$, (11.120).

11.6 Motion in Central Field

In this section the motion of an electron in a central field is studied. The Hamiltonian is given in (11.121).

In my notes on *The Undergraduate Course* section 9.2, (11.125) has been derived.

It is about p_r, with (8.20)-(8.25), *Undergraduate Course,*

$\frac{\partial}{\partial r} = \frac{\partial}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial}{\partial y}\frac{\partial y}{\partial r} + \frac{\partial}{\partial z}\frac{\partial z}{\partial r} = \frac{x}{r}\frac{\partial}{\partial x} + \frac{y}{r}\frac{\partial}{\partial y} + \frac{z}{r}\frac{\partial}{\partial z}$.

Multiply $\frac{\partial}{\partial r}$ with $-i\hbar$:

$-i\hbar\ \frac{\partial}{\partial r} = \frac{1}{r}\left(-xi\hbar\frac{\partial}{\partial x} - yi\hbar\frac{\partial}{\partial y} - zi\hbar\frac{\partial}{\partial z}\right) = \frac{1}{r}\left(xp_x + yp_y + zp_z\right) = \frac{\boldsymbol{p}\cdot\boldsymbol{r}}{r} \equiv p_r\ .$ (C.11 32)

Fine, however in (11.123):

$p_r = \boldsymbol{x}\cdot\boldsymbol{p}\ .$

How does (11.123) relate with $\frac{\boldsymbol{p}\cdot\boldsymbol{r}}{r}$? I think: $\boldsymbol{x} = \frac{\boldsymbol{r}}{r}$.

Then, (11.124), with (11.124)

$[r, p_r] = r\frac{\boldsymbol{r}}{r}\cdot\boldsymbol{p} - \frac{\boldsymbol{r}}{r}\cdot\boldsymbol{p}r = \boldsymbol{r}\cdot\boldsymbol{p} - \boldsymbol{r}\cdot\boldsymbol{p} + \frac{i\hbar}{r}\left(x\frac{\partial r}{\partial x} + y\frac{\partial r}{\partial y} + z\frac{\partial r}{\partial z}\right) = i\hbar\ .$

The total angular momentum is presented in (11.126).

For convenience I present here (11.95):

$(\boldsymbol{\Sigma}\cdot\boldsymbol{a})(\boldsymbol{\Sigma}\cdot\boldsymbol{b}) = \boldsymbol{a}\cdot\boldsymbol{b} + \mathrm{i}\boldsymbol{\Sigma}\cdot(\boldsymbol{a}\times\boldsymbol{b})$,

then (11.127) is found.

Furthermore, (4.11)→ (11.128).

Plug (11.126) and (11.128)→ (11.129).

So, with $\Sigma^2 = 3$ and (11,129)→ (11.130).

See also Dirac page 268.

To obtain (11.131) and (11.132) with (11.95) make use of:

$\boldsymbol{L}\cdot\boldsymbol{p} = 0 \rightarrow \sum_{k=1,3} L_k\, p_k\ .$

Then with (4.1)-(4.3) and $p_k = -i\hbar\frac{\partial}{\partial x_k} \rightarrow \sum_{k=1,3} L_k\, p_k = 0.$

The next step is to derive (11.133). To this end, the right-hand side of (11.131) and (11.132) is analysed. It is about:

$\boldsymbol{L}\times\boldsymbol{p}$ and $\boldsymbol{p}\times\boldsymbol{L}$

Let's take as one of the terms in (11.131), similar to $L_1 = x_2p_3 - x_3p_2$, resulting from $\boldsymbol{L} = \boldsymbol{x}\times\boldsymbol{p}$,

$\Sigma_1\cdot[(\boldsymbol{L}\times\boldsymbol{p})_1 + (\boldsymbol{p}\times\boldsymbol{L})_1] = \Sigma_1\cdot[L_2p_3 - L_3p_2 + p_2L_3 - p_3L_2]$

$= \Sigma_1\cdot[(x_3p_1 - x_1p_3)p_3 - (x_1p_2 - x_2p_1)p_2 + p_2(x_1p_2 - x_2p_1) - p_3(x_3p_1 - x_1p_3)] =$

$= \Sigma_1\cdot(i\hbar p_1 + i\hbar p_1) = 2i\hbar\Sigma_1p_1.$

So the terms contributing to $2i\hbar\Sigma_1p_1$ are:

$-p_2x_2p_1$ and $-p_3x_3p_1$.

Similarly for $\Sigma_2\cdot[(\boldsymbol{L}\times\boldsymbol{p})_2 + (\boldsymbol{p}\times\boldsymbol{L})_2]$ and $\Sigma_3\cdot[(\boldsymbol{L}\times\boldsymbol{p})_3 + (\boldsymbol{p}\times\boldsymbol{L})_3]$, we find:

$2i\hbar\Sigma_2p_2$ and $2i\hbar\Sigma_3p_3$.

Hence,

$\Sigma_1\cdot[(\boldsymbol{L}\times\boldsymbol{p})_1 + (\boldsymbol{p}\times\boldsymbol{L})_1] = 2i\hbar(\Sigma_1p_1 + \Sigma_2p_2 + \Sigma_3p_3) = 2i\hbar\boldsymbol{\Sigma}\cdot\boldsymbol{p}.$

With this result, (11.134) and (11.135) are obtained[10].

With (11.90), $\gamma^5\boldsymbol{\Sigma} = \boldsymbol{\alpha}$, (11.136) is found.

β is presented in (11.28) and ζ is defined by (11.138).

Use the above result, then (11.139), using (4.1)-(4.3), is obtained:

$(\boldsymbol{L}\times\boldsymbol{x})_1 + (\boldsymbol{x}\times\boldsymbol{L})_1 = L_2x_3 - L_3x_2 + x_2L_3 - x_3L_2 = 2i\hbar x_1.$

The terms contributing to $2i\hbar x_1$ are:

$-x_1p_3x_3$ and $-x_1p_2x_2$.

To obtain (11.142) and (11.142):

[10] This result took me some time to obtain. I mistook $\boldsymbol{L}\times\boldsymbol{p} + \boldsymbol{p}\times\boldsymbol{L}$ for a vector product. Then $\boldsymbol{L}\times\boldsymbol{p} + \boldsymbol{p}\times\boldsymbol{L} = 0$. We are dealing with operators operating on a wave function.

$[\beta, \Sigma_i] = 0.$
This is demonstrated with (11.28) and (11.92):
$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix} - \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = 0$.
For the eigenvalues of ζ^2, see Chapter 6 on Addition of Angular Momentum.
To obtain (11.145), use is made of (C.11.32) and section 4.1:
$\boldsymbol{x} \cdot \boldsymbol{p} = \left(xp_x + yp_y + zp_z\right) = rp_r$ (not equal to (11.123),
$\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}$ **.**
With (11.138) and (11.22), we have:
$\beta\, \zeta = \beta^2(\boldsymbol{\Sigma} \cdot \boldsymbol{L} + \hbar) = \boldsymbol{\Sigma} \cdot \boldsymbol{L} + \hbar.$
Finally, with these results (11.145) is obtained.
In (11.146) a new operator ϵ is defined.
Since $r\epsilon$ is a (complex) number ϵ and r commute, (11.147).
With (11.20), (11.146) and $\{\alpha_i, \alpha_j\} = 2\delta_{ij}$, (11.148) is found.
(11.151):
$-(\boldsymbol{x} \cdot \boldsymbol{p})\ (\boldsymbol{\Sigma} \cdot \boldsymbol{x}) \rightarrow -(\boldsymbol{\Sigma} \cdot \boldsymbol{x})(\boldsymbol{x} \cdot \boldsymbol{p}) + i\hbar\boldsymbol{\Sigma} \cdot \boldsymbol{x} \rightarrow (11.151).$
To find (11.152), some expressions are needed:
- $\gamma^5\boldsymbol{\Sigma} = \boldsymbol{\alpha}$,top page 185,
- $r\epsilon = \boldsymbol{\alpha} \cdot \mathbf{x}$ **,** (11.146),
- $\boldsymbol{x} \cdot \boldsymbol{p} = rp_r$,
and
$\boldsymbol{\Sigma} \cdot \boldsymbol{x} = \gamma^5 r\epsilon$.
$\gamma^5\boldsymbol{\Sigma} \cdot \mathbf{x} = \boldsymbol{\alpha} \cdot \mathbf{x} = r\epsilon$. Multiply this expression to the left and to the right with γ^5 and with (11.91), $\boldsymbol{\Sigma} \cdot \mathbf{x} = \gamma^5\, r\epsilon$, is obtained.
With these results and (11.152):
$\gamma^5\boldsymbol{\Sigma} \cdot [\boldsymbol{x}(\boldsymbol{x} \cdot \boldsymbol{p}) - (\boldsymbol{x} \cdot \boldsymbol{p})\boldsymbol{x}] = r\epsilon rp_r - rp_r r\epsilon = i\hbar\gamma^5\boldsymbol{\Sigma} \cdot \mathbf{x} = i\hbar r\epsilon \rightarrow$
$\rightarrow r^2\epsilon p_r - rp_r r\epsilon = i\hbar r\epsilon$, (11.152).

Note: $r^2\epsilon p_r - rp_r r\epsilon$ an operator operating on a wave function ψ, with (11.125):
$(r^2\epsilon p_r - rp_r r\epsilon)\psi = r^2\epsilon p_r\psi - r^2\epsilon p_r\psi - r\epsilon\psi p_r r = i\hbar r\epsilon.$

$r\epsilon rp_r - rp_r r\epsilon = i\hbar r\epsilon \rightarrow \epsilon rp_r - p_r r\epsilon = i\hbar\epsilon.$ (C.11.33)
Now (11.124):
$[r, p_r] = i\hbar \rightarrow\ i\hbar\epsilon = rp_r\epsilon - p_r r\epsilon.$
Then with (C.11.33):
$rp_r\epsilon - p_r r\epsilon = \epsilon rp_r - p_r r\epsilon \rightarrow rp_r\epsilon - \epsilon rp_r = p_r\epsilon - \epsilon p_r = [\epsilon, p_r] = 0$, (11.153).
(11.145)
$(\boldsymbol{\Sigma} \cdot \boldsymbol{x})(\boldsymbol{\Sigma} \cdot \mathbf{p}) = rp_r + i(\beta\zeta - \hbar) \rightarrow \gamma^5(\boldsymbol{\Sigma} \cdot \boldsymbol{x})\gamma^5(\boldsymbol{\Sigma} \cdot \mathbf{p}) = (\gamma^5)^2[rp_r + i(\beta\zeta - \hbar)] \rightarrow$
$\rightarrow (\boldsymbol{\alpha} \cdot \mathbf{x})(\boldsymbol{\alpha} \cdot \mathbf{p}) = rp_r + i(\beta\zeta - \hbar), (11.154).$
Using $\boldsymbol{\alpha} \cdot \mathbf{x} = r\epsilon$ and $\epsilon^2 = 1$ in (11.154):
$r\epsilon(\boldsymbol{\alpha} \cdot \mathbf{p}) = rp_r - i\hbar + i\beta\zeta$, then,
$\boldsymbol{\alpha} \cdot \mathbf{p} = \epsilon\left(p_r - \frac{i\hbar}{r}\right) + \frac{i\epsilon\beta\zeta}{r}$, (11.155).
The Hamiltonian(11.121), with (11.155):

$H = -e\phi(r) + c\boldsymbol{\alpha}\cdot\mathbf{p} + m_e\beta c^2 \rightarrow H = -e\phi(r) + c\epsilon\left(p_r - \frac{i\hbar}{r}\right) + \frac{ic\epsilon\beta\zeta}{r} + m_e\beta c^2$, (11.156).
(11.143), H commutes with ζ, so an eigenstate of the Hamiltonian is an eigenstate of ζ. The eigenvalues of ζ are presented just below (11.144): $k\hbar$.
Then, (11.156) and (11.157) result in (11.158).
Just above (11.159), Fp writes: "*It is easily demonstrated that ϵ anti-commutes with β.*"
We have:
(11.150): $[\zeta, \epsilon] = 0$,
and
(11.142): $[\zeta, \beta] = 0$.

Multiply $[\zeta, \beta] = 0$, to the left with $\epsilon \rightarrow \epsilon\zeta\beta - \epsilon\beta\zeta = 0$. (C.11.34)
Multiply $[\zeta, \epsilon] = 0$, to the left with $\beta \rightarrow \beta\zeta\epsilon - \beta\epsilon\zeta = 0$. (C.11.35)
Add (C.11.34) and (C.11.35)→ $\epsilon\zeta\beta + \beta\zeta\epsilon - (\epsilon\beta + \beta\epsilon)\zeta = 0$. (C.11.36)
In (C.11.36), with (11.142) and (11.150) for the first two terms in (C.11.36):
$(\epsilon\beta + \beta\epsilon)\zeta - (\epsilon\beta + \beta\epsilon)\zeta = 0 \rightarrow \epsilon\beta + \beta\epsilon = 0 \rightarrow \{\epsilon, \beta\} = 0$. I am not sure!
Or, (C.11.34):
$\epsilon\zeta\beta - \epsilon\beta\zeta = 0 \rightarrow \epsilon\beta\zeta - \epsilon\beta\zeta = 0$. (C.11.37)
That looks trivial.
Now assume $\epsilon\beta = -\beta\epsilon \rightarrow \{\epsilon, \beta\} = 0$. Plug this assumption into (C.11.37):
$-\beta\epsilon\zeta - \epsilon\beta\zeta = 0 \rightarrow (\beta\epsilon + \epsilon\beta)\zeta = 0$.
Since $\zeta \neq 0 \rightarrow \beta\epsilon + \epsilon\beta = 0 \rightarrow \{\epsilon, \beta\} = 0$.
The assumption of ϵ anti-commutes with β is not contradicted.

I continue with (11.159). ϵ cannot be a number → 2×2 matrix.
In general, with $\{\epsilon, \beta\} = 0$ and (11.28)
$\epsilon = \begin{pmatrix} 0 & a \\ b & 0 \end{pmatrix}$.
Then with the Hamiltonian: $a = -i$ and $b = i$.
$\epsilon = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.
In (11.158), $\epsilon\beta$ is needed, with (11.28):
$\epsilon\beta = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$. (C.11.38)
An electron in a central field is investigated, so the wavefunction is presented in the spinor form, (11.160).
With (11.158), the eigenvalue equation reads:
$$\left[c\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\left(p_r - \frac{i\hbar}{r}\right) + \frac{ic\hbar k}{r}\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} - e\phi(r) + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} m_e c^2\right]\begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix} = E\begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix},$$ (C.11.39)
4 expressions in (C.11.39) have to be evaluated.
- $c\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} p_r \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix} = cip_r \begin{pmatrix} -\psi_b \\ \psi_a \end{pmatrix}$,
- $c\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \frac{i\hbar}{r}\begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix} = \frac{c\hbar}{r}\begin{pmatrix} -\psi_b \\ \psi_a \end{pmatrix}$,
- $\frac{ic\hbar k}{r}\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}\begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix} = -\frac{c\hbar k}{r}\begin{pmatrix} \psi_b \\ \psi_a \end{pmatrix}$,

and

$$-\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} m_e c^2 \begin{pmatrix}\psi_a\\ \psi_b\end{pmatrix} = m_e c^2 \begin{pmatrix}\psi_a\\ -\psi_b\end{pmatrix}.$$

Plug these expressions into (C.11.39), equate the spinor elements:

$$-cip_r\psi_b - \frac{c\hbar}{r}\psi_b - \frac{c\hbar k}{r}\psi_b - e\phi(r)\psi_a + m_e c^2\psi_a = E\psi_a\,, \qquad \text{(C.11.40)}$$

and,

$$cip_r\psi_a + \frac{c\hbar}{r}\psi_a - \frac{c\hbar k}{r}\psi_a - e\phi(r)\psi_b - m_e c^2\psi_b = E\psi_b\,. \qquad \text{(C.11.41)}$$

(C.11.40):

$$c\left(ip_r + \hbar\frac{1+k}{r}\right)\psi_b + (e\phi(r) - m_e c^2 + E)\psi_a = 0.$$

(C.11.41):

$$c\left(ip_r + \hbar\frac{1-k}{r}\right)\psi_a - (e\phi(r) + m_e c^2 + E)\psi_b = 0.$$

With $p_r = -i\hbar\frac{d}{dr}$, (11.161) and (11.162) are obtained.

I leave this section with the question: is it (11.12) or (11.13), since we are working relativistic?

11.7 Fine Structure of Hydrogen Energy Levels

The Equations (11.161) and (11.162) are applied the Hydrogen atom.

For the hydrogen atom, Fp derived the coupled differential equations (11.164) and (11.165). Substituting the expressions (11.168) and (11.169), the differential (11.171) and (11.172) are derived. Plugging into these equations power law solutions and equating powers of y, two recursion relations are obtained: (11.175) and (11.176).

The series in (11.173) and (11.74) are terminated for $s < s_0$.

In this way a relation between the fine structure constant and the Bohr radius is obtained, (11.181).

In (11.181) and (11.182), $\alpha c_s'$, $a\alpha$ and $a_2\alpha$ are neglected since $\alpha \ll 1$.

With (11.183), plug

$a_2 c_{s-1} = a c_{s-1}'$,

into (11.182)→(11.184).

Using (11.164), (11.165) and (11.170) in (11.188)→(11.189).

(11.191)→(11.192):$i \to n$.

See also Section 12.8 of *The Undergraduate Course Fine Structure of Hydrogen.*

11.8 Positron Theory

It is about the negative energy solutions.

Exercises

Exercise 11.1 About the α and β matrices

Noting that $\alpha_i = -\beta\alpha_i\beta$, prove that α_i and β matrices all have zero trace. Hence, deduce that each matrices has n eigenvalues $+1$, and n eigenvalues -1, where $2n$ is the dimension of the matrices.

(11.28) and (11.29):

$$\beta = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$

the diagonal elements add up to 0.

And

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix},$$

the diagonal elements add up to 0.

So,

Tr$\beta = 0$, and Tr$\alpha_i = 0$.

$$\alpha_i = -\beta\alpha_i\beta = -\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = -\begin{pmatrix} 0 & -\sigma_i \\ -\sigma_i & 0 \end{pmatrix} = \alpha_i.$$

A bit more elegantly:

with (11.21) and (11.22)→ $\alpha_i\beta + \beta\alpha_i = 0$.

Multiply this expression to the left with $\beta \rightarrow \beta\alpha_i\beta + \beta^2\alpha_i = 0 \rightarrow \alpha_i = -\beta\alpha_i\beta$.

The eigenvalues.

β:

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

Then,

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

Consequently, 2 eigenvalues $+1$, and 2 eigenvalues -1.

With

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \rightarrow \begin{vmatrix} 1-\lambda & 0 \\ 0 & -1-\lambda \end{vmatrix} = 0 \rightarrow \lambda = \pm 1.$$

Is $\alpha_i = -\beta\alpha_i\beta$ of some help? I do not know.

α_i:

σ_z,

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

With pivotal condensation:

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

expand by the third column:

$$\begin{vmatrix} 0 & -\lambda & -1 \\ 1-\lambda^2 & 0 & 0 \\ 0 & -1 & -\lambda \end{vmatrix} = 0 \rightarrow (1-\lambda^2)(\lambda^2-1) = 0 .$$

Consequently, 2 eigenvalues $+1$, and 2 eigenvalues -1.

σ_x,

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

With pivotal condensation:

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

expand by the third column:

$$\begin{vmatrix} -\lambda & 0 & 1 \\ 0 & 1-\lambda^2 & 0 \\ 1 & 0 & -\lambda \end{vmatrix} = 0 \to (1-\lambda^2)(\lambda^2-1) = 0\,.$$

Consequently, 2 eigenvalues $+1$, and 2 eigenvalues -1.

σ_x,

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

Pivotal condensation:

$$\begin{vmatrix} -\lambda & 0 & 0 & -i \\ 0 & i\lambda & 1 & 0 \\ 0 & -i+i\lambda^2 & 0 & 0 \\ i & 0 & 0 & -\lambda \end{vmatrix} = 0,$$

expand by the third column:

$$\begin{vmatrix} -\lambda & 0 & -i \\ 0 & -i+i\lambda^2 & 0 \\ i & 0 & -\lambda \end{vmatrix} = 0 \to (\lambda^2-1)(\lambda^2-1) = 0\,.$$

Consequently, 2 eigenvalues $+1$, and 2 eigenvalues -1.

Exercise 11.2 About the α and β matrices continued

Verify that the matrices (11.28) and (11.29) satisfy Equations (11.20)-(11.22).

(11.28):

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and

(11.29):

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}.$$

Use (11.20)-(11.22):

$\{\alpha_i, \alpha_j\} = 2\delta_{ij}$,

$\{\alpha_i, \beta\} = 0$,

$\beta^2 = 1$.

First,

$\alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij}$.

With (11.29):

$$\alpha_i\alpha_j + \alpha_j\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} + \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} = 2\delta_{ij},$$

or

$$\begin{pmatrix} \sigma_i\sigma_j & 0 \\ 0 & \sigma_i\sigma_j \end{pmatrix} + \begin{pmatrix} \sigma_j\sigma_i & 0 \\ 0 & \sigma_j\sigma_i \end{pmatrix} = \begin{pmatrix} \sigma_i\sigma_j + \sigma_j\sigma_i & 0 \\ 0 & \sigma_i\sigma_j + \sigma_j\sigma_i \end{pmatrix} = 2\delta_{ij}.$$

Plug into this expression the Pauli matrices and $\{\alpha_i, \alpha_j\} = 2\delta_{ij}$ is satisfied.

Next,

$\alpha_i\beta + \beta\alpha_i = 0$.
With (11.28):
$$\alpha_i\beta + \beta\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{pmatrix} + \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} = 0.$$
So,
$\{\alpha_i, \beta\} = 0$, is satisfied.

Exercise 11.3 About the γ matrices

Verify that the matrices (11.26) and (11.27) satisfy the anti-commutation relation (11.25).
(11.26):
$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \beta.$$
(11.27):
$$\gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}.$$
(11.25):
$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$.
See my notes on pages 171 and 172. Use Exercise 11.2.
With (11.24):
$\gamma^i\gamma^0 = -\alpha_i$.
Then
$\gamma^i\gamma^0 + \gamma^0\gamma^i = 0 \rightarrow g^{i0} = 0.$
$$\gamma^i\gamma^j + \gamma^j\gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_j \\ -\sigma_j & 0 \end{pmatrix} + \begin{pmatrix} 0 & \sigma_j \\ -\sigma_j & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} =$$
$$= -\begin{pmatrix} \sigma_i\sigma_j + \sigma_j\sigma_i & 0 \\ 0 & \sigma_i\sigma_j + \sigma_j\sigma_i \end{pmatrix} = -2\delta_{ij} = 2g^{ij}, \text{ (11.11).}$$

Exercise 11.4 The Lorenz invariance of the integral of a 4-vectorfield

Verify that if $\partial_\mu j^\mu = 0$,
where j^μ is 4-vectorfield, then
$\int d^3x j^0$,
is Lorentz invariant, where the integral is over all space, and it is assumed that $j^\mu \rightarrow 0$ as $|\boldsymbol{x}| \rightarrow \infty$.
See also pages 175 and 176: Eqs (11.41)-(11.47).
So, j^0 can considered to be the relativistic probability density and j^μ $(\mu = 1,2,3)$ the relativistic probability current.
(11.46), integration over all space and with (11.42):
$\frac{d}{dt}\int d^3x j^0 = 0.$
Fp writes: *"This ensures that the wave function is properly normalized at time $t = 0$, such that*
$\int d^3x j^0 = 1$,
……This is the case provided $\partial_\mu j^\mu = 0$ is Lorentz invariant ……which is true as the j^μ transform as …… under Lorentz transformation".
Suppose two inertial frames, S and S'. Then we have to prove $\int d^3x j^0$ takes the same form in the two frames, S and S'.
May I assume, j^μ transform as the contravariant components of a 4-vector under Lorentz

transformation? If so, j^0 transforms as the contravariant component of a 4-vector under Lorentz transformation. In addition, $\int d^3x j^0 = 1$ is a number. So, it is Lorentz invariant. On the other hand, with the Eqs. (11.48)-(11.55) it follows $\int d^3x j^0$ is Lorentz invariant.

Exercise 11.5 About the transformation matrix A

Verify that (11.71) is a solution of (11.70).
Having obtained (11.70), Fp writes it can be shown (11.71) is a suitable solution of (11.70). Let's find out. Here are summarize my notes about page section 11.3.
I will make use of the inverse γ's: $\gamma^\nu = -\gamma_\nu$ for $\nu = 1,2,3$ and $g_\mu^\nu = 1$, for $\mu = \nu$ and $g_\mu^\nu = 0$, for $\mu \neq \nu$.
In addition, (11.25),
$\mu \neq \nu \rightarrow \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 0$,
and
$\mu = \nu \rightarrow \gamma^\nu\gamma^\nu = -2I$, contraction, i.e, the summation convention.
The inverse of γ^ν:
$\gamma^\nu = g^{\mu\nu}\gamma_\mu$.
Then,
$\gamma^0 = \gamma_0$, (C.11.20)
and $\nu = 1,2,3$
$\gamma^\nu = -\gamma_\nu$. (C.11.21)
So, $\gamma_\nu\gamma^\nu = 2I$.
Multiply (11.70) to the left with γ_ν:
$2i(\gamma_\nu g_\alpha^\nu\gamma_\beta - \gamma_\nu g_\beta^\nu\gamma_\alpha) = \gamma_\nu\gamma^\nu\sigma_{\alpha\beta} - \gamma_\nu\sigma_{\alpha\beta}\gamma^\nu = 2\sigma_{\alpha\beta} - \gamma_\nu\sigma_{\alpha\beta}\gamma^\nu$. (C.11.22)
Now, evaluate $\gamma_\nu g_\alpha^\nu$:
$\alpha = 0 \rightarrow \gamma_0 g_0^0 + \gamma_1 g_0^1 + \gamma_2 g_0^2 + \gamma_3 g_0^3 = \gamma_0$,
$\alpha = 1 \rightarrow \gamma_0 g_1^0 + \gamma_1 g_1^1 + \gamma_2 g_1^2 + \gamma_3 g_1^3 = \gamma_1$,
$\alpha = 2 \rightarrow \gamma_0 g_2^0 + \gamma_1 g_2^1 + \gamma_2 g_2^2 + \gamma_3 g_2^3 = \gamma_2$,
and
$\alpha = 3 \rightarrow \gamma_0 g_3^0 + \gamma_1 g_3^1 + \gamma_2 g_3^2 + \gamma_3 g_3^3 = \gamma_3$.
So, for $\alpha = 0,3 \rightarrow \gamma_\nu g_\alpha^\nu = \gamma_\alpha$,
where use have been made of the values of g_α^ν given just below (11.11).
Similarly:
for $\beta = 0,3 \rightarrow \gamma_\nu g_\beta^\nu = \gamma_\beta$.
Next, in (C.11.22), evaluate $\gamma_\nu\gamma^\nu$, with (C.11.20) and (C.11.21):
for $\nu = 0,3 \rightarrow \quad \gamma_\nu\gamma^\nu = 2I$.
So, I found for (C.11.22):
$2i(\gamma_\alpha\gamma_\beta - \gamma_\beta\gamma_\alpha) = 2\sigma_{\alpha\beta} - \gamma_\nu\sigma_{\alpha\beta}\gamma^\nu$,
or
$2i[\gamma_\alpha, \gamma_\beta] = 2\sigma_{\alpha\beta} - \gamma_\nu\sigma_{\alpha\beta}\gamma^\nu$. (C.11.23)
What about $\gamma_\nu\sigma_{\alpha\beta}\gamma^\nu$ in (C.11.23)?
Well, contraction produces:
$\gamma_\nu\sigma_{\alpha\beta}\gamma^\nu = -2\sigma_{\alpha\beta}$. (C.11.24)
Plug (C.11.24) into (C.11.23)→ $\sigma_{\alpha\beta} = \frac{i}{2}[\gamma_\alpha, \gamma_\beta]$, (11.71).
So, (11.710 is a suitable solution of (11.70).

Exercise 11.6. Σ_i and the Pauli matrices

Verify that the 4×4 matrices Σ_i defined in (11.92), satisfy the standard anti-commutation relations for Pauli matrices: i.e.,:

$\{\Sigma_i, \Sigma_j\} = 2\delta_{ij}$.

(11.92):

$\Sigma_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}$.

Similar to Exercise 11.2.

$$\{\Sigma_i, \Sigma_j\} = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} + \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} = \begin{pmatrix} \sigma_i\sigma_j & 0 \\ 0 & \sigma_i\sigma_j \end{pmatrix} + \begin{pmatrix} \sigma_j\sigma_i & 0 \\ 0 & \sigma_j\sigma_i \end{pmatrix} =$$

$$= \begin{pmatrix} \sigma_i\sigma_j + \sigma_j\sigma_i & 0 \\ 0 & \sigma_i\sigma_j + \sigma_j\sigma_i \end{pmatrix}.$$

Plug into this expression the Pauli matrices, and

$\{\Sigma_i, \Sigma_j\} = 2\delta_{ij}$,

is satisfied.

End of Graduate Course

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Appendix 1: Details on the CGC's in *Intermezzo* 7.7.1

$|l+\frac{1}{2},l-\frac{3}{2}\rangle = \sqrt{\frac{2l-1}{2l+1}}|l-2,\frac{1}{2}\rangle + \sqrt{\frac{2}{2l+1}}|l-1,-\frac{1}{2}\rangle.$

Then

$$J^-\,|l+\tfrac{1}{2},l-\tfrac{3}{2}\rangle = \sqrt{6l-3}\,|l+\tfrac{1}{2},l-\tfrac{5}{2}\rangle\,. \qquad \text{(C.A.1.1)}$$

$$(J_1^- + J_2^-)\left(\sqrt{\tfrac{2l-1}{2l+1}}|l-2,\tfrac{1}{2}\rangle + \sqrt{\tfrac{2}{2l+1}}|l-1,-\tfrac{1}{2}\rangle\right).$$

So,

$$(J_1^- + J_2^-)\sqrt{\tfrac{2l-1}{2l+1}}|l-2,\tfrac{1}{2}\rangle = \sqrt{\tfrac{2l-1}{2l+1}}[\sqrt{l(l+1)-(l-2)(l-3)}\,|l-3,\tfrac{1}{2}\rangle +$$

$$+\sqrt{s(s+1)-\tfrac{1}{2}(-\tfrac{1}{2})}\,|l-2,-\tfrac{1}{2}\rangle]\,. \qquad \text{(C.A.1.2)}$$

$$(J_1^- + J_2^-)\sqrt{\tfrac{2}{2l+1}}|l-1,-\tfrac{1}{2}\rangle = \sqrt{\tfrac{2}{2l+1}}[\sqrt{l(l+1)-(l-1)(l-2)}\,|l-2,-\tfrac{1}{2}\rangle +$$

$$\sqrt{s(s+1)-(-\tfrac{1}{2})(-\tfrac{1}{2}-1)}\,|l-1,-\tfrac{3}{2}\rangle]\,. \qquad \text{(C.A.1.3)}$$

The sum of (C.A.1.2) and (C.A.1.3):

$$\sqrt{\tfrac{2l-1}{2l+1}}\sqrt{6l-6}\,|l-3,\tfrac{1}{2}\rangle + [\sqrt{\tfrac{2l-1}{2l+1}} + \sqrt{\tfrac{2}{2l+1}}\sqrt{4l-2}]\,|l-2,-\tfrac{1}{2}\rangle. \qquad \text{(C.A.1.4)}$$

Then with (C.A.1.1) and (C.A.1.1):

$$|l+\tfrac{1}{2},l-\tfrac{5}{2}\rangle = \tfrac{1}{\sqrt{6l-3}}\{\sqrt{\tfrac{2l-1}{2l+1}}\sqrt{6l-6}\,|l-3,\tfrac{1}{2}\rangle + [\sqrt{\tfrac{2l-1}{2l+1}} + \sqrt{\tfrac{2}{2l+1}}\sqrt{4l-2}]\,|l-2,-\tfrac{1}{2}\rangle\}, \qquad \text{(C.A.1.5)}$$

$|l+\frac{1}{2},l-\frac{5}{2}\rangle = \sqrt{\frac{2l-2}{2l+1}}|l-3,\frac{1}{2}\rangle + \sqrt{\frac{3}{2l+1}}|l-2,-\frac{1}{2}\rangle$, (C.7.44).