PEETER JOOT PEETERJOOT@PROTONMAIL.COM

GRADUATE QUANTUM MECHANICS

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PEETER JOOT PEETERJOOT@PROTONMAIL.COM

Notes and problems from UofT PHY1520H 2015

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DOCUMENT VERSION

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Dedicated to:
Aurora and Lance, my awesome kids, and
Sofia, who not only tolerates and encourages my studies, but is also awesome enough to think that math is sexy.

PREFACE

This document was produced while taking the Spring 2015, University of Toronto Graduate Quantum Mechanics course (PHY1520H), taught by Prof. Arun Paramekanti.

Course Syllabus This course will discuss the following topics in quantum mechanics (time permitting)

1. Basics - Postulates, Wavefunctions, Density matrices, Measurements
2. Time evolution - Schrodinger picture, Heisenberg picture, Interaction picture
3. Harmonic oscillator - Operator method, Wavefunctions, Coherent states
4. Particle in a magnetic field - Local gauge invariance, 2D Landau levels
5. Symmetries - Parity, Translations, Rotations, Time-reversal
6. Angular momentum, Spin, and Angular momentum addition
7. Time-independent perturbation theory
8. Time-dependent perturbation theory
9. Variation approach
10. Scattering theory
11. Dirac equation - one dimension
12. Path integrals

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This document contains:

- Lecture notes.
- Personal notes exploring auxiliary details.

- Worked practice problems.
- Links to Mathematica notebooks associated with the course material and problems (but not problem sets).

My thanks go to Professor Paramekanti for teaching this course, and to Nishant Bhatt for providing me with a copy his notes for lecture 18, which are incorporated herein.

Peeter Joot   peeterjoot@protonmail.com

CONTENTS

LIST OF FIGURES

Part I

READING AND LECTURE NOTES

1 FUNDAMENTAL CONCEPTS

1.1 CLASSICAL MECHANICS

We'll be talking about one body physics for most of this course. In classical mechanics we can figure out the particle trajectories using both of ($\mathbf{r}, \mathbf{p}$, where

$$\begin{aligned}\frac{d\mathbf{r}}{dt} &= \frac{1}{m}\mathbf{p} \\ \frac{d\mathbf{p}}{dt} &= \boldsymbol{\nabla} V\end{aligned} \tag{1.1}$$

A two dimensional phase space as sketched in fig. 1.1 shows the trajectory of a point particle subject to some equations of motion

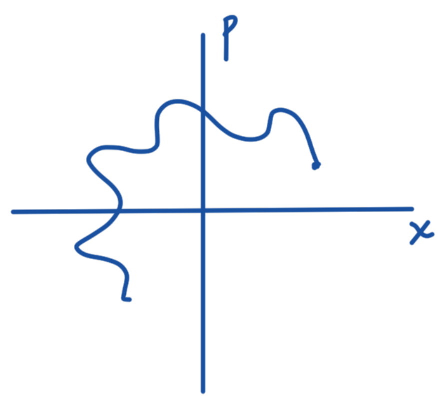

Figure 1.1: One dimensional classical phase space example.

1.2 QUANTUM MECHANICS

For this lecture, we'll work with natural units, setting

$$\boxed{\hbar = 1.} \tag{1.2}$$

In QM we are no longer allowed to think of position and momentum, but have to start asking about state vectors $|\Psi\rangle$.

We'll consider the state vector with respect to some basis, for example, in a position basis, we write

$$\langle x|\Psi\rangle = \Psi(x), \tag{1.3}$$

a complex numbered "wave function", the probability amplitude for a particle in $|\Psi\rangle$ to be in the vicinity of x.

We could also consider the state in a momentum basis

$$\langle p|\Psi\rangle = \Psi(p), \tag{1.4}$$

a probability amplitude with respect to momentum p.

More precisely,

$$|\Psi(x)|^2 dx \geq 0 \tag{1.5}$$

is the probability of finding the particle in the range $(x, x + dx)$. To have meaning as a probability, we require

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1. \tag{1.6}$$

The average position can be calculated using this probability density function. For example

$$\langle x\rangle = \int_{-\infty}^{\infty} |\Psi(x)|^2 x dx, \tag{1.7}$$

or

$$\langle f(x)\rangle = \int_{-\infty}^{\infty} |\Psi(x)|^2 f(x) dx. \tag{1.8}$$

Similarly, calculation of an average of a function of momentum can be expressed as

$$\langle f(p)\rangle = \int_{-\infty}^{\infty} |\Psi(p)|^2 f(p) dp. \tag{1.9}$$

1.3 TRANSFORMATION FROM A POSITION TO MOMENTUM BASIS

We have a problem, if we which to compute an average in momentum space such as $\langle p\rangle$, when given a wavefunction $\Psi(x)$.

How do we convert

$$\Psi(p) \stackrel{?}{\leftrightarrow} \Psi(x), \tag{1.10}$$

or equivalently

$$\langle p|\Psi\rangle \stackrel{?}{\leftrightarrow} \langle x|\Psi\rangle . \tag{1.11}$$

Such a conversion can be performed by virtue of an the assumption that we have a complete orthonormal basis, for which we can introduce identity operations such as

$$\int_{-\infty}^{\infty} dp\,|p\rangle\langle p| = 1, \tag{1.12}$$

or

$$\int_{-\infty}^{\infty} dx\,|x\rangle\langle x| = 1 \tag{1.13}$$

Some interpretations:

1. $|x_0\rangle \leftrightarrow$ sits at$x = x_0$
2. $\langle x|x'\rangle \leftrightarrow \delta(x - x')$
3. $\langle p|p'\rangle \leftrightarrow \delta(p - p')$
4. $\langle x|p'\rangle = \frac{e^{ipx}}{\sqrt{V}}$, where V is the volume of the box containing the particle. We'll define the appropriate normalization for an infinite box volume later.

The delta function interpretation of the braket $\langle p|p'\rangle$ justifies the identity operator, since we recover any state in the basis when operating with it. For example, in momentum space

$$\begin{aligned}
1\,|p\rangle &= \left(\int_{-\infty}^{\infty} dp'\,\left|p'\right\rangle\left\langle p'\right|\right)|p\rangle \\
&= \int_{-\infty}^{\infty} dp'\,\left|p'\right\rangle\left\langle p'\middle|p\right\rangle \\
&= \int_{-\infty}^{\infty} dp'\,\left|p'\right\rangle\delta(p - p') \\
&= |p\rangle .
\end{aligned} \tag{1.14}$$

This also the determination of an integral operator representation for the delta function

$$\begin{aligned}
\delta(x - x') &= \left\langle x\middle|x'\right\rangle \\
&= \int dp\,\langle x|p\rangle\left\langle p\middle|x'\right\rangle \\
&= \frac{1}{V}\int dp e^{ipx}e^{-ipx'},
\end{aligned} \tag{1.15}$$

or

$$\delta(x - x') = \frac{1}{V} \int dp e^{ip(x-x')}. \tag{1.16}$$

Here we used the fact that $\langle p|x\rangle = \langle x|p\rangle^*$.
FIXME: do we have a justification for that conjugation with what was defined here so far?
The conversion from a position basis to momentum space is now possible

$$\langle p|\Psi\rangle = \Psi(p) = \int_{-\infty}^{\infty} \langle p|x\rangle \langle x|\Psi\rangle \, dx = \int_{-\infty}^{\infty} \frac{e^{-ipx}}{\sqrt{V}} \Psi(x) dx. \tag{1.17}$$

The momentum space to position space conversion can be written as

$$\Psi(x) = \int_{-\infty}^{\infty} \frac{e^{ipx}}{\sqrt{V}} \Psi(p) dp. \tag{1.18}$$

Now we can go back and figure out the an expectation

$$\begin{aligned}
\langle p\rangle &= \int \Psi^*(p)\Psi(p) p dp \\
&= \int dp \left(\int_{-\infty}^{\infty} \frac{e^{ipx}}{\sqrt{V}} \Psi^*(x) dx \right) \left(\int_{-\infty}^{\infty} \frac{e^{-ipx'}}{\sqrt{V}} \Psi(x') dx' \right) p \\
&= \int dp dx dx' \Psi^*(x) \frac{1}{V} e^{ip(x-x')} \Psi(x') p \\
&= \int dp dx dx' \Psi^*(x) \frac{1}{V} \left(-i \frac{\partial e^{ip(x-x')}}{\partial x} \right) \Psi(x') \\
&= \int dp dx \Psi^*(x) \left(-i \frac{\partial}{\partial x} \right) \frac{1}{V} \int dx' e^{ip(x-x')} \Psi(x') \\
&= \int dx \Psi^*(x) \left(-i \frac{\partial}{\partial x} \right) \int dx' \left(\frac{1}{V} \int dp e^{ip(x-x')} \right) \Psi(x') \\
&= \int dx \Psi^*(x) \left(-i \frac{\partial}{\partial x} \right) \int dx' \delta(x - x') \Psi(x') \\
&= \int dx \Psi^*(x) \left(-i \frac{\partial}{\partial x} \right) \Psi(x)
\end{aligned} \tag{1.19}$$

Here we've essentially calculated the position space representation of the momentum operator, allowing identifications of the following form

$$p \leftrightarrow -i \frac{\partial}{\partial x} \tag{1.20}$$

$$p^2 \leftrightarrow -\frac{\partial^2}{\partial x^2}. \tag{1.21}$$

Alternate starting point. Most of the above results followed from the claim that $\langle x|p\rangle = e^{ipx}$. Note that this position space representation of the momentum operator can also be taken as the starting point. Given that, the exponential representation of the position-momentum braket follows

$$\langle x| P |p\rangle = -i\hbar \frac{\partial}{\partial x} \langle x|p\rangle \,, \tag{1.22}$$

but $\langle x| P |p\rangle = p \langle x|p\rangle$, providing a differential equation for $\langle x|p\rangle$

$$p \langle x|p\rangle = -i\hbar \frac{\partial}{\partial x} \langle x|p\rangle \,, \tag{1.23}$$

with solution

$$ipx/\hbar = \ln \langle x|p\rangle + \text{const}, \tag{1.24}$$

or

$$\langle x|p\rangle \propto e^{ipx/\hbar}. \tag{1.25}$$

1.4 MATRIX INTERPRETATION

1. Ket's $|\Psi\rangle \leftrightarrow$ column vector
2. Bra's $\langle\Psi| \leftrightarrow$ (row vector)*
3. Operators $\leftrightarrow$ matrices that act on vectors.

$$\hat{p}\,|\Psi\rangle \rightarrow \left|\Psi'\right\rangle \tag{1.26}$$

1.5 TIME EVOLUTION

For a state subject to the equations of motion given by the Hamiltonian operator $\hat{H}$

$$i \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle \,, \tag{1.27}$$

the time evolution is given by

$$|\Psi(t)\rangle = e^{-i\hat{H}t} |\Psi(0)\rangle \,. \tag{1.28}$$

1.6 REVIEW: BASIC CONCEPTS

We've reviewed the basic concepts that we will encounter in Quantum Mechanics.

1. Abstract state vector. $|\psi\rangle$
2. Basis states. $|x\rangle$
3. Observables, special Hermitian operators. We'll only deal with linear observables.
4. Measurement.

We can either express the wave functions $\psi(x) = \langle x|\psi\rangle$ in terms of a basis for the observable, or can express the observable in terms of the basis of the wave function (position or momentum for example).

We saw that the position space representation of a momentum operator (also an observable) was

$$\hat{p} \rightarrow -i\hbar\frac{\partial}{\partial x}. \tag{1.29}$$

In general we can find the matrix element representation of any operator by considering its representation in a given basis. For example, in a position basis, that would be

$$\langle x'\middle|\hat{A}\,|x\rangle \leftrightarrow A_{xx'} \tag{1.30}$$

The Hermitian property of the observable means that $A_{xx'} = A^*_{x'x}$

$$\int dx\,\langle x'\middle|\hat{A}\,|x\rangle\,\langle x|\psi\rangle = \langle x'\middle|\phi\rangle \leftrightarrow A_{x'x}\psi_x = \phi_{x'}. \tag{1.31}$$

Example 1.1: Measurement example

Consider a polarization apparatus as sketched in fig. 1.2, where the output is of the form $I_{\text{out}} = I_{\text{in}}\cos^2\theta$.

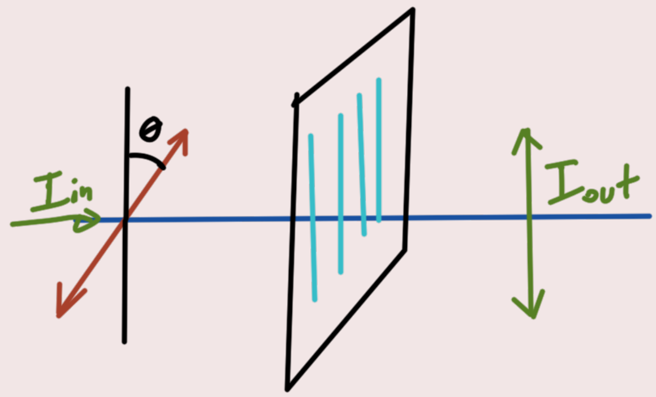

Figure 1.2: Polarizer apparatus.

A general input state can be written in terms of each of the possible polarizations

$$\alpha \left|\updownarrow\right\rangle + \beta \left|\leftrightarrow\right\rangle \sim \cos\theta \left|\updownarrow\right\rangle + \sin\theta \left|\leftrightarrow\right\rangle \tag{1.32}$$

Here $|\alpha|^2$ is the probability that the input state is in the upwards polarization state, and $|\beta|^2$ is the probability that the input state is in the downwards polarization state.

The measurement of the polarization results in an output state that has a specific polarization. That measurement is said to collapse the wavefunction.

When attempting a measurement, looking for a specific value, effects the state of the system, and is call a strong or projective measurement. Such a measurement is

(i) Probabilistic.

(ii) Requires many measurements.

This measurement process results a determination of the eigenvalue of the operator. The eigenvalue production of measurement is why we demand that operators be Hermitian.

It is also possible to try to do a weaker (perturbative) measurement, where some information is extracted from the input state without completely altering it.

Time evolution

1. Schrödinger picture. The time evolution process is governed by a Schrödinger equation of the following form

$$i\hbar \frac{\partial}{\partial t} \left|\Psi(t)\right\rangle = \hat{H} \left|\Psi(t)\right\rangle . \tag{1.33}$$

This Hamiltonian could be, for example,

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x), \tag{1.34}$$

Such a representation of time evolution is expressed in terms of operators $\hat{x}, \hat{p}, \hat{H}, \cdots$ that are independent of time.

2. Heisenberg picture.

   Suppose we have a state $|\Psi(t)\rangle$ and operate on this with an operator

   $$\hat{A}\,|\Psi(t)\rangle\,. \tag{1.35}$$

   This will have time evolution of the form

   $$\hat{A}e^{-i\hat{H}t/\hbar}\,|\Psi(0)\rangle\,, \tag{1.36}$$

   or in matrix element form

   $$\langle\phi(t)|\,\hat{A}\,|\Psi(t)\rangle = \langle\phi(0)|\,e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}\,|\Psi(0)\rangle\,. \tag{1.37}$$

   We work with states that do not evolve in time $|\phi(0)\rangle\,, |\Psi(0)\rangle\,, \cdots$, but operators do evolve in time according to

   $$\hat{A}(t) = e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}. \tag{1.38}$$

Density operator We can have situations where it is impossible to determine a single state that describes the system. For example, given the gas in the room that you are sitting in, there are things that we can measure, but it is impossible to describe the state that describes all the particles and also impossible to construct a Hamiltonian that governs all the interactions of those many many particles.

We need a probabilistic description to even describe such a complex system, and to be able to deal with concepts like entanglement.

Suppose we have a complex system that can be partitioned into two subsets, left and right, as sketched in fig. 1.3.

If the states in each partition can be enumerated separately, we can write the state of the system as sums over the probability amplitudes that for the combined states.

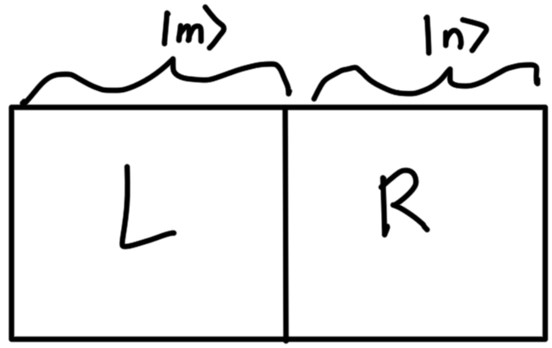

Figure 1.3: System partitioned into separate set of states.

$$|\Psi\rangle = \sum_{m,n} C_{m,n} |m\rangle |n\rangle \tag{1.39}$$

Here $C_{m,n}$ is the probability amplitude to find the state in the combined state $|m\rangle |n\rangle$.

As an example of such a system, we could investigate a two particle configuration where spin up or spin down can be separately measured for each particle.

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle |\downarrow\rangle + |\downarrow\rangle |\uparrow\rangle \right) \tag{1.40}$$

Considering such a system we could ask questions such as

- What is the probability that the left half is in state m? This would be

$$\sum_n \left| C_{m,n} \right|^2 \tag{1.41}$$

- Probability that the left half is in state m, and the probability that the right half is in state n? That is

$$\left| C_{m,n} \right|^2 \tag{1.42}$$

We define the density operator

$$\hat{\rho} = |\Psi\rangle \langle\Psi| . \tag{1.43}$$

This is idempotent

$$
\begin{aligned}
\hat{\rho}^2 &= (|\Psi\rangle\langle\Psi|)(|\Psi\rangle\langle\Psi|) \\
&= |\Psi\rangle\langle\Psi|
\end{aligned}
\tag{1.44}
$$

An example of a partitioned system with four total states (two spin 1/2 particles) is sketched in fig. 1.4.

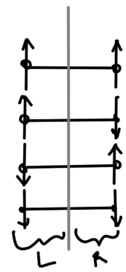

Figure 1.4: Two spins.

An example of a partitioned system with eight total states (three spin 1/2 particles) is sketched in fig. 1.5.

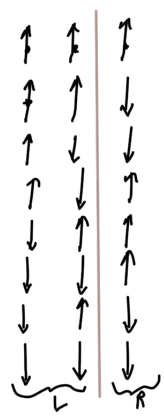

Figure 1.5: Three spins.

The density matrix

$$
\hat{\rho} = |\Psi\rangle\langle\Psi| \tag{1.45}
$$

is clearly an operator as can be seen by applying it to a state

$$
\hat{\rho}\,|\phi\rangle = |\Psi\rangle\,(\langle\Psi|\phi\rangle)\,. \tag{1.46}
$$

The quantity in braces is just a complex number.
After expanding the pure state $|\Psi\rangle$ in terms of basis states for each of the two partitions

$$|\Psi\rangle = \sum_{m,n} C_{m,n} |m\rangle_{\mathrm{L}} |n\rangle_{\mathrm{R}} , \tag{1.47}$$

With L and R implied for $|m\rangle, |n\rangle$ indexed states respectively, this can be written

$$|\Psi\rangle = \sum_{m,n} C_{m,n} |m\rangle |n\rangle . \tag{1.48}$$

The density operator is

$$\hat{\rho} = \sum_{m,n} C_{m,n} C^*_{m',n'} |m\rangle |n\rangle \sum_{m',n'} \langle m'| \langle n'| . \tag{1.49}$$

Suppose we trace over the right partition of the state space, defining such a trace as the reduced density operator $\hat{\rho}_{\mathrm{red}}$

$$\begin{aligned}
\hat{\rho}_{\mathrm{red}} &\equiv \mathrm{tr}_{\mathrm{R}}(\hat{\rho}) \\
&= \sum_{\tilde{n}} \langle \tilde{n}| \hat{\rho} |\tilde{n}\rangle \\
&= \sum_{\tilde{n}} \langle \tilde{n}| \left(\sum_{m,n} C_{m,n} |m\rangle |n\rangle \right) \left(\sum_{m',n'} C^*_{m',n'} \langle m'| \langle n'| \right) |\tilde{n}\rangle \\
&= \sum_{\tilde{n}} \sum_{m,n} \sum_{m',n'} C_{m,n} C^*_{m',n'} |m\rangle \delta_{\tilde{n}n} \langle m'| \delta_{\tilde{n}n'} \\
&= \sum_{\tilde{n},m,m'} C_{m,\tilde{n}} C^*_{m',\tilde{n}} |m\rangle \langle m'|
\end{aligned} \tag{1.50}$$

Computing the matrix element of $\hat{\rho}_{\mathrm{red}}$, we have

$$\begin{aligned}
\langle \tilde{m}| \hat{\rho}_{\mathrm{red}} |\tilde{m}\rangle &= \sum_{m,m',\tilde{n}} C_{m,\tilde{n}} C^*_{m',\tilde{n}} \langle \tilde{m}|m\rangle \langle m'|\tilde{m}\rangle \\
&= \sum_{\tilde{n}} \left| C_{\tilde{m},\tilde{n}} \right|^2 .
\end{aligned} \tag{1.51}$$

This is the probability that the left partition is in state $\tilde{m}$.

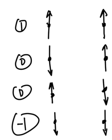

Figure 1.6: Magnetic moments from two spins.

1.7 AVERAGE OF AN OBSERVABLE

Suppose we have two spin half particles. For such a system the total magnetization is

$$S_{\text{Total}} = S_1^z + S_1^z, \tag{1.52}$$

as sketched in fig. 1.6.
The average of some observable is

$$\left\langle \hat{A} \right\rangle = \sum_{m,n,m',n'} C^*_{m,n} C_{m',n'} \langle m| \langle n| \hat{A} \left|n'\right\rangle \left|m'\right\rangle . \tag{1.53}$$

Consider the trace of the density operator observable product

$$\text{tr}(\hat{\rho}\hat{A}) = \sum_{m,n} \langle mn|\Psi\rangle \langle\Psi| \hat{A} |m,n\rangle . \tag{1.54}$$

Let

$$|\Psi\rangle = \sum_{m,n} C_{mn} |m,n\rangle , \tag{1.55}$$

so that

$$\begin{aligned} \text{tr}(\hat{\rho}\hat{A}) &= \sum_{m,n,m',n',m'',n''} C_{m',n'} C^*_{m'',n''} \left\langle mn \middle| m',n' \right\rangle \left\langle m'',n'' \right| \hat{A} |m,n\rangle \\ &= \sum_{m,n,m'',n''} C_{m,n} C^*_{m'',n''} \left\langle m'',n'' \right| \hat{A} |m,n\rangle . \end{aligned} \tag{1.56}$$

This is just

$$\boxed{\langle\Psi| \hat{A} |\Psi\rangle = \text{tr}(\hat{\rho}\hat{A}).} \tag{1.57}$$

1.8 LEFT OBSERVABLES

Consider

$$\begin{aligned}
\langle\Psi|\,\hat{A}_{\mathrm{L}}\,|\Psi\rangle &= \mathrm{tr}(\hat{\rho}\hat{A}_{\mathrm{L}}) \\
&= \mathrm{tr}_{\mathrm{L}}\,\mathrm{tr}_{\mathrm{R}}(\hat{\rho}\hat{A}_{\mathrm{L}}) \\
&= \mathrm{tr}_{\mathrm{L}}\left((\mathrm{tr}_{\mathrm{R}}\,\hat{\rho})\,\hat{A}_{\mathrm{L}})\right) \\
&= \mathrm{tr}_{\mathrm{L}}\left(\hat{\rho}_{\mathrm{red}}\hat{A}_{\mathrm{L}})\right).
\end{aligned} \tag{1.58}$$

We see

$$\langle\Psi|\,\hat{A}_{\mathrm{L}}\,|\Psi\rangle = \mathrm{tr}_{\mathrm{L}}\left(\hat{\rho}_{\mathrm{red,L}}\hat{A}_{\mathrm{L}}\right). \tag{1.59}$$

We find that we don't need to know the state of the complete system to answer questions about portions of the system, but instead just need $\hat{\rho}$, a "probability operator" that provides all the required information about the partitioning of the system.

1.9 PURE STATES VS. MIXED STATES

For pure states we can assign a state vector and talk about reduced scenarios. For mixed states we must work with reduced density matrices.

Example 1.2: Two particle spin half pure states

Consider

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \tag{1.60}$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\uparrow\uparrow\rangle\right). \tag{1.61}$$

For the first pure state the density operator is

$$\hat{\rho} = \frac{1}{2}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)\left(\langle\uparrow\downarrow| - \langle\downarrow\uparrow|\right) \tag{1.62}$$

What are the reduced density matrices?

$$\begin{aligned}
\hat{\rho}_{\mathrm{L}} &= \mathrm{tr}_{\mathrm{R}}\,(\hat{\rho}) \\
&= \frac{1}{2}(-1)(-1)\,|\downarrow\rangle\,\langle\downarrow| + \frac{1}{2}(+1)(+1)\,|\uparrow\rangle\,\langle\uparrow|\,,
\end{aligned} \tag{1.63}$$

so the matrix representation of this reduced density operator is

$$\hat{\rho}_{\mathrm{L}} = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{1.64}$$

For the second pure state the density operator is

$$\hat{\rho} = \frac{1}{2}\left(\lvert\uparrow\downarrow\rangle + \lvert\uparrow\uparrow\rangle\right)\left(\langle\uparrow\downarrow\rvert + \langle\uparrow\uparrow\rvert\right). \tag{1.65}$$

This has a reduced density matrix

$$\begin{aligned} \hat{\rho}_{\mathrm{L}} &= \mathrm{tr}_{\mathrm{R}}\left(\hat{\rho}\right) \\ &= \frac{1}{2}\lvert\uparrow\rangle\langle\uparrow\rvert + \frac{1}{2}\lvert\uparrow\rangle\langle\uparrow\rvert \\ &= \lvert\uparrow\rangle\langle\uparrow\rvert. \end{aligned} \tag{1.66}$$

This has a matrix representation

$$\hat{\rho}_{\mathrm{L}} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{1.67}$$

In this second example, we have more information about the left partition. That will be seen as a zero entanglement entropy in the problem set. In contrast we have less information about the first state, and will find a non-zero positive entanglement entropy in that case.

1.10 ENTROPY WHEN DENSITY OPERATOR HAS ZERO EIGENVALUES

In the class notes and the text [11] the Von Neumann entropy is defined as

$$S = -\,\mathrm{tr}(\rho \ln \rho). \tag{1.68}$$

In one of our problems I had trouble evaluating this, having calculated a density operator matrix representation

$$\rho = E \wedge E^{-1}, \tag{1.69}$$

where

$$E = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \tag{1.70}$$

and

$$\wedge = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{1.71}$$

The usual method of evaluating a function of a matrix is to assume the function has a power series representation, and that a similarity transformation of the form $A = E \wedge E^{-1}$ is possible, so that

$$f(A) = Ef(\wedge)E^{-1}, \tag{1.72}$$

however, when attempting to do this with the matrix of eq. (1.69) leads to an undesirable result

$$\ln \rho = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \ln 1 & 0 \\ 0 & \ln 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{1.73}$$

The $\ln 0$ makes the evaluation of this matrix logarithm rather unpleasant. To give meaning to the entropy expression, we have to do two things, the first is treating the trace operation as a higher precedence than the logarithms that it contains. That is

$$\begin{aligned} -\operatorname{tr}(\rho \ln \rho) &= -\operatorname{tr}(E \wedge E^{-1} E \ln \wedge E^{-1}) \\ &= -\operatorname{tr}(E \wedge \ln \wedge E^{-1}) \\ &= -\operatorname{tr}(E^{-1} E \wedge \ln \wedge) \\ &= -\operatorname{tr}(\wedge \ln \wedge) \\ &= -\sum_k \wedge_{kk} \ln \wedge_{kk}. \end{aligned} \tag{1.74}$$

Now the matrix of the logarithm need not be evaluated, but we still need to give meaning to $\wedge_{kk} \ln \wedge_{kk}$ for zero diagonal entries. This can be done by considering a limiting scenario

$$\begin{aligned} -\lim_{a \to 0} a \ln a &= -\lim_{x \to \infty} e^{-x} \ln e^{-x} \\ &= \lim_{x \to \infty} x e^{-x} \\ &= 0. \end{aligned} \tag{1.75}$$

The entropy can now be expressed in the unambiguous form, summing over all the non-zero eigenvalues of the density operator

$$\boxed{S = -\sum_{\wedge_{kk} \neq 0} \wedge_{kk} \ln \wedge_{kk}.} \tag{1.76}$$

1.11 PROBLEMS

Exercise 1.1 Representation of 2×2 matrix with Pauli matrices. ([11] pr. 1.2)

Given an arbitrary 2×2 matrix $X = a_0 + \boldsymbol{\sigma} \cdot \mathbf{a}$, show the relationships between a_μ and $\operatorname{tr}(X)$, $\operatorname{tr}(\sigma_k X)$, and X_{ij}.

Answer for Exercise 1.1

Observe that each of the Pauli matrices σ_k are traceless

$$
\begin{aligned}
\sigma_x &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\
\sigma_y &= \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \\
\sigma_z &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}
\end{aligned}
\tag{1.77}
$$

so $\operatorname{tr}(X) = 2a_0$. Note that $\operatorname{tr}(\sigma_k \sigma_m) = 2\delta_{km}$, so $\operatorname{tr}(\sigma_k X) = 2a_k$.

Notationally, it would seem to make sense to define $\sigma_0 \equiv I$, so that $\operatorname{tr}(\sigma_\mu X) = a_\mu$. I don't know if that is common practice.

For the opposite relations, given

$$
\begin{aligned}
X &= a_0 + \boldsymbol{\sigma} \cdot \mathbf{a} \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} a_0 + \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} a_1 + \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} a_2 + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} a_3 \\
&= \begin{bmatrix} a_0 + a_3 & a_1 - i a_2 \\ a_1 + i a_2 & a_0 - a_3 \end{bmatrix} \\
&= \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix},
\end{aligned}
\tag{1.78}
$$

so

$$
\begin{aligned}
a_0 &= \frac{1}{2}\left(X_{11} + X_{22}\right) \\
a_1 &= \frac{1}{2}\left(X_{12} + X_{21}\right) \\
a_2 &= \frac{1}{2i}\left(X_{21} - X_{12}\right) \\
a_3 &= \frac{1}{2}\left(X_{11} - X_{22}\right)
\end{aligned}
.
\tag{1.79}
$$

Exercise 1.2 Rotation transformation. ([11] pr. 1.3)

Determine the structure and determinant of the transformation

$$\boldsymbol{\sigma} \cdot \mathbf{a} \rightarrow \boldsymbol{\sigma} \cdot \mathbf{a}' = \exp\left(i\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}\phi/2\right) \boldsymbol{\sigma} \cdot \mathbf{a} \exp\left(-i\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}\phi/2\right). \tag{1.80}$$

Answer for Exercise 1.2

Knowing Geometric Algebra, this is recognized as a rotation transformation. In GA, i is treated as a pseudoscalar (which commutes with all grades in $\mathbb{R}^3$), and the expression can be reduced to one involving dot and wedge products. Let's see how can this be reduced using only the Pauli matrix toolbox.

First, consider the determinant of one of the exponentials. Showing that one such exponential has unit determinant is sufficient. The matrix representation of the unit normal is

$$\begin{aligned} \boldsymbol{\sigma} \cdot \hat{\mathbf{n}} &= n_x \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + n_y \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + n_z \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ &= \begin{bmatrix} n_z & n_x - i n_y \\ n_x + i n_y & -n_z \end{bmatrix}. \end{aligned} \tag{1.81}$$

This is expected to have a unit square, and does

$$\begin{aligned} (\boldsymbol{\sigma} \cdot \hat{\mathbf{n}})^2 &= \begin{bmatrix} n_z & n_x - i n_y \\ n_x + i n_y & -n_z \end{bmatrix} \begin{bmatrix} n_z & n_x - i n_y \\ n_x + i n_y & -n_z \end{bmatrix} \\ &= \left(n_x^2 + n_y^2 + n_z^2\right) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ &= 1. \end{aligned} \tag{1.82}$$

This allows for a cosine and sine expansion of the exponential, as in

$$\begin{aligned} \exp\left(i\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}\theta\right) &= \cos\theta + i\boldsymbol{\sigma} \cdot \hat{\mathbf{n}} \sin\theta \\ &= \cos\theta \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + i \sin\theta \begin{bmatrix} n_z & n_x - i n_y \\ n_x + i n_y & -n_z \end{bmatrix} \\ &= \begin{bmatrix} \cos\theta + i n_z \sin\theta & \left(n_x - i n_y\right) i \sin\theta \\ \left(n_x + i n_y\right) i \sin\theta & \cos\theta - i n_z \sin\theta \end{bmatrix}. \end{aligned} \tag{1.83}$$

This has determinant

$$
\begin{aligned}
\left|\exp\left(i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\theta\right)\right| &= \cos^2\theta + n_z^2\sin^2\theta - \left(-n_x^2 + -n_y^2\right)\sin^2\theta \\
&= \cos^2\theta + \left(n_x^2 + n_y^2 + n_z^2\right)\sin^2\theta \\
&= 1,
\end{aligned}
\tag{1.84}
$$

as expected.

Next step is to show that this transformation is a rotation, and determine the sense of the rotation. Let $C = \cos\phi/2, S = \sin\phi/2$, so that

$$
\begin{aligned}
\boldsymbol{\sigma}\cdot\mathbf{a}' &= \exp\left(i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi/2\right)\boldsymbol{\sigma}\cdot\mathbf{a}\exp\left(-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi/2\right) \\
&= \left(C + i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}S\right)\boldsymbol{\sigma}\cdot\mathbf{a}\left(C - i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}S\right) \\
&= \left(C + i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}S\right)\left(C\boldsymbol{\sigma}\cdot\mathbf{a} - i\boldsymbol{\sigma}\cdot\mathbf{a}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}S\right) \\
&= C^2\boldsymbol{\sigma}\cdot\mathbf{a} + \boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\boldsymbol{\sigma}\cdot\mathbf{a}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}S^2 + i\left(-\boldsymbol{\sigma}\cdot\mathbf{a}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}} + \boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\boldsymbol{\sigma}\cdot\mathbf{a}\right)SC \\
&= \frac{1}{2}\left(1+\cos\phi\right)\boldsymbol{\sigma}\cdot\mathbf{a} + \boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\boldsymbol{\sigma}\cdot\mathbf{a}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\frac{1}{2}\left(1-\cos\phi\right) + i\left[\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\right]\frac{1}{2}\sin\phi \\
&= \frac{1}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\{\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\} + \frac{1}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\left[\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\right]\cos\phi + \frac{1}{2}i\left[\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\right]\sin\phi.
\end{aligned}
\tag{1.85}
$$

Observe that the angle dependent portion can be written in a compact exponential form

$$
\begin{aligned}
\boldsymbol{\sigma}\cdot\mathbf{a}' &= \frac{1}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\{\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\} + \left(\cos\phi + i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\sin\phi\right)\frac{1}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\left[\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\right] \\
&= \frac{1}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\{\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\} + \exp\left(i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi\right)\frac{1}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\left[\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\right].
\end{aligned}
\tag{1.86}
$$

The anticommutator and commutator products with the unit normal can be identified as projections and rejections respectively. Consider the symmetric product first

$$
\begin{aligned}
\frac{1}{2}\{\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\} &= \frac{1}{2}\sum n_r a_s\left(\sigma_r\sigma_s + \sigma_s\sigma_r\right) \\
&= \frac{1}{2}\sum_{r\neq s} n_r a_s\left(\sigma_r\sigma_s + \sigma_s\sigma_r\right) + \frac{1}{2}\sum_r n_r a_r 2 \\
&= 2\hat{\mathbf{n}}\cdot\mathbf{a}.
\end{aligned}
\tag{1.87}
$$

This shows that

$$
\frac{1}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\{\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\} = \left(\hat{\mathbf{n}}\cdot\mathbf{a}\right)\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},
\tag{1.88}
$$

which is the projection of **a** in the direction of the normal $\hat{\mathbf{n}}$. To show that the commutator term is the rejection, consider the sum of the two

$$\frac{1}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\{\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\}+\frac{1}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\left[\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\right]=\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\boldsymbol{\sigma}\cdot\mathbf{a} \\ =\boldsymbol{\sigma}\cdot\mathbf{a}, \tag{1.89}$$

so we must have

$$\boldsymbol{\sigma}\cdot\mathbf{a}-(\hat{\mathbf{n}}\cdot\mathbf{a})\,\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}=\frac{1}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\left[\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\right]. \tag{1.90}$$

This is the component of $\mathbf{a}$ that has the projection in the $\hat{\mathbf{n}}$ direction removed. Looking back to eq. (1.86), the transformation leaves components of the vector that are colinear with the unit normal unchanged, and applies an exponential operation to the component that lies in what is presumed to be the rotation plane. To verify that this latter portion of the transformation is a rotation, and to determine the sense of the rotation, let's expand the factor of the sine of eq. (1.85).

That is

$$\begin{aligned}\frac{i}{2}\left[\boldsymbol{\sigma}\cdot\hat{\mathbf{n}},\boldsymbol{\sigma}\cdot\mathbf{a}\right]&=\frac{i}{2}\sum n_r a_s\left[\sigma_r,\sigma_s\right]\\&=\frac{i}{2}\sum n_r a_s 2i\epsilon_{rst}\sigma_t\\&=-\sum\sigma_t n_r a_s\epsilon_{rst}\\&=-\boldsymbol{\sigma}\cdot(\hat{\mathbf{n}}\times\mathbf{a})\\&=\boldsymbol{\sigma}\cdot(\mathbf{a}\times\hat{\mathbf{n}}).\end{aligned} \tag{1.91}$$

Since $\mathbf{a}\times\hat{\mathbf{n}}=\left(\mathbf{a}-\hat{\mathbf{n}}(\hat{\mathbf{n}}\cdot\mathbf{a})\right)\times\hat{\mathbf{n}}$, this vector is seen to lie in the plane normal to $\hat{\mathbf{n}}$, but perpendicular to the rejection of $\hat{\mathbf{n}}$ from $\mathbf{a}$. That completes the demonstration that this is a rotation transformation.

To understand the sense of this rotation, consider $\hat{\mathbf{n}}=\hat{\mathbf{z}}, \mathbf{a}=\hat{\mathbf{x}}$, so

$$\begin{aligned}\boldsymbol{\sigma}\cdot(\mathbf{a}\times\hat{\mathbf{n}})&=\boldsymbol{\sigma}\cdot(\hat{\mathbf{x}}\times\hat{\mathbf{z}})\\&=-\boldsymbol{\sigma}\cdot\hat{\mathbf{y}},\end{aligned} \tag{1.92}$$

and

$$\boldsymbol{\sigma}\cdot\mathbf{a}'=\hat{\mathbf{x}}\cos\phi-\hat{\mathbf{y}}\sin\phi, \tag{1.93}$$

showing that this rotation transformation has a clockwise sense.

Exercise 1.3 Some bra-ket manipulation problems. (*[11] pr. 1.4*)

Using braket logic expand

a.

$$\operatorname{tr} XY \tag{1.94}$$

b.

$$(XY)^\dagger \tag{1.95}$$

c.

$$e^{if(A)}, \tag{1.96}$$

where A is Hermitian with a complete set of eigenvalues.

d.

$$\sum_{a'} \Psi_{a'}(\mathbf{x}')^* \Psi_{a'}(\mathbf{x}''), \tag{1.97}$$

where $\Psi_{a'}(\mathbf{x}'') = \langle \mathbf{x}' | a' \rangle$.

Answer for Exercise 1.3

Part a.

$$\begin{aligned}
\operatorname{tr} XY &= \sum_a \langle a| XY |a\rangle \\
&= \sum_{a,b} \langle a| X |b\rangle \langle b| Y |a\rangle \\
&= \sum_{a,b} \langle b| Y |a\rangle \langle a| X |b\rangle \\
&= \sum_{a,b} \langle b| YX |b\rangle \\
&= \operatorname{tr} YX.
\end{aligned} \tag{1.98}$$

Part b.

$$
\begin{aligned}
\langle a| (XY)^\dagger |b\rangle &= (\langle b| XY |a\rangle)^* \\
&= \sum_c (\langle b| X |c\rangle \langle c| Y |a\rangle)^* \\
&= \sum_c (\langle b| X |c\rangle)^* (\langle c| Y |a\rangle)^* \\
&= \sum_c (\langle c| Y |a\rangle)^* (\langle b| X |c\rangle)^* \\
&= \sum_c \langle a| Y^\dagger |c\rangle \langle c| X^\dagger |b\rangle \\
&= \langle a| Y^\dagger X^\dagger |b\rangle ,
\end{aligned}
\tag{1.99}
$$

so $(XY)^\dagger = Y^\dagger X^\dagger$.

Part c. Let's presume that the function f has a Taylor series representation

$$
f(A) = \sum_r b_r A^r. \tag{1.100}
$$

If the eigenvalues of A are given by

$$
A |a_s\rangle = a_s |a_s\rangle , \tag{1.101}
$$

this operator can be expanded like

$$
\begin{aligned}
A &= \sum_{a_s} A |a_s\rangle \langle a_s| \\
&= \sum_{a_s} a_s |a_s\rangle \langle a_s| ,
\end{aligned}
\tag{1.102}
$$

To compute powers of this operator, consider first the square

$$
\begin{aligned}
A^2 &= \\
&= \sum_{a_s} a_s |a_s\rangle \langle a_s| \sum_{a_r} a_r |a_r\rangle \langle a_r| \\
&= \sum_{a_s, a_r} a_s a_r |a_s\rangle \langle a_s| |a_r\rangle \langle a_r| \\
&= \sum_{a_s, a_r} a_s a_r |a_s\rangle \delta_{sr} \langle a_r| \\
&= \sum_{a_s} a_s^2 |a_s\rangle \langle a_s| .
\end{aligned}
\tag{1.103}
$$

The pattern for higher powers will clearly just be

$$A^k = \sum_{a_s} a_s^k \left| a_s \right\rangle \left\langle a_s \right|, \tag{1.104}$$

so the expansion of $f(A)$ will be

$$\begin{aligned} f(A) &= \sum_r b_r A^r \\ &= \sum_r b_r \sum_{a_s} a_s^r \left| a_s \right\rangle \left\langle a_s \right| \\ &= \sum_{a_s} \left(\sum_r b_r a_s^r \right) \left| a_s \right\rangle \left\langle a_s \right| \\ &= \sum_{a_s} f(a_s) \left| a_s \right\rangle \left\langle a_s \right|. \end{aligned} \tag{1.105}$$

The exponential expansion is

$$\begin{aligned} e^{if(A)} &= \sum_t \frac{i^t}{t!} f^t(A) \\ &= \sum_t \frac{i^t}{t!} \left(\sum_{a_s} f(a_s) \left| a_s \right\rangle \left\langle a_s \right| \right)^t \\ &= \sum_t \frac{i^t}{t!} \sum_{a_s} f^t(a_s) \left| a_s \right\rangle \left\langle a_s \right| \\ &= \sum_{a_s} e^{if(a_s)} \left| a_s \right\rangle \left\langle a_s \right|. \end{aligned} \tag{1.106}$$

Part d.

$$\begin{aligned} \sum_{a'} \Psi_{a'}(\mathbf{x}')^* \Psi_{a'}(\mathbf{x}'') &= \sum_{a'} \left\langle \mathbf{x}' \middle| a' \right\rangle^* \left\langle \mathbf{x}'' \middle| a' \right\rangle \\ &= \sum_{a'} \left\langle a' \middle| \mathbf{x}' \right\rangle \left\langle \mathbf{x}'' \middle| a' \right\rangle \\ &= \sum_{a'} \left\langle \mathbf{x}'' \middle| a' \right\rangle \left\langle a' \middle| \mathbf{x}' \right\rangle \\ &= \left\langle \mathbf{x}'' \middle| \mathbf{x}' \right\rangle \\ &= \delta\left(\mathbf{x}'' - \mathbf{x}'\right). \end{aligned} \tag{1.107}$$

Exercise 1.4 Operator matrix representation. (*[11] pr. 1.5*)

a. Determine the matrix representation of $|\alpha\rangle\langle\beta|$ given a complete set of eigenvectors $|a^r\rangle$.
b. Verify with $|\alpha\rangle = |s_z = \hbar/2\rangle, |s_x = \hbar/2\rangle$.

Answer for Exercise 1.4

Part a. Forming the matrix element

$$\begin{aligned}\left\langle a^r\right|\left(|\alpha\rangle\langle\beta|\right)\left|a^s\right\rangle &= \left\langle a^r|\alpha\right\rangle\left\langle\beta|a^s\right\rangle \\ &= \left\langle a^r|\alpha\right\rangle\left\langle a^s|\beta\right\rangle^*,\end{aligned} \tag{1.108}$$

the matrix representation is seen to be

$$\begin{aligned}|\alpha\rangle\langle\beta| &\sim \begin{bmatrix}\left\langle a^1\right|\left(|\alpha\rangle\langle\beta|\right)\left|a^1\right\rangle & \left\langle a^1\right|\left(|\alpha\rangle\langle\beta|\right)\left|a^2\right\rangle & \cdots \\ \left\langle a^2\right|\left(|\alpha\rangle\langle\beta|\right)\left|a^1\right\rangle & \left\langle a^2\right|\left(|\alpha\rangle\langle\beta|\right)\left|a^2\right\rangle & \cdots \\ \vdots & \vdots & \ddots\end{bmatrix} \\ &= \begin{bmatrix}\left\langle a^1|\alpha\right\rangle\left\langle a^1|\beta\right\rangle^* & \left\langle a^1|\alpha\right\rangle\left\langle a^2|\beta\right\rangle^* & \cdots \\ \left\langle a^2|\alpha\right\rangle\left\langle a^1|\beta\right\rangle^* & \left\langle a^2|\alpha\right\rangle\left\langle a^2|\beta\right\rangle^* & \cdots \\ \vdots & \vdots & \ddots\end{bmatrix}.\end{aligned} \tag{1.109}$$

Part b. First compute the spin-z representation of $|s_x = \hbar/2\rangle$.

$$(S_x - \hbar/2I)\begin{bmatrix}a \\ b\end{bmatrix} = \left(\begin{bmatrix}0 & \hbar/2 \\ \hbar/2 & 0\end{bmatrix} - \begin{bmatrix}\hbar/2 & 0 \\ 0 & \hbar/2\end{bmatrix}\right) = \begin{bmatrix}a \\ b\end{bmatrix} = \frac{\hbar}{2}\begin{bmatrix}-1 & 1 \\ 1 & -1\end{bmatrix}\begin{bmatrix}a \\ b\end{bmatrix}, \tag{1.110}$$

so $|s_x = \hbar/2\rangle \propto (1, 1)$.
Normalized we have

$$\begin{aligned}|\alpha\rangle &= |s_z = \hbar/2\rangle = \begin{bmatrix}1 \\ 0\end{bmatrix} \\ |\beta\rangle &= |s_z = \hbar/2\rangle\,\frac{1}{\sqrt{2}}\begin{bmatrix}1 \\ 1\end{bmatrix}.\end{aligned} \tag{1.111}$$

Using eq. (1.109) the matrix representation is

$$\begin{aligned}|\alpha\rangle\langle\beta| &\sim \begin{bmatrix}(1)(1/\sqrt{2})^* & (1)(1/\sqrt{2})^* \\ (0)(1/\sqrt{2})^* & (0)(1/\sqrt{2})^*\end{bmatrix} \\ &= \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1 \\ 0 & 0\end{bmatrix}.\end{aligned} \tag{1.112}$$

This can be confirmed with direct computation

$$\begin{aligned}|\alpha\rangle\langle\beta| &= \begin{bmatrix}1\\0\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\end{bmatrix}\\ &= \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\0 & 0\end{bmatrix}.\end{aligned} \tag{1.113}$$

Exercise 1.5 Eigenvalue of sum of kets. ([11] pr. 1.6)

Given eigenkets $|i\rangle, |j\rangle$ of an operator A, what are the conditions that $|i\rangle + |j\rangle$ is also an eigenvector?

Answer for Exercise 1.5

Let $A|i\rangle = i|i\rangle, A|j\rangle = j|j\rangle$, and suppose that the sum is an eigenket. Then there must be a value a such that

$$A(|i\rangle + |j\rangle) = a(|i\rangle + |j\rangle), \tag{1.114}$$

so

$$i|i\rangle + j|j\rangle = a(|i\rangle + |j\rangle). \tag{1.115}$$

Operating with $\langle i|, \langle j|$ respectively, gives

$$\begin{aligned}i &= a\\ j &= a,\end{aligned} \tag{1.116}$$

so for the sum to be an eigenket, both of the corresponding energy eigenvalues must be identical (i.e. linear combinations of degenerate eigenkets are also eigenkets).

Exercise 1.6 Null operator. ([11] pr. 1.7)

Given eigenkets $|a'\rangle$ of operator A

a. show that

$$\prod_{a'}(A - a') \tag{1.117}$$

is the null operator.

b.

$$\prod_{a''\neq a'}\frac{(A - a'')}{a' - a''} \tag{1.118}$$

c. Illustrate using S_z for a spin 1/2 system.

Answer for Exercise 1.6

Part a. Application of $|a\rangle$, the eigenket of A with eigenvalue a to any term $A - a'$ scales $|a\rangle$ by $a - a'$, so the product operating on $|a\rangle$ is

$$\prod_{a'} (A - a') |a\rangle = \prod_{a'} (a - a') |a\rangle . \tag{1.119}$$

Since $|a\rangle$ is one of the $\{|a'\rangle\}$ eigenkets of A, one of these terms must be zero.

Part b. Again, consider the action of the operator on $|a\rangle$,

$$\prod_{a'' \neq a'} \frac{(A - a'')}{a' - a''} |a\rangle = \prod_{a'' \neq a'} \frac{(a - a'')}{a' - a''} |a\rangle . \tag{1.120}$$

If $|a\rangle = |a'\rangle$, then $\prod_{a'' \neq a'} \frac{(A-a'')}{a'-a''} |a\rangle = |a\rangle$, whereas if it does not, then it equals one of the a'' energy eigenvalues. This is a representation of the Kronecker delta function

$$\prod_{a'' \neq a'} \frac{(A - a'')}{a' - a''} |a\rangle \equiv \delta_{a',a} |a\rangle \tag{1.121}$$

Part c. For operator S_z the eigenvalues are $\{\hbar/2, -\hbar/2\}$, so the null operator must be

$$\begin{aligned}
\prod_{a'} (A - a') &= \left(\frac{\hbar}{2}\right)^2 \left(\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right) \left(\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right) \\
&= \begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} \\
&= \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}
\end{aligned} \tag{1.122}$$

For the delta representation, consider the $|\pm\rangle$ states and their eigenvalue. The delta operators are

$$\prod_{a'' \neq \hbar/2} \frac{(A - a'')}{\hbar/2 - a''} = \frac{S_z - (-\hbar/2)I}{\hbar/2 - (-\hbar/2)} = \frac{1}{2} (\sigma_z + I) = \frac{1}{2} \left(\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right) = \frac{1}{2} \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{1.123}$$

$$\prod_{a'' \neq -\hbar/2} \frac{(A - a'')}{-\hbar/2 - a''} = \frac{S_z - (\hbar/2)I}{-\hbar/2 - \hbar/2} = \frac{1}{2} (\sigma_z - I) = \frac{1}{2} \left(\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right) = \frac{1}{2} \begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \tag{1.124}$$

These clearly have the expected delta function property acting on kets $|+\rangle = (1,0)^{\mathrm{T}}, |-\rangle = (0,1)^{\mathrm{T}}$.

Exercise 1.7 Spin half general normal. ([11] pr. 1.9)

Construct $|\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle$, where $\hat{\mathbf{n}} = (\cos\alpha\sin\beta, \sin\alpha\sin\beta, \cos\beta)^{\mathrm{T}}$ such that

$$\mathbf{S}\cdot\hat{\mathbf{n}}\,|\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle = \frac{\hbar}{2}|\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle, \tag{1.125}$$

Solve this as an eigenvalue problem.

Answer for Exercise 1.7

The spin operator for this direction is

$$\begin{aligned}
\mathbf{S}\cdot\hat{\mathbf{n}} &= \frac{\hbar}{2}\boldsymbol{\sigma}\cdot\hat{\mathbf{n}} \\
&= \frac{\hbar}{2}\left(\cos\alpha\sin\beta\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} + \sin\alpha\sin\beta\begin{bmatrix}0 & -i\\i & 0\end{bmatrix} + \cos\beta\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\right) \\
&= \frac{\hbar}{2}\begin{bmatrix}\cos\beta & e^{-i\alpha}\sin\beta\\ e^{i\alpha}\sin\beta & -\cos\beta\end{bmatrix}.
\end{aligned} \tag{1.126}$$

Observed that this is traceless and has a $-\hbar/2$ determinant like any of the x, y, z spin operators.

Assuming that this has an $\hbar/2$ eigenvalue (to be verified later), the eigenvalue problem is

$$\begin{aligned}
0 &= \mathbf{S}\cdot\hat{\mathbf{n}} - \hbar/2I \\
&= \frac{\hbar}{2}\begin{bmatrix}\cos\beta - 1 & e^{-i\alpha}\sin\beta\\ e^{i\alpha}\sin\beta & -\cos\beta - 1\end{bmatrix} \\
&= \hbar\begin{bmatrix}-\sin^2\frac{\beta}{2} & e^{-i\alpha}\sin\frac{\beta}{2}\cos\frac{\beta}{2}\\ e^{i\alpha}\sin\frac{\beta}{2}\cos\frac{\beta}{2} & -\cos^2\frac{\beta}{2}\end{bmatrix}
\end{aligned} \tag{1.127}$$

This has a zero determinant as expected, and the eigenvector (a, b) will satisfy

$$\begin{aligned}
0 &= -\sin^2\frac{\beta}{2}a + e^{-i\alpha}\sin\frac{\beta}{2}\cos\frac{\beta}{2}b \\
&= \sin\frac{\beta}{2}\left(-\sin\frac{\beta}{2}a + e^{-i\alpha}b\cos\frac{\beta}{2}\right)
\end{aligned} \tag{1.128}$$

$$\begin{bmatrix}a\\b\end{bmatrix} \propto \begin{bmatrix}\cos\frac{\beta}{2}\\ e^{i\alpha}\sin\frac{\beta}{2}\end{bmatrix}. \tag{1.129}$$

This is appropriately normalized, so the ket for $\mathbf{S}\cdot\hat{\mathbf{n}}$ is

$$|\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle = \cos\frac{\beta}{2}\,|+\rangle + e^{i\alpha}\sin\frac{\beta}{2}\,|-\rangle\,. \tag{1.130}$$

Note that the other eigenvalue is

$$|\mathbf{S}\cdot\hat{\mathbf{n}};-\rangle = -\sin\frac{\beta}{2}\,|+\rangle + e^{i\alpha}\cos\frac{\beta}{2}\,|-\rangle\,. \tag{1.131}$$

It is straightforward to show that these are orthogonal and that this has the $-\hbar/2$ eigenvalue.

Exercise 1.8 Two state Hamiltonian. (*[11] pr. 1.10*)

Solve the eigenproblem for

$$H = a\big(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|\big) \tag{1.132}$$

Answer for Exercise 1.8

In matrix form the Hamiltonian is

$$H = a\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{1.133}$$

The eigenvalue problem is

$$\begin{aligned} 0 &= |H-\lambda I| \\ &= (a-\lambda)(-a-\lambda) - a^2 \\ &= (-a+\lambda)(a+\lambda) - a^2 \\ &= \lambda^2 - a^2 - a^2, \end{aligned} \tag{1.134}$$

or

$$\lambda = \pm\sqrt{2}a. \tag{1.135}$$

An eigenket proportional to (α,β) must satisfy

$$0 = (1\mp\sqrt{2})\alpha + \beta, \tag{1.136}$$

so

$$|\pm\rangle \propto \begin{bmatrix} -1 \\ 1\mp\sqrt{2} \end{bmatrix}, \tag{1.137}$$

or

$$\begin{aligned} |\pm\rangle &= \frac{1}{2(2-\sqrt{2})}\begin{bmatrix} -1 \\ 1 \mp \sqrt{2} \end{bmatrix} \\ &= \frac{2+\sqrt{2}}{4}\begin{bmatrix} -1 \\ 1 \mp \sqrt{2} \end{bmatrix}. \end{aligned} \tag{1.138}$$

That is

$$|\pm\rangle = \frac{2+\sqrt{2}}{4}\left(-|1\rangle + (1 \mp \sqrt{2})\,|2\rangle\right). \tag{1.139}$$

Exercise 1.9 Spin half probability and dispersion. ([11] pr. 1.12, phy1520 2015 ps1.3)

A spin 1/2 system $\mathbf{S}\cdot\hat{\mathbf{n}}$, with $\hat{\mathbf{n}} = \sin\theta\hat{\mathbf{x}} + \cos\theta\hat{\mathbf{z}}$, is in state with eigenvalue $\hbar/2$.

a. If S_x is measured. What is the probability of getting $+\hbar/2$?

b. Evaluate the dispersion in S_x, that is,

$$\left\langle (S_x - \langle S_x\rangle)^2 \right\rangle. \tag{1.140}$$

Answer for Exercise 1.9

Part a. In matrix form the spin operator for the system is

$$\begin{aligned} \mathbf{S}\cdot\hat{\mathbf{n}} &= \frac{\hbar}{2}\left(\cos\theta\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \sin\theta\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right) \\ &= \frac{\hbar}{2}\begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix} \end{aligned} \tag{1.141}$$

An eigenket $|\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle = (a, b)^{\mathrm{T}}$ must satisfy

$$\begin{aligned} 0 &= (\cos\theta - 1)\,a + \sin\theta b \\ &= \left(-2\sin^2\frac{\theta}{2}\right)a + 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}b \\ &= -\sin\frac{\theta}{2}a + \cos\frac{\theta}{2}b, \end{aligned} \tag{1.142}$$

so the eigenstate is

$$|\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle = \begin{bmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{bmatrix}. \tag{1.143}$$

Pick $|S_x; \pm\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm 1 \end{bmatrix}$ as the basis for the S_x operator. Then, for the probability that the system will end up in the $+\hbar/2$ state of S_x, we have

$$
\begin{aligned}
P &= |\langle S_x; + | \mathbf{S} \cdot \hat{\mathbf{n}}; + \rangle|^2 \\
&= \left| \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}^\dagger \begin{bmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{bmatrix} \right|^2 \\
&= \frac{1}{2} \left| \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{bmatrix} \right|^2 \\
&= \frac{1}{2} \left(\cos \frac{\theta}{2} + \sin \frac{\theta}{2} \right)^2 \\
&= \frac{1}{2} \left(1 + 2 \cos \frac{\theta}{2} \sin \frac{\theta}{2} \right) \\
&= \frac{1}{2} \left(1 + \sin \theta \right).
\end{aligned}
\tag{1.144}
$$

This is a reasonable seeming result, with $P \in [0, 1]$. Some special values also further validate this

$$
\begin{aligned}
&\theta = 0, |\mathbf{S} \cdot \hat{\mathbf{n}}; + \rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |S_z; + \rangle = \frac{1}{\sqrt{2}} |S_x; + \rangle + \frac{1}{\sqrt{2}} |S_x; - \rangle \\
&\theta = \pi/2, |\mathbf{S} \cdot \hat{\mathbf{n}}; + \rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = |S_x; + \rangle \\
&\theta = \pi, |\mathbf{S} \cdot \hat{\mathbf{n}}; + \rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |S_z; - \rangle = \frac{1}{\sqrt{2}} |S_x; + \rangle - \frac{1}{\sqrt{2}} |S_x; - \rangle,
\end{aligned}
\tag{1.145}
$$

where we see that the probabilities are in proportion to the projection of the initial state onto the measured state $|S_x; + \rangle$.

Part b. The S_x expectation is

$$
\begin{aligned}
\langle S_x \rangle &= \frac{\hbar}{2} \begin{bmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{bmatrix} \\
&= \frac{\hbar}{2} \begin{bmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \end{bmatrix} \begin{bmatrix} \sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{bmatrix} \\
&= \frac{\hbar}{2} 2 \sin\frac{\theta}{2} \cos\frac{\theta}{2} \\
&= \frac{\hbar}{2} \sin\theta.
\end{aligned}
\tag{1.146}
$$

Note that $S_x^2 = (\hbar/2)^2 I$, so

$$
\begin{aligned}
\left\langle S_x^2 \right\rangle &= \left(\frac{\hbar}{2}\right)^2 \begin{bmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \end{bmatrix} \begin{bmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{bmatrix} \\
&= \left(\frac{\hbar}{2}\right)^2 \cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2} \\
&= \left(\frac{\hbar}{2}\right)^2 .
\end{aligned}
\tag{1.147}
$$

The dispersion is

$$
\begin{aligned}
\left\langle (S_x - \langle S_x \rangle)^2 \right\rangle &= \left\langle S_x^2 \right\rangle - \langle S_x \rangle^2 \\
&= \left(\frac{\hbar}{2}\right)^2 \left(1 - \sin^2\theta\right) \\
&= \left(\frac{\hbar}{2}\right)^2 \cos^2\theta.
\end{aligned}
\tag{1.148}
$$

At $\theta = \pi/2$ the dispersion is 0, which is expected since $|\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle = |S_x;+\rangle$ at that point. Similarly, the dispersion is maximized at $\theta = 0, \pi$ where the $|\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle$ component in the $|S_x;+\rangle$ direction is minimized.

Exercise 1.10 Cascading Stern-Gerlach. (*[11] pr. 1.13*)

Three Stern-Gerlach type measurements are performed, the first that prepares the state in a $|S_z;+\rangle$ state, the next in a $|\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle$ state where $\hat{\mathbf{n}} = \cos\beta\hat{\mathbf{z}} + \sin\beta\hat{\mathbf{x}}$, and the last performing a S_z $\hbar/2$ state measurement, as illustrated in fig. 1.7.

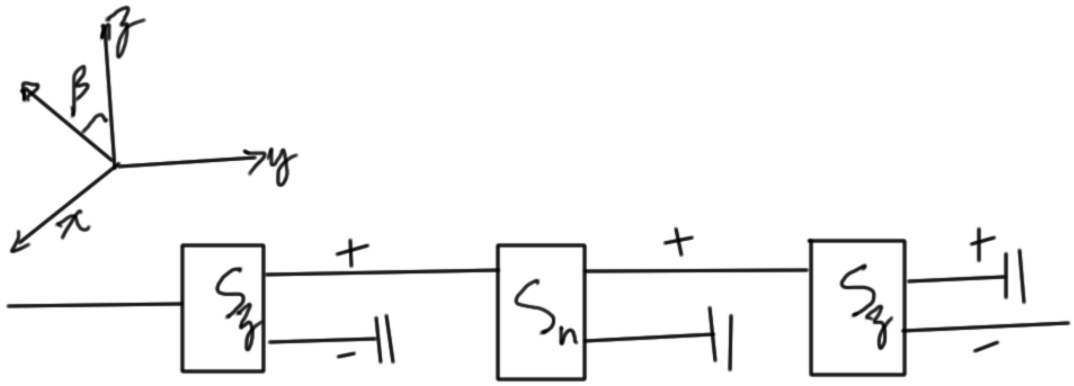

Figure 1.7: Cascaded Stern-Gerlach type measurements.

What is the intensity of the final $s_z = -\hbar/2$ beam? What is the orientation for the second measuring apparatus to maximize the intensity of this beam?

Answer for Exercise 1.10

The spin operator for the second apparatus is

$$\begin{aligned}\mathbf{S}\cdot\hat{\mathbf{n}} &= \frac{\hbar}{2}\left(\sin\beta\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} + \cos\beta\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\right)\\ &= \frac{\hbar}{2}\begin{bmatrix}\cos\beta & \sin\beta\\ \sin\beta & -\cos\beta\end{bmatrix}.\end{aligned} \tag{1.149}$$

The intensity of the final $|S_z; -\rangle$ beam is

$$P = |\langle - | \mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle \langle \mathbf{S}\cdot\hat{\mathbf{n}}; + | + \rangle|^2, \tag{1.150}$$

(i.e. the second apparatus applies a projection operator $|\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle\langle\mathbf{S}\cdot\hat{\mathbf{n}}; +|$ to the initial $|+\rangle$ state, and then the $|-\rangle$ states are selected out of that.

The $\mathbf{S}\cdot\hat{\mathbf{n}}$ eigenket is found to be

$$|\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle = \begin{bmatrix}\cos\frac{\beta}{2}\\ \sin\frac{\beta}{2}\end{bmatrix}, \tag{1.151}$$

so

$$
\begin{aligned}
P &= \left| \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\frac{\beta}{2} \\ \sin\frac{\beta}{2} \end{bmatrix} \begin{bmatrix} \cos\frac{\beta}{2} & \sin\frac{\beta}{2} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right|^2 \\
&= \left| \cos\frac{\beta}{2} \sin\frac{\beta}{2} \right|^2 \\
&= \left| \frac{1}{2} \sin\beta \right|^2 \\
&= \frac{1}{4} \sin^2\beta.
\end{aligned}
\tag{1.152}
$$

This is maximized when $\beta = \pi/2$, or $\hat{\mathbf{n}} = \hat{\mathbf{x}}$. At this angle the state leaving the second apparatus is

$$
\begin{aligned}
\begin{bmatrix} \cos\frac{\beta}{2} \\ \sin\frac{\beta}{2} \end{bmatrix} \begin{bmatrix} \cos\frac{\beta}{2} & \sin\frac{\beta}{2} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} &= \frac{1}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\
&= \frac{1}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\
&= \frac{1}{2} \left|+\right\rangle + \frac{1}{2} \left|-\right\rangle,
\end{aligned}
\tag{1.153}
$$

so the state after filtering the $\left|-\right\rangle$ states is $\frac{1}{2} \left|-\right\rangle$ with intensity (probability density) of $1/4$ relative to a unit normalize input $\left|+\right\rangle$ state to the $\mathbf{S} \cdot \hat{\mathbf{n}}$ apparatus.

Exercise 1.11 Can anticommuting operators have a simultaneous eigenket? (*[11] pr. 1.16*)

Two Hermitian operators anticommute

$$
\begin{aligned}
\{A, B\} &= AB + BA \\
&= 0.
\end{aligned}
\tag{1.154}
$$

Is it possible to have a simultaneous eigenket of A and B? Prove or illustrate your assertion.

Answer for Exercise 1.11

Suppose that such a simultaneous non-zero eigenket $\left|\alpha\right\rangle$ exists, then

$$
A \left|\alpha\right\rangle = a \left|\alpha\right\rangle,
\tag{1.155}
$$

and

$$
B \left|\alpha\right\rangle = b \left|\alpha\right\rangle
\tag{1.156}
$$

This gives

$$\begin{aligned}(AB + BA)\left|\alpha\right\rangle &= (Ab + Ba)\left|\alpha\right\rangle \\ &= 2ab\left|\alpha\right\rangle.\end{aligned} \tag{1.157}$$

If this is zero, one of the operators must have a zero eigenvalue. Knowing that we can construct an example of such operators. In matrix form, let

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & a \end{bmatrix} \tag{1.158a}$$

$$B = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & b \end{bmatrix}. \tag{1.158b}$$

These are both Hermitian, and anticommute provided at least one of a, b is zero. These have a common eigenket

$$\left|\alpha\right\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \tag{1.159}$$

A zero eigenvalue of one of the commuting operators may not be a sufficient condition for such anticommutation.

Exercise 1.12 Degeneracy in non-commuting observables that both commute with the Hamiltonian.

Show that non-commuting operators that both commute with the Hamiltonian, have, in general, degenerate energy eigenvalues. That is

$$[A, H] = [B, H] = 0, \tag{1.160}$$

but

$$[A, B] \neq 0. \tag{1.161}$$

a. Consider L_x, L_z and a central force Hamiltonian $H = \mathbf{p}^2/2m + V(r)$ as examples.
b. Construct some simple matrix examples that illustrate the degeneracy conditions.
c. Prove the general case.

Answer for Exercise 1.12

Part a. Let's start with demonstrate these commutators act as expected in these cases. With $\mathbf{L} = \mathbf{x} \times \mathbf{p}$, we have

$$\begin{aligned}
L_x &= y p_z - z p_y \\
L_y &= z p_x - x p_z \\
L_z &= x p_y - y p_x.
\end{aligned} \tag{1.162}$$

The L_x, L_z commutator is

$$\begin{aligned}
[L_x, L_z] &= [y p_z - z p_y, x p_y - y p_x] \\
&= [y p_z, x p_y] - [y p_z, y p_x] - [z p_y, x p_y] + [z p_y, y p_x] \\
&= x p_z [y, p_y] + z p_x [p_y, y] \\
&= i\hbar (x p_z - z p_x) \\
&= -i\hbar L_y
\end{aligned} \tag{1.163}$$

cyclically permuting the indexes shows that no pairs of different $\mathbf{L}$ components commute. For L_y, L_x that is

$$\begin{aligned}
[L_y, L_x] &= [z p_x - x p_z, y p_z - z p_y] \\
&= [z p_x, y p_z] - [z p_x, z p_y] - [x p_z, y p_z] + [x p_z, z p_y] \\
&= y p_x [z, p_z] + x p_y [p_z, z] \\
&= i\hbar (y p_x - x p_y) \\
&= -i\hbar L_z,
\end{aligned} \tag{1.164}$$

and for L_z, L_y

$$\begin{aligned}
[L_z, L_y] &= [x p_y - y p_x, z p_x - x p_z] \\
&= [x p_y, z p_x] - [x p_y, x p_z] - [y p_x, z p_x] + [y p_x, x p_z] \\
&= z p_y [x, p_x] + y p_z [p_x, x] \\
&= i\hbar (z p_y - y p_z) \\
&= -i\hbar L_x.
\end{aligned} \tag{1.165}$$

If these angular momentum components are also shown to commute with themselves (which they do), the commutator relations above can be summarized as

$$[L_a, L_b] = i\hbar \epsilon_{abc} L_c. \tag{1.166}$$

In the example to consider, we'll have to consider the commutators with $\mathbf{p}^2$ and $V(r)$. Picking any one component of $\mathbf{L}$ is sufficient due to the symmetries of the problem. For example

$$\begin{aligned}
\left[L_x, \mathbf{p}^2\right] &= \left[y p_z - z p_y, p_x^2 + p_y^2 + p_z^2\right] \\
&= \left[y p_z, \cancel{p_x^2} + p_y^2 + \cancel{p_z^2}\right] - \left[z p_y, \cancel{p_x^2} + \cancel{p_y^2} + p_z^2\right] \\
&= p_z \left[y, p_y^2\right] - p_y \left[z, p_z^2\right] \\
&= p_z 2 i \hbar p_y - p_y 2 i \hbar p_z \\
&= 0.
\end{aligned} \tag{1.167}$$

How about the commutator of $\mathbf{L}$ with the potential? It is sufficient to consider one component again, for example

$$\begin{aligned}
[L_x, V] &= [y p_z - z p_y, V] \\
&= y \left[p_z, V\right] - z \left[p_y, V\right] \\
&= -i \hbar y \frac{\partial V(r)}{\partial z} + i \hbar z \frac{\partial V(r)}{\partial y} \\
&= -i \hbar y \frac{\partial V}{\partial r} \frac{\partial r}{\partial z} + i \hbar z \frac{\partial V}{\partial r} \frac{\partial r}{\partial y} \\
&= -i \hbar y \frac{\partial V}{\partial r} \frac{z}{r} + i \hbar z \frac{\partial V}{\partial r} \frac{y}{r} \\
&= 0.
\end{aligned} \tag{1.168}$$

This has shown that all the components of $\mathbf{L}$ commute with a central force Hamiltonian, and each different component of $\mathbf{L}$ do not commute. It does not demonstrate the degeneracy, but I do recall that exists for this system.

Part b. I thought perhaps the problem at hand would be easier if I were to construct some example matrices representing operators that did not commute, but did commuted with a Hamiltonian. I came up with

$$
\begin{aligned}
A &= \begin{bmatrix} \sigma_z & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
B &= \begin{bmatrix} \sigma_x & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
H &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}
\end{aligned}
\tag{1.169}
$$

This system has $[A, H] = [B, H] = 0$, and

$$
[A, B] = \begin{bmatrix} 0 & 2 & 0 \\ -2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}
\tag{1.170}
$$

There is one shared eigenvector between all of A, B, H

$$
|3\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.
\tag{1.171}
$$

The other eigenvectors for A are

$$
\begin{aligned}
|a_1\rangle &= \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \\
|a_2\rangle &= \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix},
\end{aligned}
\tag{1.172}
$$

and for B

$$
\begin{aligned}
|b_1\rangle &= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \\
|b_2\rangle &= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix},
\end{aligned}
\tag{1.173}
$$

This clearly has the degeneracy sought.

Looking to [1], it appears that it is possible to construct an even simpler example. Let

$$
\begin{aligned}
A &= \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \\
B &= \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \\
H &= \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.
\end{aligned}
\tag{1.174}
$$

Here $[A, B] = -A$, and $[A, H] = [B, H] = 0$, but the Hamiltonian isn't interesting at all physically.

A less boring example builds on this. Let

$$
\begin{aligned}
A &= \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
B &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
H &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}.
\end{aligned}
\tag{1.175}
$$

Here $[A, B] \neq 0$, and $[A, H] = [B, H] = 0$. I don't see a way for any exception to be constructed.

Part c. The concrete examples above give some intuition for solving the more abstract problem. Suppose that we are working in a basis that simultaneously diagonalizes operator A and the Hamiltonian H. To make life easy consider the simplest case where this basis is also an eigenbasis for the second operator B for all but two of that operators eigenvectors. For such a system let's write

$$\begin{aligned} H |1\rangle &= \epsilon_1 |1\rangle \\ H |2\rangle &= \epsilon_2 |2\rangle \\ A |1\rangle &= a_1 |1\rangle \\ A |2\rangle &= a_2 |2\rangle , \end{aligned} \tag{1.176}$$

where $|1\rangle$, and $|2\rangle$ are not eigenkets of B. Because B also commutes with H, we must have

$$\begin{aligned} HB |1\rangle &= H |n\rangle \langle n| B |1\rangle \\ &= \epsilon_n |n\rangle B_{n1}, \end{aligned} \tag{1.177}$$

and

$$\begin{aligned} BH |1\rangle &= B\epsilon_1 |1\rangle \\ &= \epsilon_1 |n\rangle \langle n| B |1\rangle \\ &= \epsilon_1 |n\rangle B_{n1}. \end{aligned} \tag{1.178}$$

The commutator is

$$[B, H] |1\rangle = (\epsilon_1 - \epsilon_n) |n\rangle B_{n1}. \tag{1.179}$$

Similarly

$$[B, H] |2\rangle = (\epsilon_2 - \epsilon_n) |n\rangle B_{n2}. \tag{1.180}$$

For those kets $|m\rangle \in \{|3\rangle, |4\rangle, \cdots\}$ that are eigenkets of B, with $B |m\rangle = b_m |m\rangle$, we have

$$\begin{aligned} [B, H] |m\rangle &= B\epsilon_m |m\rangle - Hb_m |m\rangle \\ &= b_m\epsilon_m |m\rangle - \epsilon_m b_m |m\rangle \\ &= 0. \end{aligned} \tag{1.181}$$

If the commutator is zero, then we require all its matrix elements

$$\begin{aligned} \langle 1| \left[B, H\right] |1\rangle &= \left(\epsilon_1 - \epsilon_1\right) B_{11} \\ \langle 2| \left[B, H\right] |1\rangle &= \left(\epsilon_1 - \epsilon_2\right) B_{21} \\ \langle 1| \left[B, H\right] |2\rangle &= \left(\epsilon_2 - \epsilon_1\right) B_{12} \\ \langle 2| \left[B, H\right] |2\rangle &= \left(\epsilon_2 - \epsilon_2\right) B_{22}, \end{aligned} \tag{1.182}$$

to be zero. Because of eq. (1.181) only the matrix elements with respect to states $|1\rangle, |2\rangle$ need be considered. Two of the matrix elements above are clearly zero, regardless of the values of B_{11}, and B_{22}, and for the other two to be zero, we must either have

- $B_{21} = B_{12} = 0$, or
- $\epsilon_1 = \epsilon_2$.

If the first condition were true we would have

$$\begin{aligned} B|1\rangle &= |n\rangle \langle n| B |1\rangle \\ &= |n\rangle B_{n1} \\ &= |1\rangle B_{11}, \end{aligned} \tag{1.183}$$

and $B|2\rangle = B_{22}|2\rangle$. This contradicts the requirement that $|1\rangle, |2\rangle$ not be eigenkets of B, leaving only the second option. That second option means there must be a degeneracy in the system.

Exercise 1.13 Uncertainty relation. ([11] pr. 1.20)

Find the ket that maximizes the uncertainty product

$$\left\langle (\Delta S_x)^2 \right\rangle \left\langle \left(\Delta S_y\right)^2 \right\rangle, \tag{1.184}$$

and compare to the uncertainty bound $\frac{1}{4}\left|\left\langle [S_x, S_y] \right\rangle\right|^2$.

Answer for Exercise 1.13

To parameterize the ket space, consider first the kets that where both components are both not zero, where a single complex number can parameterize the ket

$$\begin{aligned} |s\rangle &= \begin{bmatrix} \beta' e^{i\phi'} \\ \alpha' e^{i\theta'} \end{bmatrix} \\ &\propto \begin{bmatrix} 1 \\ \alpha e^{i\theta} \end{bmatrix} \end{aligned} \tag{1.185}$$

The expectation values with respect to this ket are

$$\begin{aligned}\langle S_x \rangle &= \frac{\hbar}{2}\begin{bmatrix}1 & \alpha e^{-i\theta}\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}1\\ \alpha e^{i\theta}\end{bmatrix}\\ &= \frac{\hbar}{2}\begin{bmatrix}1 & \alpha e^{-i\theta}\end{bmatrix}\begin{bmatrix}\alpha e^{i\theta}\\ 1\end{bmatrix}\\ &= \frac{\hbar}{2}\alpha e^{i\theta} + \alpha e^{-i\theta}\\ &= \frac{\hbar}{2}2\alpha\cos\theta\\ &= \hbar\alpha\cos\theta.\end{aligned} \tag{1.186}$$

$$\begin{aligned}\left\langle S_y \right\rangle &= \frac{\hbar}{2}\begin{bmatrix}1 & \alpha e^{-i\theta}\end{bmatrix}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}\begin{bmatrix}1\\ \alpha e^{i\theta}\end{bmatrix}\\ &= \frac{i\hbar}{2}\begin{bmatrix}1 & \alpha e^{-i\theta}\end{bmatrix}\begin{bmatrix}-\alpha e^{i\theta}\\ 1\end{bmatrix}\\ &= \frac{-i\alpha\hbar}{2}2i\sin\theta\\ &= \alpha\hbar\sin\theta.\end{aligned} \tag{1.187}$$

The variances are

$$\begin{aligned}(\Delta S_x)^2 &= \left(\frac{\hbar}{2}\begin{bmatrix}-2\alpha\cos\theta & 1\\ 1 & -2\alpha\cos\theta\end{bmatrix}\right)^2\\ &= \frac{\hbar^2}{4}\begin{bmatrix}-2\alpha\cos\theta & 1\\ 1 & -2\alpha\cos\theta\end{bmatrix}\begin{bmatrix}-2\alpha\cos\theta & 1\\ 1 & -2\alpha\cos\theta\end{bmatrix}\\ &= \frac{\hbar^2}{4}\begin{bmatrix}4\alpha^2\cos^2\theta + 1 & -4\alpha\cos\theta\\ -4\alpha\cos\theta & 4\alpha^2\cos^2\theta + 1\end{bmatrix},\end{aligned} \tag{1.188}$$

and

$$
\begin{aligned}
\left(\Delta S_y\right)^2 &= \left(\frac{\hbar}{2}\begin{bmatrix} -2\alpha\sin\theta & -i \\ i & -2\alpha\sin\theta \end{bmatrix}\right)^2 \\
&= \frac{\hbar^2}{4}\begin{bmatrix} -2\alpha\sin\theta & -i \\ i & -2\alpha\sin\theta \end{bmatrix}\begin{bmatrix} -2\alpha\sin\theta & -i \\ i & -2\alpha\sin\theta \end{bmatrix} \\
&= \frac{\hbar^2}{4}\begin{bmatrix} 4\alpha^2\sin^2\theta + 1 & 4\alpha i\sin\theta \\ -4\alpha i\sin\theta & 4\alpha^2\sin^2\theta + 1 \end{bmatrix}.
\end{aligned}
\tag{1.189}
$$

The uncertainty factors are

$$
\begin{aligned}
\left\langle (\Delta S_x)^2 \right\rangle &= \frac{\hbar^2}{4}\begin{bmatrix} 1 & \alpha e^{-i\theta} \end{bmatrix}\begin{bmatrix} 4\alpha^2\cos^2\theta + 1 & -4\alpha\cos\theta \\ -4\alpha\cos\theta & 4\alpha^2\cos^2\theta + 1 \end{bmatrix}\begin{bmatrix} 1 \\ \alpha e^{i\theta} \end{bmatrix} \\
&= \frac{\hbar^2}{4}\begin{bmatrix} 1 & \alpha e^{-i\theta} \end{bmatrix}\begin{bmatrix} 4\alpha^2\cos^2\theta + 1 - 4\alpha^2\cos\theta e^{i\theta} \\ -4\alpha\cos\theta + 4\alpha^3\cos^2\theta e^{i\theta} + \alpha e^{i\theta} \end{bmatrix} \\
&= \frac{\hbar^2}{4}\left(4\alpha^2\cos^2\theta + 1 - 4\alpha^2\cos\theta e^{i\theta} - 4\alpha^2\cos\theta e^{-i\theta} + 4\alpha^4\cos^2\theta + \alpha^2\right) \\
&= \frac{\hbar^2}{4}\left(4\alpha^2\cos^2\theta + 1 - 8\alpha^2\cos^2\theta + 4\alpha^4\cos^2\theta + \alpha^2\right) \\
&= \frac{\hbar^2}{4}\left(-4\alpha^2\cos^2\theta + 1 + 4\alpha^4\cos^2\theta + \alpha^2\right) \\
&= \frac{\hbar^2}{4}\left(4\alpha^2\cos^2\theta\left(\alpha^2 - 1\right) + \alpha^2 + 1\right),
\end{aligned}
\tag{1.190}
$$

and

$$
\begin{aligned}
\left\langle \left(\Delta S_y\right)^2 \right\rangle &= \frac{\hbar^2}{4}\begin{bmatrix} 1 & \alpha e^{-i\theta} \end{bmatrix}\begin{bmatrix} 4\alpha^2\sin^2\theta + 1 & 4\alpha i\sin\theta \\ -4\alpha i\sin\theta & 4\alpha^2\sin^2\theta + 1 \end{bmatrix}\begin{bmatrix} 1 \\ \alpha e^{i\theta} \end{bmatrix} \\
&= \frac{\hbar^2}{4}\begin{bmatrix} 1 & \alpha e^{-i\theta} \end{bmatrix}\begin{bmatrix} 4\alpha^2\sin^2\theta + 1 + 4\alpha^2 i\sin\theta e^{i\theta} \\ -4\alpha i\sin\theta + 4\alpha^3\sin^2\theta e^{i\theta} + \alpha e^{i\theta} \end{bmatrix} \\
&= \frac{\hbar^2}{4}\left(4\alpha^2\sin^2\theta + 1 + 4\alpha^2 i\sin\theta e^{i\theta} - 4\alpha^2 i\sin\theta e^{-i\theta} + 4\alpha^4\sin^2\theta + \alpha^2\right) \\
&= \frac{\hbar^2}{4}\left(-4\alpha^2\sin^2\theta + 1 + 4\alpha^4\sin^2\theta + \alpha^2\right) \\
&= \frac{\hbar^2}{4}\left(4\alpha^2\sin^2\theta\left(\alpha^2 - 1\right) + \alpha^2 + 1\right).
\end{aligned}
\tag{1.191}
$$

The uncertainty product can finally be calculated

$$\begin{aligned}\left\langle (\Delta S_x)^2 \right\rangle \left\langle \left(\Delta S_y\right)^2 \right\rangle &= \left(\frac{\hbar}{2}\right)^4 \left(4\alpha^2 \cos^2\theta\left(\alpha^2 - 1\right) + \alpha^2 + 1\right)\left(4\alpha^2 \sin^2\theta\left(\alpha^2 - 1\right) + \alpha^2 + 1\right) \\ &= \left(\frac{\hbar}{2}\right)^4 \left(4\alpha^4 \sin^2(2\theta)\left(\alpha^2 - 1\right) + 4\alpha^2\left(\alpha^4 - 1\right) + \left(\alpha^2 + 1\right)^2\right)\end{aligned} \tag{1.192}$$

The maximum occurs when $f = \sin^2 2\theta$ is extremized. Those points are

$$\begin{aligned} 0 &= \frac{\partial f}{\partial \theta} \\ &= 2\sin 2\theta \cos 2\theta \\ &= 4 \sin 4\theta. \end{aligned} \tag{1.193}$$

Those points are at $4\theta = \pi n$, for integer n, or

$$\theta = \frac{\pi}{4} n, n \in [0, 7], \tag{1.194}$$

Minimums will occur when

$$\begin{aligned} 0 &< \frac{\partial^2 f}{\partial \theta^2} \\ &= 8 \cos 4\theta, \end{aligned} \tag{1.195}$$

or

$$n = 0, 2, 4, 6. \tag{1.196}$$

At these points $\sin^2 2\theta$ takes the values

$$\begin{aligned} \sin^2\left(2\frac{\pi}{4}\{0, 2, 4, 6\}\right) &= \sin^2(\pi\{0, 1, 2, 3\}) \\ &\in \{0\}, \end{aligned} \tag{1.197}$$

so the maximization of the uncertainty product can be reduced to that of

$$\left\langle (\Delta S_x)^2 \right\rangle \left\langle \left(\Delta S_y\right)^2 \right\rangle = \left(\frac{\hbar}{2}\right)^4 \left(4\alpha^2\left(\alpha^4 - 1\right) + \left(\alpha^2 + 1\right)^2\right) \tag{1.198}$$

We seek

$$\begin{aligned}
0 &= \frac{\partial}{\partial\alpha}\left(4\alpha^2\left(\alpha^4-1\right)+\left(\alpha^2+1\right)^2\right) \\
&= \left(8\alpha\left(\alpha^4-1\right)+16\alpha^5+4\left(\alpha^2+1\right)\alpha\right) \\
&= 4\alpha\left(2\alpha^4-2+4\alpha^4+4\alpha^2+4\right) \\
&= 8\alpha\left(3\alpha^4+2\alpha^2+1\right).
\end{aligned} \tag{1.199}$$

The only real root of this polynomial is $\alpha = 0$, so the ket where both $|+\rangle$ and $|-\rangle$ are not zero that maximizes the uncertainty product is

$$\begin{aligned}
|s\rangle &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\
&= |+\rangle .
\end{aligned} \tag{1.200}$$

The search for this maximizing value excluded those kets proportional to $\begin{bmatrix} 0 \\ 1 \end{bmatrix} = |-\rangle$. Let's see the values of this uncertainty product at both $|\pm\rangle$, and compare to the uncertainty commutator. First $|s\rangle = |+\rangle$

$$\begin{aligned}
\langle S_x \rangle &= \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} \\
&= 0.
\end{aligned} \tag{1.201}$$

$$\begin{aligned}
\left\langle S_y \right\rangle &= \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} \\
&= 0.
\end{aligned} \tag{1.202}$$

so

$$\begin{aligned}
\left\langle (\Delta S_x)^2 \right\rangle &= \left(\frac{\hbar}{2}\right)^2 \begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} \\
&= \left(\frac{\hbar}{2}\right)^2
\end{aligned} \tag{1.203}$$

$$\begin{aligned}\left\langle\left(\Delta S_y\right)^2\right\rangle &= \left(\frac{\hbar}{2}\right)^2 \begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}1 \\ 0\end{bmatrix} \\ &= \left(\frac{\hbar}{2}\right)^2.\end{aligned} \tag{1.204}$$

For the commutator side of the uncertainty relation we have

$$\begin{aligned}\frac{1}{4}\left|\left\langle\left[S_x, S_y\right]\right\rangle\right|^2 &= \frac{1}{4}|\langle i\hbar S_z\rangle|^2 \\ &= \left(\frac{\hbar}{2}\right)^4 \left|\begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}1 & 0 \\ 0 & -1\end{bmatrix}\begin{bmatrix}1 \\ 0\end{bmatrix}\right|^2,\end{aligned} \tag{1.205}$$

so for the $|+\rangle$ state we have an equality condition for the uncertainty relation

$$\begin{aligned}\left\langle(\Delta S_x)^2\right\rangle\left\langle\left(\Delta S_y\right)^2\right\rangle &= \frac{1}{4}\left|\left\langle\left[S_x, S_y\right]\right\rangle\right|^2 \\ &= \left(\frac{\hbar}{2}\right)^4.\end{aligned} \tag{1.206}$$

It's reasonable to guess that the $|-\rangle$ state also matches the equality condition. Let's check

$$\begin{aligned}\langle S_x\rangle &= \begin{bmatrix}0 & 1\end{bmatrix}\begin{bmatrix}0 & 1 \\ 1 & 0\end{bmatrix}\begin{bmatrix}0 \\ 1\end{bmatrix} \\ &= 0.\end{aligned} \tag{1.207}$$

$$\begin{aligned}\left\langle S_y\right\rangle &= \begin{bmatrix}0 & 1\end{bmatrix}\begin{bmatrix}0 & -i \\ i & 0\end{bmatrix}\begin{bmatrix}0 \\ 1\end{bmatrix} \\ &= 0.\end{aligned} \tag{1.208}$$

so $\left\langle(\Delta S_x)^2\right\rangle = \left\langle(\Delta S_y)^2\right\rangle = \left(\frac{\hbar}{2}\right)^2$.

For the commutator side of the uncertainty relation will be identical, so the equality of eq. (1.206) is satisfied for both $|\pm\rangle$. Note that it wasn't explicitly verified that $|-\rangle$ maximized the uncertainty product, but I don't feel like working through that second set of algebraic mess.

We can see by example that equality does not mean that the equality condition means that the product is maximized. For example, it is straightforward to show that $|S_x; \pm\rangle$ also satisfy the equality condition of the uncertainty relation. However, in that case the product is not maximized, but is zero.

Exercise 1.14 Degenerate ket space example. ([11] pr. 1.23)

Consider operators with representation

$$A = \begin{bmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{bmatrix}, \qquad B = \begin{bmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{bmatrix}. \tag{1.209}$$

Show that these both have degeneracies, commute, and compute a simultaneous ket space for both operators.

Answer for Exercise 1.14

The eigenvalues and eigenvectors for A can be read off by inspection, with values of $a, -a, -a$, and kets

$$\left|a_1\right\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \left|a_2\right\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \left|a_3\right\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \tag{1.210}$$

Notice that the lower-right 2×2 submatrix of B is proportional to σ_y, so it's eigenvalues can be formed by inspection

$$\left|b_1\right\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \left|b_2\right\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ i \end{bmatrix}, \left|b_3\right\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ -i \end{bmatrix}. \tag{1.211}$$

Computing $B \left|b_i\right\rangle$ shows that the eigenvalues are $b, b, -b$ respectively.

Because of the two-fold degeneracy in the $-a$ eigenvalues of A, any linear combination of $\left|a_2\right\rangle, \left|a_3\right\rangle$ will also be an eigenket. In particular,

$$\begin{aligned} \left|a_2\right\rangle + i \left|a_3\right\rangle &= \left|b_2\right\rangle \\ \left|a_2\right\rangle - i \left|a_3\right\rangle &= \left|b_3\right\rangle, \end{aligned} \tag{1.212}$$

so the basis $\{\left|b_i\right\rangle\}$ is a simultaneous eigenspace for both A and B. Because there is a simultaneous eigenspace, the matrices must commute. This can be confirmed with direct computation

$$
\begin{aligned}
AB &= ab \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix} \\
&= ab \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & 0 \end{bmatrix},
\end{aligned}
\tag{1.213}
$$

and

$$
\begin{aligned}
BA &= ab \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \\
&= ab \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & 0 \end{bmatrix}.
\end{aligned}
\tag{1.214}
$$

Exercise 1.15 Unitary transformation. (*[11] pr. 1.26*)

Construct the transformation matrix that maps between the S_z diagonal basis, to the S_x diagonal basis.

Answer for Exercise 1.15

Based on the definition

$$
U \left| a^{(r)} \right\rangle = \left| b^{(r)} \right\rangle,
\tag{1.215}
$$

the matrix elements can be computed

$$
\left\langle a^{(s)} \right| U \left| a^{(r)} \right\rangle = \left\langle a^{(s)} \middle| b^{(r)} \right\rangle,
\tag{1.216}
$$

that is

$$
\begin{aligned}
U &= \begin{bmatrix} \left\langle a^{(1)} \right| U \left| a^{(1)} \right\rangle & \left\langle a^{(1)} \right| U \left| a^{(2)} \right\rangle \\ \left\langle a^{(2)} \right| U \left| a^{(1)} \right\rangle & \left\langle a^{(2)} \right| U \left| a^{(2)} \right\rangle \end{bmatrix} \\
&= \begin{bmatrix} \left\langle a^{(1)} \middle| b^{(1)} \right\rangle & \left\langle a^{(1)} \middle| b^{(2)} \right\rangle \\ \left\langle a^{(2)} \middle| b^{(1)} \right\rangle & \left\langle a^{(2)} \middle| b^{(2)} \right\rangle \end{bmatrix} \\
&= \frac{1}{\sqrt{2}} \begin{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} & \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \\ \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} & \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \end{bmatrix} \\
&= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.
\end{aligned}
\tag{1.217}
$$

As a similarity transformation, we have

$$
\begin{aligned}
\left\langle b^{(r)} \right| S_z \left| b^{(s)} \right\rangle &= \left\langle b^{(r)} \middle| a^{(t)} \right\rangle \left\langle a^{(t)} \right| S_z \left| a^{(u)} \right\rangle \left\langle a^{(u)} \middle| b^{(s)} \right\rangle \\
&= \left\langle a^{(r)} \middle| U \right\rangle^\dagger a^{(t)} \left\langle a^{(t)} \right| S_z \left| a^{(u)} \right\rangle \left\langle a^{(u)} \right| U \left| a^{(s)} \right\rangle,
\end{aligned}
\tag{1.218}
$$

or

$$
S_z' = U^\dagger S_z U. \tag{1.219}
$$

Let's check that the computed similarity transformation does it's job.

$$
\begin{aligned}
\sigma_z' &= U^\dagger \sigma_z U \\
&= \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \\
&= \frac{1}{2} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \\
&= \frac{1}{2} \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix} \\
&= \sigma_x.
\end{aligned}
\tag{1.220}
$$

The transformation matrix can also be computed more directly

$$
\begin{aligned}
U &= U \left|a^{(r)}\right\rangle \left\langle a^{(r)}\right| \\
&= \left|b^{(r)}\right\rangle \left\langle a^{(r)}\right| \\
&= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} + \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} \\
&= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix} + \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix} \\
&= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.
\end{aligned} \tag{1.221}
$$

Exercise 1.16 One dimensional translation operator. (*[11] pr. 1.28*)

a. Evaluate the classical Poisson bracket

$$[x, F(p)]_{\text{classical}} \tag{1.222}$$

b. Evaluate the commutator

$$\left[x, e^{ipa/\hbar}\right] \tag{1.223}$$

c. Using the result in b, prove that

$$e^{ipa/\hbar} \left|x'\right\rangle, \tag{1.224}$$

is an eigenstate of the coordinate operator x.

Answer for Exercise 1.16

Part a.

$$
\begin{aligned}
[x, F(p)]_{\text{classical}} &= \frac{\partial x}{\partial x}\frac{\partial F(p)}{\partial p} - \frac{\partial x}{\partial p}\frac{\partial F(p)}{\partial x} \\
&= \frac{\partial F(p)}{\partial p}.
\end{aligned} \tag{1.225}
$$

Part b. Having worked backwards through these problems, the answer for this one dimensional problem can be obtained from eq. (1.246) and is

$$\left[x, e^{ipa/\hbar}\right] = a e^{ipa/\hbar}. \tag{1.226}$$

Part c.

$$xe^{ipa/\hbar}\left|x'\right\rangle = \left(\left[x, e^{ipa/\hbar}\right] e^{ipa/\hbar} x+\right)\left|x'\right\rangle = \left(ae^{ipa/\hbar} + e^{ipa/\hbar} x'\right)\left|x'\right\rangle = (a + x')\left|x'\right\rangle. \quad (1.227)$$

This demonstrates that $e^{ipa/\hbar}\left|x'\right\rangle$ is an eigenstate of x with eigenvalue $a + x'$.

Exercise 1.17 Polynomial commutators. (*[11] pr. 1.29*)

a. For power series F, G, verify

$$[x_k, G(\mathbf{p})] = i\hbar \frac{\partial G}{\partial p_k}, \qquad [p_k, F(\mathbf{x})] = -i\hbar \frac{\partial F}{\partial x_k}. \quad (1.228)$$

b. Evaluate $\left[x^2, p^2\right]$, and compare to the classical Poisson bracket $\left[x^2, p^2\right]_{\text{classical}}$.

Answer for Exercise 1.17

Part a. Let

$$\begin{aligned} G(\mathbf{p}) &= \sum_{klm} a_{klm} p_1^k p_2^l p_3^m \\ F(\mathbf{x}) &= \sum_{klm} b_{klm} x_1^k x_2^l x_3^m. \end{aligned} \quad (1.229)$$

It is simpler to work with a specific x_k, say $x_k = y$. The validity of the general result will still be clear doing so. Expanding the commutator gives

$$\begin{aligned} [y, G(\mathbf{p})] &= \sum_{klm} a_{klm}\left[y, p_1^k p_2^l p_3^m\right] \\ &= \sum_{klm} a_{klm}\left(y p_1^k p_2^l p_3^m - p_1^k p_2^l p_3^m y\right) \\ &= \sum_{klm} a_{klm}\left(p_1^k y p_2^l p_3^m - p_1^k y p_2^l p_3^m\right) \\ &= \sum_{klm} a_{klm} p_1^k \left[y, p_2^l\right] p_3^m. \end{aligned} \quad (1.230)$$

From eq. (1.244), we have $\left[y, p_2^l\right] = l i\hbar p_2^{l-1}$, so

$$\begin{aligned} [y, G(\mathbf{p})] &= \sum_{klm} a_{klm} p_1^k \left[y, p_2^l\right]\left(l i\hbar p_2^{l-1}\right) p_3^m \\ &= i\hbar \frac{\partial G(\mathbf{p})}{\partial y}. \end{aligned} \quad (1.231)$$

It is straightforward to show that $\left[p, x^l\right] = -l i \hbar x^{l-1}$, allowing for a similar computation of the momentum commutator

$$\begin{aligned}
\left[p_y, F(\mathbf{x})\right] &= \sum_{klm} b_{klm} \left[p_y, x_1^k x_2^l x_3^m\right] \\
&= \sum_{klm} b_{klm} \left(p_y x_1^k x_2^l x_3^m - x_1^k x_2^l x_3^m p_y\right) \\
&= \sum_{klm} b_{klm} \left(x_1^k p_y x_2^l x_3^m - x_1^k p_y x_2^l x_3^m\right) \\
&= \sum_{klm} b_{klm} x_1^k \left[p_y, x_2^l\right] x_3^m \\
&= \sum_{klm} b_{klm} x_1^k \left(-l i \hbar x_2^{l-1}\right) x_3^m \\
&= -i\hbar \frac{\partial F(\mathbf{x})}{\partial p_y}.
\end{aligned} \tag{1.232}$$

Part b. It isn't clear to me how the results above can be used directly to compute $\left[x^2, p^2\right]$. However, when the first term of such a commutator is a mononomial, it can be expanded in terms of an x commutator

$$\begin{aligned}
\left[x^2, G(\mathbf{p})\right] &= x^2 G - G x^2 \\
&= x\,(xG) - Gx^2 \\
&= x\,([x, G] + Gx) - Gx^2 \\
&= x\,[x, G] + (xG)\,x - Gx^2 \\
&= x\,[x, G] + ([x, G] + \cancel{Gx})\,x - \cancel{Gx^2} \\
&= x\,[x, G] + [x, G]\,x.
\end{aligned} \tag{1.233}$$

Similarly,

$$\left[x^3, G(\mathbf{p})\right] = x^2\,[x, G] + x\,[x, G]\,x + [x, G]\,x^2. \tag{1.234}$$

An induction hypothesis can be formed

$$\left[x^k, G(\mathbf{p})\right] = \sum_{j=0}^{k-1} x^{k-1-j}\,[x, G]\,x^j, \tag{1.235}$$

and demonstrated

$$\begin{aligned}
\left[x^{k+1}, G(\mathbf{p})\right] &= x^{k+1}G - Gx^{k+1} \\
&= x\left(x^k G\right) - Gx^{k+1} \\
&= x\left(\left[x^k, G\right] + Gx^k\right) - Gx^{k+1} \\
&= x\left[x^k, G\right] + (xG)\, x^k - Gx^{k+1} \\
&= x\left[x^k, G\right] + ([x, G] + Gx)\, x^k - Gx^{k+1} \\
&= x\left[x^k, G\right] + [x, G]\, x^k \\
&= x\sum_{j=0}^{k-1} x^{k-1-j}\, [x, G]\, x^j + [x, G]\, x^k \\
&= \sum_{j=0}^{k-1} x^{(k+1)-1-j}\, [x, G]\, x^j + [x, G]\, x^k \\
&= \sum_{j=0}^{k} x^{(k+1)-1-j}\, [x, G]\, x^j. \qquad \square
\end{aligned} \tag{1.236}$$

That was a bit overkill for this problem, but may be useful later. Application of this to the problem gives

$$\begin{aligned}
\left[x^2, p^2\right] &= x\left[x, p^2\right] + \left[x, p^2\right] x \\
&= xi\hbar\frac{\partial p^2}{\partial x} + i\hbar\frac{\partial p^2}{\partial x} x \\
&= x2i\hbar p + 2i\hbar p x \\
&= i\hbar\,(2xp + 2px)\,.
\end{aligned} \tag{1.237}$$

The classical commutator is

$$\begin{aligned}
\left[x^2, p^2\right]_{\text{classical}} &= \frac{\partial x^2}{\partial x}\frac{\partial p^2}{\partial p} - \frac{\partial x^2}{\partial p}\frac{\partial p^2}{\partial x} \\
&= 2x2p \\
&= 2xp + 2px.
\end{aligned} \tag{1.238}$$

This demonstrates the expected relation between the classical and quantum commutators

$$\left[x^2, p^2\right] = i\hbar\left[x^2, p^2\right]_{\text{classical}}. \tag{1.239}$$

Exercise 1.18 Translation operator and position expectation. (*[11] pr. 1.30*)

The translation operator for a finite spatial displacement is given by

$$\mathcal{T}(\mathbf{l}) = \exp\left(-i\mathbf{p}\cdot\mathbf{l}/\hbar\right), \tag{1.240}$$

where $\mathbf{p}$ is the momentum operator.

a. Evaluate

$$\left[x_i, \mathcal{T}(\mathbf{l})\right]. \tag{1.241}$$

b. Demonstrate how the expectation value $\langle \mathbf{x} \rangle$ changes under translation.

Answer for Exercise 1.18

Part a. For clarity, let's set $x_i = y$. The general result will be clear despite doing so.

$$\left[y, \mathcal{T}(\mathbf{l})\right] = \sum_{k=0} \frac{1}{k!}\left(\frac{-i}{\hbar}\right)\left[y, (\mathbf{p}\cdot\mathbf{l})^k\right]. \tag{1.242}$$

The commutator expands as

$$\begin{aligned}
\left[y, (\mathbf{p}\cdot\mathbf{l})^k\right] + (\mathbf{p}\cdot\mathbf{l})^k y &= y\,(\mathbf{p}\cdot\mathbf{l})^k \\
&= y\left(p_x l_x + p_y l_y + p_z l_z\right)(\mathbf{p}\cdot\mathbf{l})^{k-1} \\
&= \left(p_x l_x y + y p_y l_y + p_z l_z y\right)(\mathbf{p}\cdot\mathbf{l})^{k-1} \\
&= \left(p_x l_x y + l_y\left(p_y y + i\hbar\right) + p_z l_z y\right)(\mathbf{p}\cdot\mathbf{l})^{k-1} \\
&= (\mathbf{p}\cdot\mathbf{l})\, y\,(\mathbf{p}\cdot\mathbf{l})^{k-1} + i\hbar l_y\,(\mathbf{p}\cdot\mathbf{l})^{k-1} \\
&= \cdots \\
&= (\mathbf{p}\cdot\mathbf{l})^{k-1}\, y\,(\mathbf{p}\cdot\mathbf{l})^{k-(k-1)} + (k-1)i\hbar l_y\,(\mathbf{p}\cdot\mathbf{l})^{k-1} \\
&= (\mathbf{p}\cdot\mathbf{l})^{k}\, y + k i\hbar l_y\,(\mathbf{p}\cdot\mathbf{l})^{k-1}.
\end{aligned} \tag{1.243}$$

In the above expansion, the commutation of y with p_x, p_z has been used. This gives, for $k \neq 0$,

$$\left[y, (\mathbf{p}\cdot\mathbf{l})^k\right] = k i\hbar l_y\,(\mathbf{p}\cdot\mathbf{l})^{k-1}. \tag{1.244}$$

Note that this also holds for the $k = 0$ case, since y commutes with the identity operator. Plugging back into the $\mathcal{T}$ commutator, we have

$$\begin{aligned}
\left[y, \mathcal{T}(\mathbf{l})\right] &= \sum_{k=1} \frac{1}{k!}\left(\frac{-i}{\hbar}\right) k i\hbar l_y\,(\mathbf{p}\cdot\mathbf{l})^{k-1} \\
&= l_y \sum_{k=1} \frac{1}{(k-1)!}\left(\frac{-i}{\hbar}\right)(\mathbf{p}\cdot\mathbf{l})^{k-1} \\
&= l_y \mathcal{T}(\mathbf{l}).
\end{aligned} \tag{1.245}$$

The same pattern clearly applies with the other x_i values, providing the desired relation.

$$[\mathbf{x}, \mathcal{T}(\mathbf{l})] = \sum_{m=1}^{3} \mathbf{e}_m l_m \mathcal{T}(\mathbf{l}) = \mathbf{l}\mathcal{T}(\mathbf{l}). \tag{1.246}$$

Part b. Suppose that the translated state is defined as $|\alpha_\mathbf{l}\rangle = \mathcal{T}(\mathbf{l})|\alpha\rangle$. The expectation value with respect to this state is

$$\begin{aligned}
\langle \mathbf{x}' \rangle &= \langle \alpha_\mathbf{l} | \mathbf{x} | \alpha_\mathbf{l} \rangle \\
&= \langle \alpha | \mathcal{T}^\dagger(\mathbf{l}) \mathbf{x} \mathcal{T}(\mathbf{l}) | \alpha \rangle \\
&= \langle \alpha | \mathcal{T}^\dagger(\mathbf{l}) (\mathbf{x} \mathcal{T}(\mathbf{l})) | \alpha \rangle \\
&= \langle \alpha | \mathcal{T}^\dagger(\mathbf{l}) (\mathcal{T}(\mathbf{l}) \mathbf{x} + \mathbf{l}\mathcal{T}(\mathbf{l})) | \alpha \rangle \\
&= \langle \alpha | \mathcal{T}^\dagger \mathcal{T} \mathbf{x} + \mathbf{l} \mathcal{T}^\dagger \mathcal{T} | \alpha \rangle \\
&= \langle \alpha | \mathbf{x} | \alpha \rangle + \mathbf{l} \langle \alpha | \alpha \rangle \\
&= \langle \mathbf{x} \rangle + \mathbf{l}.
\end{aligned} \tag{1.247}$$

Exercise 1.19 **Density matrix.** (*phy1520 2015 ps1.1*)

Consider a spin-1/2 particle. The Hilbert space is two-dimensional, let us label the two states as $|\uparrow\rangle$ and $|\downarrow\rangle$. Write down the 2×2 density matrix which corresponds to the following pure states.

(i) $|\uparrow\rangle$

(ii) $\frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$

(iii) $\frac{1}{\sqrt{2}}\left(|\uparrow\rangle + i|\downarrow\rangle\right)$

(iv) At time $t = 0$, let us start with the state $\frac{1}{\sqrt{2}}\left(|\uparrow\rangle + i|\downarrow\rangle\right)$, and consider time-evolution under the Hamiltonian $\hat{H} = -BS_z$, where S_z is the z-component of the spin operator. This leads to eigenstates $|\uparrow\rangle$ with energy $-B\hbar/2$, and $|\downarrow\rangle$ with energy $+B\hbar/2$. The state $\frac{1}{\sqrt{2}}\left(|\uparrow\rangle + i|\downarrow\rangle\right)$ is not an eigenstate of this Hamiltonian and it will evolve in time. Find the state and the corresponding 2×2 density matrix of this system at a later time t.

Answer for Exercise 1.19

PROBLEM SET RELATED MATERIAL REDACTED IN THIS DOCUMENT.PLEASE FEEL FREE TO EMAIL ME FOR THE FULL VERSION IF YOU AREN'T TAKING PHY1520. [redacted]

[redacted]. END-REDACTION

Exercise 1.20 **Reduced density matrix.** (*phy1520 2015 ps1.2*)

Consider two spin-1/2 particles, the Hilbert space is now 4-dimensional, with states $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$. Let us consider the following pure states:

(i) $\frac{1}{2}\left(|\uparrow\uparrow\rangle - |\uparrow\downarrow\rangle - |\downarrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$

(ii) $\frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right)$

(iii) $\frac{1}{\sqrt{5}}\left(|\uparrow\uparrow\rangle + 2\,|\downarrow\downarrow\rangle\right)$

In each case, obtain the reduced 2×2 density matrix which describes the first spin, when we trace over the second spin. The von Neumann entanglement entropy is defined via $S_{\mathrm{vN}} = -\operatorname{tr}(\rho_{\mathrm{R}} \ln \rho_{\mathrm{R}})$ where ρ_{R} is the reduced density matrix you have obtained above and the tr now refers to tracing over the first spin. Using the reduced density matrices you have obtained above, compute the corresponding S_{vN}, and simply explain your result in words. Consider the Renyi entropy $S_n = \frac{1}{1-n} \ln\left(\operatorname{tr}(\rho_{\mathrm{R}}^n)\right)$. Prove that $S_{n\rightarrow 1} = S_{\mathrm{vN}}$, and compute $S_{n=2}$ for the above ρ_{R}.

Answer for Exercise 1.20

PROBLEM SET RELATED MATERIAL REDACTED IN THIS DOCUMENT.PLEASE FEEL FREE TO EMAIL ME FOR THE FULL VERSION IF YOU AREN'T TAKING PHY1520. [redacted]. END-REDACTION

Exercise 1.21 **Ensembles for spin one half.** ([11] *pr. 3.10*)

a. Sakurai leaves it to the reader to verify that knowledge of the three ensemble averages [S_x], [S_y],[S_z] is sufficient to reconstruct the density operator for a spin one half system. Show this.
b. Show how the expectation values $\langle S_x \rangle, \left\langle S_y \right\rangle, \langle S_x \rangle$ fully determine the spin orientation for a pure ensemble.

Answer for Exercise 1.21

Part a. I'll do this in two parts, the first using a spin-up/down ensemble to see what form this has, then the general case. The general case is a bit messy algebraically. After first attempting it the hard way, I did the grunt work portion of that calculation in Mathematica, but then realized it's not so bad to do it manually.

Consider first an ensemble with density operator

$$\rho = w_+ \left| + \right\rangle \left\langle + \right| + w_- \left| - \right\rangle \left\langle - \right|, \tag{1.248}$$

where these are the $\mathbf{S} \cdot (\pm \hat{\mathbf{z}})$ eigenstates. The traces are

$$\begin{aligned}
\mathrm{tr}(\rho\sigma_x) &= \left\langle + \right| \rho\sigma_x \left| + \right\rangle + \left\langle - \right| \rho\sigma_x \left| - \right\rangle \\
&= \left\langle + \right| \rho \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \left| + \right\rangle + \left\langle - \right| \rho \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \left| - \right\rangle \\
&= \left\langle + \right| \left(w_+ \left| + \right\rangle \left\langle + \right| + w_- \left| - \right\rangle \left\langle - \right| \right) \left| - \right\rangle + \left\langle - \right| \left(w_+ \left| + \right\rangle \left\langle + \right| + w_- \left| - \right\rangle \left\langle - \right| \right) \left| + \right\rangle \\
&= \left\langle + \right| w_- \left| - \right\rangle + \left\langle - \right| w_+ \left| + \right\rangle \\
&= 0,
\end{aligned} \tag{1.249}$$

$$\begin{aligned}
\mathrm{tr}(\rho\sigma_y) &= \left\langle + \right| \rho\sigma_y \left| + \right\rangle + \left\langle - \right| \rho\sigma_y \left| - \right\rangle \\
&= \left\langle + \right| \rho \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \left| + \right\rangle + \left\langle - \right| \rho \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \left| - \right\rangle \\
&= i \left\langle + \right| \left(w_+ \left| + \right\rangle \left\langle + \right| + w_- \left| - \right\rangle \left\langle - \right| \right) \left| - \right\rangle - i \left\langle - \right| \left(w_+ \left| + \right\rangle \left\langle + \right| + w_- \left| - \right\rangle \left\langle - \right| \right) \left| + \right\rangle \\
&= i \left\langle + \right| w_- \left| - \right\rangle - i \left\langle - \right| w_+ \left| + \right\rangle \\
&= 0,
\end{aligned} \tag{1.250}$$

and

$$\begin{aligned}
\mathrm{tr}(\rho\sigma_z) &= \left\langle + \right| \rho\sigma_z \left| + \right\rangle + \left\langle - \right| \rho\sigma_z \left| - \right\rangle \\
&= \left\langle + \right| \rho \left| + \right\rangle - \left\langle - \right| \rho \left| - \right\rangle \\
&= \left\langle + \right| \left(w_+ \left| + \right\rangle \left\langle + \right| + w_- \left| - \right\rangle \left\langle - \right| \right) \left| + \right\rangle - \left\langle - \right| \left(w_+ \left| + \right\rangle \left\langle + \right| + w_- \left| - \right\rangle \left\langle - \right| \right) \left| - \right\rangle \\
&= \left\langle + \right| w_+ \left| + \right\rangle - \left\langle - \right| w_- \left| - \right\rangle \\
&= w_+ - w_-.
\end{aligned} \tag{1.251}$$

Since $w_+ + w_- = 1$, this gives

$$\boxed{\begin{aligned} w_+ &= \frac{1 + \mathrm{tr}(\rho\sigma_z)}{2} \\ w_- &= \frac{1 - \mathrm{tr}(\rho\sigma_z)}{2} \end{aligned}} \tag{1.252}$$

Attempting to do a similar set of trace expansions this way for a more general spin basis turns out to be a really bad idea and horribly messy. So much so that I resorted to spinOneHalfSymbolicManipulation.nb to do this symbolic work. However, it's not so bad if the trace is done completely in matrix form.

Using the basis

$$\begin{aligned} |\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle &= \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\phi} \end{bmatrix} \\ |\mathbf{S}\cdot\hat{\mathbf{n}}; -\rangle &= \begin{bmatrix} \sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2) \end{bmatrix}, \end{aligned} \tag{1.253}$$

the projector matrices are

$$\begin{aligned} |\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle\langle\mathbf{S}\cdot\hat{\mathbf{n}}; +| &= \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\phi} \end{bmatrix} \begin{bmatrix} \cos(\theta/2) & \sin(\theta/2)e^{-i\phi} \end{bmatrix} \\ &= \begin{bmatrix} \cos^2(\theta/2) & \cos(\theta/2)\sin(\theta/2)e^{-i\phi} \\ \sin(\theta/2)\cos(\theta/2)e^{i\phi} & \sin^2(\theta/2) \end{bmatrix}, \end{aligned} \tag{1.254}$$

$$\begin{aligned} |\mathbf{S}\cdot\hat{\mathbf{n}}; -\rangle\langle\mathbf{S}\cdot\hat{\mathbf{n}}; -| &= \begin{bmatrix} \sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2) \end{bmatrix} \begin{bmatrix} \sin(\theta/2)e^{i\phi} & -\cos(\theta/2) \end{bmatrix} \\ &= \begin{bmatrix} \sin^2(\theta/2) & -\cos(\theta/2)\sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2)\sin(\theta/2)e^{i\phi} & \cos^2(\theta/2) \end{bmatrix} \end{aligned} \tag{1.255}$$

With $C = \cos(\theta/2), S = \sin(\theta/2)$, a general density operator in this basis has the form

$$\begin{aligned} \rho &= w_+ \begin{bmatrix} C^2 & CS\,e^{-i\phi} \\ SCe^{i\phi} & S^2 \end{bmatrix} + w_- \begin{bmatrix} S^2 & -CS\,e^{-i\phi} \\ -CS\,e^{i\phi} & C^2 \end{bmatrix} \\ &= \begin{bmatrix} w_+C^2 + w_-S^2 & (w_+ - w_-)CS\,e^{-i\phi} \\ (w_+ - w_-)SCe^{i\phi} & w_+S^2 + w_-C^2 \end{bmatrix}. \end{aligned} \tag{1.256}$$

The products with the Pauli matrices are

$$\begin{aligned}\rho\sigma_x &= \begin{bmatrix} w_+C^2 + w_-S^2 & (w_+ - w_-)CS\,e^{-i\phi} \\ (w_+ - w_-)SCe^{i\phi} & w_+S^2 + w_-C^2 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ &= \begin{bmatrix} (w_+ - w_-)CS\,e^{-i\phi} & w_+C^2 + w_-S^2 \\ w_+S^2 + w_-C^2 & (w_+ - w_-)SCe^{i\phi} \end{bmatrix}\end{aligned} \tag{1.257}$$

$$\begin{aligned}\rho\sigma_y &= \begin{bmatrix} w_+C^2 + w_-S^2 & (w_+ - w_-)CS\,e^{-i\phi} \\ (w_+ - w_-)SCe^{i\phi} & w_+S^2 + w_-C^2 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \\ &= i\begin{bmatrix} (w_+ - w_-)CS\,e^{-i\phi} & -w_+C^2 - w_-S^2 \\ w_+S^2 + w_-C^2 & -(w_+ - w_-)SCe^{i\phi} \end{bmatrix}\end{aligned} \tag{1.258}$$

$$\begin{aligned}\rho\sigma_z &= \begin{bmatrix} w_+C^2 + w_-S^2 & (w_+ - w_-)CS\,e^{-i\phi} \\ (w_+ - w_-)SCe^{i\phi} & w_+S^2 + w_-C^2 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ &= \begin{bmatrix} w_+C^2 + w_-S^2 & -(w_+ - w_-)CS\,e^{-i\phi} \\ (w_+ - w_-)SCe^{i\phi} & -(w_+S^2 + w_-C^2) \end{bmatrix}\end{aligned} \tag{1.259}$$

The respective traces can be read right off the matrices

$$\begin{aligned}\operatorname{tr}(\rho\sigma_x) &= (w_+ - w_-)\sin\theta\cos\phi \\ \operatorname{tr}(\rho\sigma_y) &= (w_+ - w_-)\sin\theta\sin\phi\,. \\ \operatorname{tr}(\rho\sigma_z) &= (w_+ - w_-)\cos\theta\end{aligned} \tag{1.260}$$

This gives

$$(w_+ - w_-)\hat{\mathbf{n}} = \Big(\operatorname{tr}(\rho\sigma_x), \operatorname{tr}(\rho\sigma_y), \operatorname{tr}(\rho\sigma_z)\Big), \tag{1.261}$$

or

$$\boxed{w_\pm = \frac{1 \pm \sqrt{\operatorname{tr}^2(\rho\sigma_x) + \operatorname{tr}^2(\rho\sigma_y) + \operatorname{tr}^2(\rho\sigma_z)}}{2}.} \tag{1.262}$$

So, as claimed, it's possible to completely describe the ensemble weight factors using the ensemble averages of $[S_x], [S_y], [S_z]$. I used the Pauli matrices instead, but the difference is just an $\hbar/2$ scaling adjustment.

Alternate approach Another easier and trig free way to look at this problem is assume the density operator's representation is given by a 2×2 matrix with undetermined values

$$\rho = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \tag{1.263}$$

For such a representation we have

$$\begin{aligned}
\rho\sigma_x &= \begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} b & a \\ d & c \end{bmatrix} \\
\rho\sigma_y &= \begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = i\begin{bmatrix} b & -a \\ d & -c \end{bmatrix} \\
\rho\sigma_z &= \begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} a & -b \\ c & -d \end{bmatrix}
\end{aligned} \tag{1.264}$$

The ensemble averages can be read by inspection

$$\begin{aligned}
[\sigma_x] &= b + c \\
[\sigma_y] &= i(b - c) \\
[\sigma_z] &= a - d
\end{aligned} \tag{1.265}$$

Noting that $\mathrm{tr}\left(EAE^{-1}\right) = \mathrm{tr}\left(AE^{-1}E\right) = \mathrm{tr}\left(A\right)$, and that there must be a diagonal basis for which $\langle +|-\rangle = 0$ and

$$\rho = w_+ \left|+\right\rangle \left\langle +\right| + w_- \left|-\right\rangle \left\langle -\right|, \tag{1.266}$$

we must have

$$\begin{aligned}
\mathrm{tr}\,\rho &= a + d \\
&= w_+ + w_- \\
&= 1.
\end{aligned} \tag{1.267}$$

This provides one set of equations for each of b, c and a, d

$$\begin{aligned}
[\sigma_x] &= b + c \\
[\sigma_y] &= i(b - c),
\end{aligned} \tag{1.268}$$

and

$$\begin{aligned}
[\sigma_z] &= a - d \\
1 &= a + d.
\end{aligned} \tag{1.269}$$

These have solutions

$$\begin{aligned}
b &= \frac{[\sigma_x] - i[\sigma_y]}{2} \\
c &= \frac{[\sigma_x] + i[\sigma_y]}{2} \\
a &= \frac{1 + [\sigma_z]}{2} \\
d &= \frac{1 - [\sigma_z]}{2},
\end{aligned} \tag{1.270}$$

or

$$\boxed{\rho = \frac{1}{2}\begin{bmatrix} 1 + [\sigma_z] & [\sigma_x] - i[\sigma_y] \\ [\sigma_x] + i[\sigma_y] & 1 - [\sigma_z] \end{bmatrix}.} \tag{1.271}$$

The characteristic equation for this operator is

$$0 = \left(\left(\frac{1}{2} - \lambda\right) + \frac{[\sigma_z]}{2}\right)\left(\left(\frac{1}{2} - \lambda\right) - \frac{[\sigma_z]}{2}\right) - \frac{1}{4}\left([\sigma_x] + i[\sigma_y]\right)\left([\sigma_x] - i[\sigma_y]\right), \tag{1.272}$$

or

$$\boxed{\lambda = \frac{1 \pm \sqrt{[\sigma_x]^2 + [\sigma_y]^2 + [\sigma_z]^2}}{2},} \tag{1.273}$$

as found above.

Part b. Suppose that the system is in the state $|\mathbf{S}\cdot\hat{\mathbf{n}};+\rangle$ as defined in eq. (1.253), then the expectation values of $\sigma_x, \sigma_y, \sigma_z$ with respect to this state are

$$\begin{aligned}
\langle\sigma_x\rangle &= \begin{bmatrix} \cos(\theta/2) & \sin(\theta/2)e^{-i\phi} \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\phi} \end{bmatrix} \\
&= \begin{bmatrix} \cos(\theta/2) & \sin(\theta/2)e^{-i\phi} \end{bmatrix}\begin{bmatrix} \sin(\theta/2)e^{i\phi} \\ \cos(\theta/2) \end{bmatrix} \\
&= \sin\theta\cos\phi,
\end{aligned} \tag{1.274}$$

$$\begin{aligned}\left\langle \sigma_y \right\rangle &= \begin{bmatrix}\cos(\theta/2) & \sin(\theta/2)e^{-i\phi}\end{bmatrix}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}\begin{bmatrix}\cos(\theta/2)\\ \sin(\theta/2)e^{i\phi}\end{bmatrix}\\ &= i\begin{bmatrix}\cos(\theta/2) & \sin(\theta/2)e^{-i\phi}\end{bmatrix}\begin{bmatrix}-\sin(\theta/2)e^{i\phi}\\ \cos(\theta/2)\end{bmatrix}\\ &= \sin\theta\sin\phi,\end{aligned} \tag{1.275}$$

$$\begin{aligned}\langle \sigma_z \rangle &= \begin{bmatrix}\cos(\theta/2) & \sin(\theta/2)e^{-i\phi}\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}\cos(\theta/2)\\ \sin(\theta/2)e^{i\phi}\end{bmatrix}\\ &= \begin{bmatrix}\cos(\theta/2) & \sin(\theta/2)e^{-i\phi}\end{bmatrix}\begin{bmatrix}\cos(\theta/2)\\ -\sin(\theta/2)e^{i\phi}\end{bmatrix}\\ &= \cos\theta.\end{aligned} \tag{1.276}$$

So we have

$$\boxed{\hat{\mathbf{n}} = \left(\langle\sigma_x\rangle, \left\langle\sigma_y\right\rangle, \langle\sigma_z\rangle\right).} \tag{1.277}$$

The spin direction is completely determined by this vector of expectation values (or equivalently, the expectation values of S_x, S_y, S_z).

2 QUANTUM DYNAMICS

2.1 CLASSICAL HARMONIC OSCILLATOR

Recall the classical Harmonic oscillator equations in their Hamiltonian form

$$\frac{dx}{dt} = \frac{p}{m} \tag{2.1a}$$

$$\frac{dp}{dt} = -kx. \tag{2.1b}$$

With

$$\begin{aligned} x(t=0) &= x_0 \\ p(t=0) &= p_0 \\ k &= m\omega^2, \end{aligned} \tag{2.2}$$

the solutions are ellipses in phase space

$$x(t) = x_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t) \tag{2.3a}$$

$$p(t) = p_0 \cos(\omega t) - m\omega x_0 \sin(\omega t). \tag{2.3b}$$

After a suitable scaling of the variables, these elliptical orbits can be transformed into circular trajectories.

2.2 QUANTUM HARMONIC OSCILLATOR

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 \tag{2.4}$$

Set

$$\hat{X} = \sqrt{\frac{m\omega}{\hbar}}\hat{x} \tag{2.5a}$$

$$\hat{P} = \sqrt{\frac{1}{m\omega\hbar}}\hat{p} \tag{2.5b}$$

The commutators after this change of variables goes from

$$[\hat{x}, \hat{p}] = i\hbar, \tag{2.6}$$

to

$$\left[\hat{X}, \hat{P}\right] = i. \tag{2.7}$$

The Hamiltonian takes the form

$$\begin{aligned}\hat{H} &= \frac{\hbar\omega}{2}\left(\hat{X}^2 + \hat{P}^2\right) \\ &= \hbar\omega\left(\left(\frac{\hat{X} - i\hat{P}}{\sqrt{2}}\right)\left(\frac{\hat{X} + i\hat{P}}{\sqrt{2}}\right) + \frac{1}{2}\right).\end{aligned} \tag{2.8}$$

Define ladder operators (raising and lowering operators respectively)

$$\hat{a}^\dagger = \frac{\hat{X} - i\hat{P}}{\sqrt{2}} \tag{2.9a}$$

$$\hat{a} = \frac{\hat{X} + i\hat{P}}{\sqrt{2}} \tag{2.9b}$$

so

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right). \tag{2.10}$$

We can show

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1, \tag{2.11}$$

and

$$N|n\rangle \equiv \hat{a}^\dagger a = n|n\rangle, \tag{2.12}$$

where $n \geq 0$ is an integer. Recall that

$$\hat{a}|0\rangle = 0, \tag{2.13}$$

and

$$\langle X|\, X + iP\, |0\rangle = 0. \tag{2.14}$$

With

$$\langle x|0\rangle = \Psi_0(x), \tag{2.15}$$

we can show

$$\frac{1}{\sqrt{2}}\left(X + \frac{\partial}{\partial X}\right)\Psi_0(X) = 0. \tag{2.16}$$

Also recall that

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \tag{2.17a}$$

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{2.17b}$$

2.3 COHERENT STATES

Coherent states for the quantum harmonic oscillator are the eigenkets for the creation and annihilation operators

$$\hat{a}\,|z\rangle = z\,|z\rangle \tag{2.18a}$$

$$\hat{a}^\dagger\,|\tilde{z}\rangle = \tilde{z}\,|\tilde{z}\rangle\,, \tag{2.18b}$$

where

$$|z\rangle = \sum_{n=0}^{\infty} c_n\,|n\rangle\,, \tag{2.19}$$

and z is allowed to be a complex number.
Looking for such a state, we compute

$$\begin{aligned}\hat{a}\,|z\rangle &= \sum_{n=1}^{\infty} c_n \hat{a}\,|n\rangle \\ &= \sum_{n=1}^{\infty} c_n\,\sqrt{n}\,|n-1\rangle\end{aligned} \tag{2.20}$$

compare this to

$$\begin{aligned} z\,|z\rangle &= z\sum_{n=0}^{\infty} c_n\,|n\rangle \\ &= \sum_{n=1}^{\infty} c_n\,\sqrt{n}\,|n-1\rangle \\ &= \sum_{n=0}^{\infty} c_{n+1}\,\sqrt{n+1}\,|n\rangle\,, \end{aligned} \tag{2.21}$$

so

$$c_{n+1}\,\sqrt{n+1} = zc_n \tag{2.22}$$

This gives

$$c_{n+1} = \frac{zc_n}{\sqrt{n+1}} \tag{2.23}$$

$$\begin{aligned} c_1 &= c_0 z \\ c_2 &= \frac{zc_1}{\sqrt{2}} = \frac{z^2 c_0}{\sqrt{2}} \\ &\vdots \end{aligned} \tag{2.24}$$

or

$$c_n = \frac{z^n}{\sqrt{n!}}. \tag{2.25}$$

So the desired state is

$$|z\rangle = c_0\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\,|n\rangle\,. \tag{2.26}$$

Also recall that

$$|n\rangle = \frac{\left(\hat{a}^{\dagger}\right)^n}{\sqrt{n!}}\,|0\rangle\,, \tag{2.27}$$

which gives

$$\begin{aligned} |z\rangle &= c_0\sum_{n=0}^{\infty}\frac{\left(z\hat{a}^{\dagger}\right)^n}{n!}\,|0\rangle \\ &= c_0 e^{z\hat{a}^{\dagger}}\,|0\rangle\,. \end{aligned} \tag{2.28}$$

The normalization is

$$c_0 = e^{-|z|^2/2}. \tag{2.29}$$

While we have $\langle n_1|n_2\rangle = \delta_{n_1,n_2}$, these $|z\rangle$ states are not orthonormal. Figuring out that this overlap

$$\langle z_1|z_2\rangle \neq 0, \tag{2.30}$$

will be left for homework.

2.4 COHERENT STATE TIME EVOLUTION

We don't know much about these coherent states. For example does a coherent state at time zero evolve to a coherent state?

$$|z\rangle \stackrel{?}{\rightarrow} |z(t)\rangle \tag{2.31}$$

It turns out that these questions are best tackled in the Heisenberg picture, considering

$$e^{-i\hat{H}t/\hbar}\,|z\rangle\,. \tag{2.32}$$

For example, what is the average of the position operator

$$\langle z|\, e^{i\hat{H}t/\hbar}\hat{x}e^{-i\hat{H}t/\hbar}\,|z\rangle = \sum_{n,n'=0}^{\infty} \langle n|\, c_n^* e^{iE_n t/\hbar} \left(a + a^\dagger\right) \sqrt{\frac{\hbar}{m\omega}} c_{n'} e^{iE_{n'}t/\hbar}\,|n\rangle\,. \tag{2.33}$$

This is very messy to attempt. Instead if we know how the operator evolves we can calculate

$$\langle z|\, \hat{x}_{\mathrm{H}}(t)\,|z\rangle\,, \tag{2.34}$$

that is

$$\langle \hat{x}\rangle\,(t) = \langle z|\, \hat{x}_{\mathrm{H}}(t)\,|z\rangle\,, \tag{2.35}$$

and for momentum

$$\langle \hat{p}\rangle\,(t) = \langle z|\, \hat{p}_{\mathrm{H}}(t)\,|z\rangle\,. \tag{2.36}$$

The question to ask is what are the expansions of

$$\hat{a}_{\mathrm{H}}(t) = e^{i\hat{H}t/\hbar}\hat{a}e^{-i\hat{H}t/\hbar}. \tag{2.37a}$$

$$\hat{a}_{\mathrm{H}}^\dagger(t) = e^{i\hat{H}t/\hbar}\hat{a}^\dagger e^{-i\hat{H}t/\hbar}. \tag{2.37b}$$

The question to ask is how do these operators ask on the basis states

$$\begin{aligned} \hat{a}_{\mathrm{H}}(t)\left|n\right\rangle &= e^{i\hat{H}t/\hbar}\hat{a}e^{-i\hat{H}t/\hbar}\left|n\right\rangle \\ &= e^{i\hat{H}t/\hbar}\hat{a}e^{-it\omega(n+1/2)}\left|n\right\rangle \\ &= e^{-it\omega(n+1/2)}e^{i\hat{H}t/\hbar}\sqrt{n}\left|n-1\right\rangle \\ &= \sqrt{n}e^{-it\omega(n+1/2)}e^{it\omega(n-1/2)}\left|n-1\right\rangle \\ &= \sqrt{n}e^{-i\omega t}\left|n-1\right\rangle \\ &= e^{-i\omega t}\left|n\right\rangle . \end{aligned} \tag{2.38}$$

So we have found

$$\begin{aligned} \hat{a}_{\mathrm{H}}(t) &= ae^{-i\omega t} \\ \hat{a}^{\dagger}_{\mathrm{H}}(t) &= a^{\dagger}e^{i\omega t} \end{aligned} \tag{2.39}$$

2.5 EXPECTATION WITH RESPECT TO COHERENT STATES

A coherent state for the SHO $H = \left(N + \frac{1}{2}\right)\hbar\omega$ was given by

$$a\left|z\right\rangle = z\left|z\right\rangle , \tag{2.40}$$

where we showed that

$$\left|z\right\rangle = c_0 e^{za^{\dagger}}\left|0\right\rangle . \tag{2.41}$$

In the Heisenberg picture we found

$$\begin{aligned} a_{\mathrm{H}}(t) &= e^{iHt/\hbar}ae^{-iHt/\hbar} = ae^{-i\omega t} \\ a^{\dagger}_{\mathrm{H}}(t) &= e^{iHt/\hbar}a^{\dagger}e^{-iHt/\hbar} = a^{\dagger}e^{i\omega t}. \end{aligned} \tag{2.42}$$

Recall that the position and momentum representation of the ladder operators was

$$\begin{aligned} a &= \frac{1}{\sqrt{2}}\left(\hat{x}\sqrt{\frac{m\omega}{\hbar}} + i\hat{p}\sqrt{\frac{1}{m\hbar\omega}}\right) \\ a^{\dagger} &= \frac{1}{\sqrt{2}}\left(\hat{x}\sqrt{\frac{m\omega}{\hbar}} - i\hat{p}\sqrt{\frac{1}{m\hbar\omega}}\right), \end{aligned} \tag{2.43}$$

or equivalently

$$\begin{aligned}\hat{x} &= \left(a + a^\dagger\right) \sqrt{\frac{\hbar}{2m\omega}} \\ \hat{p} &= i\left(a^\dagger - a\right) \sqrt{\frac{m\hbar\omega}{2}}.\end{aligned} \tag{2.44}$$

Given this we can compute expectation value of position operator

$$\begin{aligned}\langle z|\,\hat{x}\,|z\rangle &= \sqrt{\frac{\hbar}{2m\omega}} \langle z| \left(a + a^\dagger\right) |z\rangle \\ &= (z + z^*) \sqrt{\frac{\hbar}{2m\omega}} \\ &= 2\,\mathrm{Re}\, z \sqrt{\frac{\hbar}{2m\omega}}.\end{aligned} \tag{2.45}$$

Similarly

$$\begin{aligned}\langle z|\,\hat{p}\,|z\rangle &= i\sqrt{\frac{m\hbar\omega}{2}} \langle z| \left(a^\dagger - a\right) |z\rangle \\ &= \sqrt{\frac{m\hbar\omega}{2}} 2\,\mathrm{Im}\, z.\end{aligned} \tag{2.46}$$

How about the expectation of the Heisenberg position operator? That is

$$\begin{aligned}\langle z|\,\hat{x}_{\mathrm{H}}(t)\,|z\rangle &= \sqrt{\frac{\hbar}{2m\omega}} \langle z| \left(a + a^\dagger\right) |z\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}} \left(z e^{-i\omega t} + z^* e^{i\omega t}\right) \\ &= \sqrt{\frac{\hbar}{2m\omega}} \left((z + z^*)\cos(\omega t) - i\,(z - z^*)\sin(\omega t)\right) \\ &= \sqrt{\frac{\hbar}{2m\omega}} \left(\langle x(0)\rangle \sqrt{\frac{2m\omega}{\hbar}} \cos(\omega t) - i\,\langle p(0)\rangle\, i \sqrt{\frac{2m\omega}{\hbar}} \sin(\omega t)\right) \\ &= \langle x(0)\rangle \cos(\omega t) + \frac{\langle p(0)\rangle}{m\omega} \sin(\omega t).\end{aligned} \tag{2.47}$$

We find that the average of the Heisenberg position operator evolves in time in exactly the same fashion as position in the classical Harmonic oscillator. This phase space like trajectory is sketched in fig. 2.1.

In the text it is shown that we have the same structure for the Heisenberg operator itself, before taking expectations

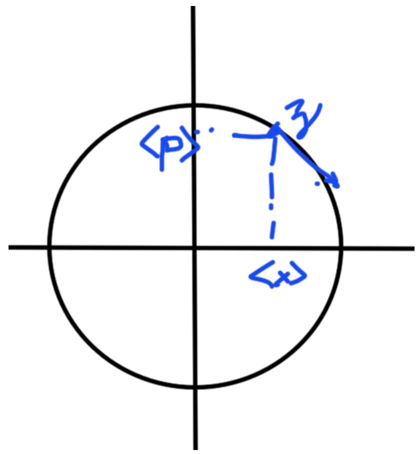

Figure 2.1: Phase space like trajectory.

$$\hat{x}_{\mathrm{H}}(t) = x(0)\cos(\omega t) + \frac{p(0)}{m\omega}\sin(\omega t). \tag{2.48}$$

Where the coherent states become useful is that we will see that the second moments of position and momentum are not time dependent with respect to the coherent states. Such states remain localized.

2.6 COHERENT STATE UNCERTAINTY

First note that using the commutator relationship we have

$$\begin{aligned} \langle z| aa^\dagger |z\rangle &= \langle z| \left(\left[a, a^\dagger \right] + a^\dagger a \right) |z\rangle \\ &= \langle z| \left(1 + a^\dagger a \right) |z\rangle . \end{aligned} \tag{2.49}$$

For the second moment we have

$$\begin{aligned} \langle z| \hat{x}^2 |z\rangle &= \frac{\hbar}{2m\omega} \langle z| \left(a + a^\dagger \right) \left(a + a^\dagger \right) |z\rangle \\ &= \frac{\hbar}{2m\omega} \langle z| \left(a^2 + (a^\dagger)^2 + aa^\dagger + a^\dagger a \right) |z\rangle \\ &= \frac{\hbar}{2m\omega} \langle z| \left(a^2 + (a^\dagger)^2 + 2a^\dagger a + 1 \right) |z\rangle \\ &= \frac{\hbar}{2m\omega} \left(z^2 + (z^*)^2 + 2z^* z + 1 \right) |z\rangle \\ &= \frac{\hbar}{2m\omega} (z + z^*)^2 + \frac{\hbar}{2m\omega}. \end{aligned} \tag{2.50}$$

We find

$$\sigma_x^2 = \frac{\hbar}{2m\omega}, \tag{2.51}$$

and

$$\sigma_p^2 = \frac{m\hbar\omega}{2} \tag{2.52}$$

so

$$\sigma_x^2\sigma_p^2 = \frac{\hbar^2}{4}, \tag{2.53}$$

or

$$\sigma_x\sigma_p = \frac{\hbar}{2}. \tag{2.54}$$

This is the minimum uncertainty.

2.7 QUANTUM FIELD THEORY

In Quantum Field theory the ideas of isolated oscillators is used to model particle creation. The lowest energy state (a no particle, vacuum state) is given the lowest energy level, with each additional quantum level modeling a new particle creation state as sketched in fig. 2.2.

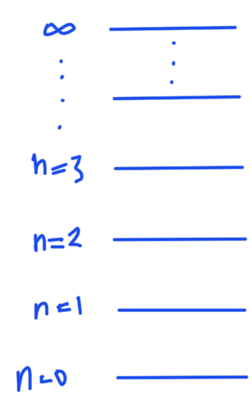

Figure 2.2: QFT energy levels.

We have to imagine many oscillators, each with a distinct vacuum energy $\sim \mathbf{k}^2$. The Harmonic oscillator can be used to model the creation of particles with $\hbar\omega$ energy differences from that "vacuum energy".

2.8 CHARGED PARTICLE IN A MAGNETIC FIELD

In the classical case (with SI units or $c = 1$) we have

$$\mathbf{F} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B}. \tag{2.55}$$

Alternately, we can look at the Hamiltonian view of the system, written in terms of potentials

$$\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}, \tag{2.56}$$

$$\mathbf{E} = -\boldsymbol{\nabla}\phi - \frac{\partial \mathbf{A}}{\partial t}. \tag{2.57}$$

Note that the curl form for the magnetic field implies one of the required Maxwell's equations $\boldsymbol{\nabla} \cdot \mathbf{B} = 0$.

Ignoring time dependence of the potentials, the Hamiltonian can be expressed as

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + q\phi. \tag{2.58}$$

In this Hamiltonian the vector $\mathbf{p}$ is called the canonical momentum, the momentum conjugate to position in phase space.

It is left as an exercise to show that the Lorentz force equation results from application of the Hamiltonian equations of motion, and that the velocity is given by $\mathbf{v} = (\mathbf{p} - q\mathbf{A})/m$.

For quantum mechanics, we use the same Hamiltonian, but promote our position, momentum and potentials to operators.

$$\hat{H} = \frac{1}{2m}\left(\hat{\mathbf{p}} - q\hat{\mathbf{A}}(\mathbf{r}, t)\right)^2 + q\hat{\phi}(\mathbf{r}, t). \tag{2.59}$$

2.9 GAUGE INVARIANCE

Can we say anything about this before looking at the question of a particle in a magnetic field?

Recall that the we can make a gauge transformation of the form

$$\mathbf{A} \rightarrow \mathbf{A} + \boldsymbol{\nabla}\chi \tag{2.60a}$$

$$\phi \rightarrow \phi - \frac{\partial \chi}{\partial t} \tag{2.60b}$$

Does this notion of gauge invariance also carry over to the Quantum Hamiltonian. After gauge transformation we have

$$\hat{H}' = \frac{1}{2m}(\hat{\mathbf{p}} - q\mathbf{A} - q\boldsymbol{\nabla}\chi)^2 + q\left(\phi - \frac{\partial \chi}{\partial t}\right) \tag{2.61}$$

Now we are in a mess, since this function χ can make the Hamiltonian horribly complicated. We don't see how gauge invariance can easily be applied to the quantum problem. Next time we will introduce a transformation that resolves some of this mess.

Particle with **E**, **B** *fields* We express our fields with vector and scalar potentials

$$\mathbf{E}, \mathbf{B} \rightarrow \mathbf{A}, \phi \tag{2.62}$$

and apply a gauge transformed Hamiltonian

$$H = \frac{1}{2m} (\mathbf{p} - q\mathbf{A})^2 + q\phi. \tag{2.63}$$

Recall that in classical mechanics we have

$$\mathbf{p} - q\mathbf{A} = m\mathbf{v} \tag{2.64}$$

where $\mathbf{p}$ is not gauge invariant, but the classical momentum $m\mathbf{v}$ is.

If given a point in phase space we must also specify the gauge that we are working with.

For the quantum case, temporarily considering a Hamiltonian without any scalar potential, but introducing a gauge transformation

$$\mathbf{A} \rightarrow \mathbf{A} + \boldsymbol{\nabla}\chi, \tag{2.65}$$

which takes the Hamiltonian from

$$H = \frac{1}{2m} (\mathbf{p} - q\mathbf{A})^2 , \tag{2.66}$$

to

$$H = \frac{1}{2m} (\mathbf{p} - q\mathbf{A} - q\boldsymbol{\nabla}\chi)^2 . \tag{2.67}$$

We care that the position and momentum operators obey

$$\left[\hat{r}_i, \hat{p}_j\right] = i\hbar\delta_{ij}. \tag{2.68}$$

We can apply a transformation that keeps $\mathbf{r}$ the same, but changes the momentum

$$\begin{aligned} \hat{\mathbf{r}}' &= \hat{\mathbf{r}} \\ \hat{\mathbf{p}}' &= \hat{\mathbf{p}} - q\boldsymbol{\nabla}\chi(\mathbf{r}) \end{aligned} \tag{2.69}$$

This maps the Hamiltonian to

$$H = \frac{1}{2m} (\mathbf{p}' - q\mathbf{A} - q\boldsymbol{\nabla}\chi)^2 , \tag{2.70}$$

We want to check if the commutator relationships have the desired structure, that is

$$\begin{aligned} \left[r_i', r_j'\right] &= 0 \\ \left[p_i', p_j'\right] &= 0 \end{aligned} \tag{2.71}$$

This is confirmed in exercise 2.3.

Another thing of interest is how are the wave functions altered by this change of variables? The wave functions must change in response to this transformation if the energies of the Hamiltonian are to remain the same.

Considering a plane wave specified by

$$e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{2.72}$$

where we alter the momentum by

$$\mathbf{k} \to \mathbf{k} - e\boldsymbol{\nabla}\chi. \tag{2.73}$$

This takes the plane wave to

$$e^{i(\mathbf{k}-q\boldsymbol{\nabla}\chi)\cdot\mathbf{r}}. \tag{2.74}$$

We want to try to find a wave function for the new Hamiltonian

$$H' = \frac{1}{2m}\left(\mathbf{p}' - q\mathbf{A} - q\boldsymbol{\nabla}\chi\right)^2, \tag{2.75}$$

of the form

$$\psi'(\mathbf{r}) \stackrel{?}{=} e^{i\theta(\mathbf{r})}\psi(\mathbf{r}), \tag{2.76}$$

where the new wave function differs from a wave function for the original Hamiltonian by only a position dependent phase factor.

Let's look at the action of the Hamiltonian on the new wave function

$$H'\psi'(\mathbf{r}). \tag{2.77}$$

Looking at just the first action

$$\begin{aligned}(-i\hbar\boldsymbol{\nabla} - q\mathbf{A} - q\boldsymbol{\nabla}\chi)\,e^{i\theta(\mathbf{r})}\psi(\mathbf{r}) &= e^{i\theta}\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A} - q\boldsymbol{\nabla}\chi\right)\psi(\mathbf{r}) + (-i\hbar i\boldsymbol{\nabla}\theta)\,e^{i\theta}\psi(\mathbf{r}) \\ &= e^{i\theta}\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A} - q\boldsymbol{\nabla}\chi + \hbar\boldsymbol{\nabla}\theta\right)\psi(\mathbf{r}).\end{aligned} \tag{2.78}$$

If we choose

$$\theta = \frac{q\chi}{\hbar}, \tag{2.79}$$

then we are left with

$$(-i\hbar\boldsymbol{\nabla} - q\mathbf{A} - q\boldsymbol{\nabla}\chi)\,e^{i\theta(\mathbf{r})}\psi(\mathbf{r}) = e^{i\theta}\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}\right)\psi(\mathbf{r}). \tag{2.80}$$

Let $\mathbf{M} = -i\hbar\boldsymbol{\nabla} - q\mathbf{A}$, and act again with $\left(-i\hbar\boldsymbol{\nabla} - q\mathbf{A} - q\boldsymbol{\nabla}\chi\right)$

$$
\begin{aligned}
(-i\hbar\boldsymbol{\nabla} - q\mathbf{A} - q\boldsymbol{\nabla}\chi)\, e^{i\theta}\mathbf{M}\psi &= e^{i\theta}\,(-i\hbar i\boldsymbol{\nabla}\theta - q\mathbf{A} - q\boldsymbol{\nabla}\chi)\, e^{i\theta}\mathbf{M}\psi + e^{i\theta}\,(-i\hbar\boldsymbol{\nabla})\,\mathbf{M}\psi \\
&= e^{i\theta}\,(-i\hbar\boldsymbol{\nabla} - q\mathbf{A} + \boldsymbol{\nabla}\,(\hbar\theta - q\chi))\,\mathbf{M}\psi \\
&= e^{i\theta}\mathbf{M}^2\psi.
\end{aligned}
\tag{2.81}
$$

Restoring factors of m, we've shown that for a choice of $\hbar\theta - q\chi$, we have

$$
\frac{1}{2m}\,(-i\hbar\boldsymbol{\nabla} - q\mathbf{A} - q\boldsymbol{\nabla}\chi)^2\, e^{i\theta}\psi = e^{i\theta}\frac{1}{2m}\,(-i\hbar\boldsymbol{\nabla} - q\mathbf{A})^2\,\psi.
\tag{2.82}
$$

When ψ is an energy eigenfunction, this means

$$
H' e^{i\theta}\psi = e^{i\theta}H\psi = e^{i\theta}E\psi = E(e^{i\theta}\psi).
\tag{2.83}
$$

We've found a transformation of the wave function that has the same energy eigenvalues as the corresponding wave functions for the original untransformed Hamiltonian.

In summary

$$
\boxed{
\begin{aligned}
H' &= \frac{1}{2m}\,(\mathbf{p} - q\mathbf{A} - q\boldsymbol{\nabla}\chi)^2 \\
\psi'(\mathbf{r}) &= e^{i\theta(\mathbf{r})}\psi(\mathbf{r}), \qquad \text{where } \theta(\mathbf{r}) = q\chi(\mathbf{r})/\hbar
\end{aligned}
}
\tag{2.84}
$$

Aharonov-Bohm effect Consider a periodic motion in a fixed ring as sketched in fig. 2.3.

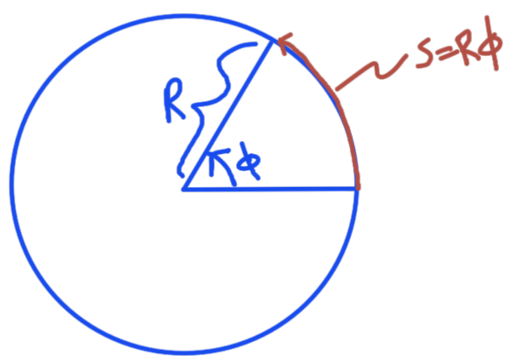

Figure 2.3: Particle confined to a ring.

Here the displacement around the perimeter is $s = R\phi$ and the Hamiltonian

$$
H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial s^2} = -\frac{\hbar^2}{2mR^2}\frac{\partial^2}{\partial \phi^2}.
\tag{2.85}
$$

Now assume that there is a magnetic field squeezed into the point at the origin, by virtue of a flux at the origin

$$\mathbf{B} = \Phi_0 \delta(\mathbf{r}) \hat{\mathbf{z}}. \tag{2.86}$$

We know that

$$\oint \mathbf{A} \cdot d\mathbf{l} = \Phi_0, \tag{2.87}$$

so that

$$\mathbf{A} = \frac{\Phi_0}{2\pi r} \hat{\boldsymbol{\phi}}. \tag{2.88}$$

The Hamiltonian for the new configuration is

$$H = -\left(-i\hbar \boldsymbol{\nabla} - q \frac{\Phi_0}{2\pi r} \hat{\boldsymbol{\phi}} \right)^2 = -\frac{1}{2m} \left(-i\hbar \frac{1}{R} \frac{\partial}{\partial \phi} - q \frac{\Phi_0}{2\pi R} \right)^2. \tag{2.89}$$

Here the replacement $r \rightarrow R$ makes use of the fact that this problem as been posed with the particle forced to move around the ring at the fixed radius R.

For this transformed Hamiltonian, what are the wave functions?

$$\psi(\phi)' \stackrel{?}{=} e^{in\phi}. \tag{2.90}$$

$$\begin{aligned} H\psi &= \frac{1}{2m} \left(-i\hbar \frac{1}{R}(in) - q \frac{\Phi_0}{2\pi R} \right)^2 e^{in\phi} \\ &= \underbrace{\boxed{\frac{1}{2m} \left(\frac{\hbar n}{R} - q \frac{\Phi_0}{2\pi R} \right)^2}}_{E_n} e^{in\phi}. \end{aligned} \tag{2.91}$$

This is very unclassical, since the energy changes in a way that depends on the flux, because particles are seeing magnetic fields that are not present at the point of the particle.

This is sketched in fig. 2.4.

we see that there are multiple points that the energies hit the minimum levels

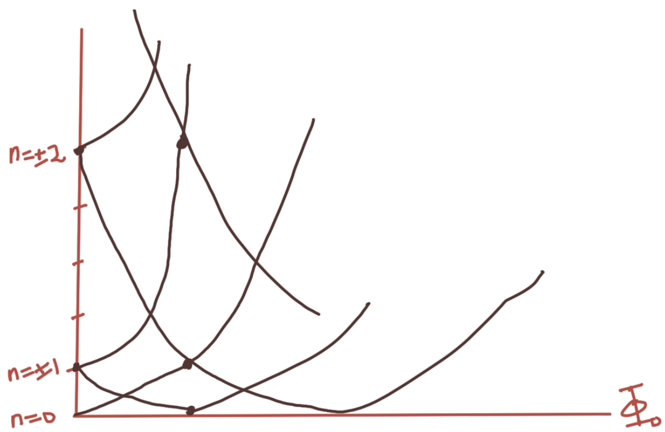

Figure 2.4: Energy variation with flux.

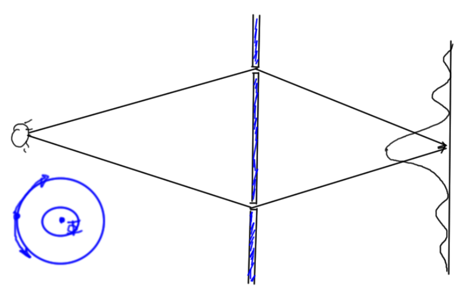

Figure 2.5: Two slit interference with magnetic whisker.

problem set note. In the problem set we'll look at interference patterns for two slit electron interference like that of fig. 2.5, where a magnetic whisker that introduces flux is added to the configuration.

Aharonov-Bohm effect (cont.) Why do we have the zeros at integral multiples of h/q? Consider a particle in a circular trajectory as sketched in fig. 2.6

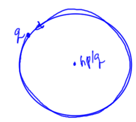

Figure 2.6: Circular trajectory.

FIXME: Prof mentioned:

$$\begin{aligned}\phi_{\text{loop}} &= q\frac{hp/q}{\hbar} \\ &= 2\pi p\end{aligned} \tag{2.92}$$

... I'm not sure what that was about now.

In classical mechanics we have

$$\oint p dq \tag{2.93}$$

The integral zero points are related to such a loop, but the $q\mathbf{A}$ portion of the momentum $\mathbf{p} - q\mathbf{A}$ needs to be considered.

Superconductors After cooling some materials sufficiently, superconductivity, a complete lack of resistance to electrical flow can be observed. A resistivity vs temperature plot of such a material is sketched in fig. 2.7.

Just like He^4 can undergo Bose condensation, superconductivity can be explained by a hybrid Bosonic state where electrons are paired into one state containing integral spin.

The Little-Parks experiment puts a superconducting ring around a magnetic whisker as sketched in fig. 2.8.

This experiment shows that the effective charge of the circulating charge was $2e$, validating the concept of Cooper-pairing, the Bosonic combination (integral spin) of electrons in superconduction.

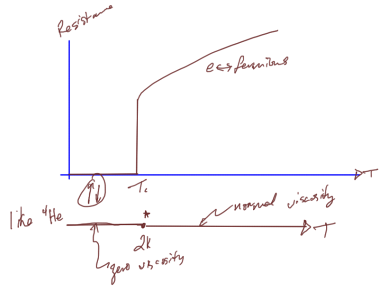

Figure 2.7: Superconductivity with comparison to superfluidity.

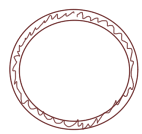

Figure 2.8: Little-Parks superconducting ring.

Motion around magnetic field

$$\omega_c = \frac{eB}{m} \tag{2.94}$$

We work with what is now called the Landau gauge

$$\mathbf{A} = (0, Bx, 0) \tag{2.95}$$

This gives

$$\begin{aligned}
\mathbf{B} &= \boldsymbol{\nabla} \times \mathbf{A} \\
&= \left(\partial_x A_y - \partial_y A_x\right) \hat{\mathbf{z}} \\
&= B\hat{\mathbf{z}}.
\end{aligned} \tag{2.96}$$

An alternate gauge choice, the symmetric gauge, is

$$\mathbf{A} = \left(-\frac{By}{2}, \frac{Bx}{2}, 0\right), \tag{2.97}$$

that also has the same magnetic field

$$\begin{aligned}
\mathbf{B} &= \boldsymbol{\nabla} \mathbf{A} \\
&= \left(\partial_x A_y - \partial_y A_x\right) \hat{\mathbf{z}} \\
&= \left(\frac{B}{2} - \left(-\frac{B}{2}\right)\right) \hat{\mathbf{z}} \\
&= B\hat{\mathbf{z}}.
\end{aligned} \tag{2.98}$$

We expect the physics for each to have the same results, although the wave functions in one gauge may be more complicated than in the other.

Our Hamiltonian is

$$\begin{aligned} H &= \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 \\ &= \frac{1}{2m}\hat{p}_x^2 + \frac{1}{2m}\left(\hat{p}_y - eB\hat{x}\right)^2 \end{aligned} \tag{2.99}$$

We can solve after noting that

$$\left[\hat{p}_y, H\right] = 0 \tag{2.100}$$

means that

$$\Psi(x, y) = e^{ik_y y}\phi(x) \tag{2.101}$$

The eigensystem

$$H\psi(x, y) = E\phi(x, y), \tag{2.102}$$

becomes

$$\left(\frac{1}{2m}\hat{p}_x^2 + \frac{1}{2m}\left(\hbar k_y - eB\hat{x}\right)^2\right)\phi(x) = E\phi(x). \tag{2.103}$$

This reduced Hamiltonian can be rewritten as

$$\begin{aligned} H_x &= \frac{1}{2m}p_x^2 + \frac{1}{2m}e^2B^2\left(\hat{x} - \frac{\hbar k_y}{eB}\right)^2 \\ &\equiv \frac{1}{2m}p_x^2 + \frac{1}{2}m\omega^2\left(\hat{x} - x_0\right)^2 \end{aligned} \tag{2.104}$$

where

$$\frac{1}{2m}e^2B^2 = \frac{1}{2}m\omega^2, \tag{2.105}$$

or

$$\begin{aligned} \omega &= \frac{eB}{m} \\ &\equiv \omega_{\mathrm{c}}. \end{aligned} \tag{2.106}$$

and

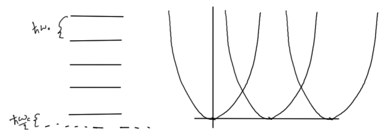

Figure 2.9: Energy levels, and Energy vs flux.

$$x_0 = \frac{\hbar}{k_y} eB. \tag{2.107}$$

But what is this x_0? Because k_y is not really specified in this problem, we can consider that we have a zero point energy for every k_y, but the oscillator position is shifted for every such value of k_y. For each set of energy levels fig. 2.9 we can consider that there is a different zero point energy for each possible k_y.

This is an infinitely degenerate system with an infinite number of states for any given energy level.

This tells us that there is a problem, and have to reconsider the assumption that any k_y is acceptable.

To resolve this we can introduce periodic boundary conditions, imagining that a square is rotated in space forming a cylinder as sketched in fig. 2.10.

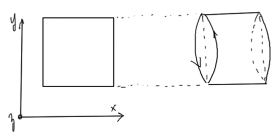

Figure 2.10: Landau degeneracy region.

Requiring quantized momentum

$$k_y L_y = 2\pi n, \tag{2.108}$$

or

$$k_y = \frac{2\pi n}{L_y}, \qquad n \in \mathbb{Z}, \tag{2.109}$$

gives

$$x_0(n) = \frac{\hbar}{eB} \frac{2\pi n}{L_y}, \tag{2.110}$$

with $x_0 \le L_x$. The range is thus restricted to

$$\frac{\hbar}{eB}\frac{2\pi n_{\text{max}}}{L_y} = L_x, \tag{2.111}$$

or

$$n_{\text{max}} = \underbrace{\boxed{L_x L_y}}_{\text{area}} \frac{eB}{2\pi\hbar} \tag{2.112}$$

That is

$$\begin{aligned} n_{\text{max}} &= \frac{\Phi_{\text{total}}}{h/e} \\ &= \frac{\Phi_{\text{total}}}{\Phi_0}. \end{aligned} \tag{2.113}$$

Attempting to measure Hall-effect systems, it was found that the Hall conductivity was quantized like

$$\sigma_{xy} = p\frac{e^2}{h}. \tag{2.114}$$

This quantization is explained by these Landau levels, and this experimental apparatus provides one of the more accurate ways to measure the fine structure constant.

2.10 DIAGONALIZATING THE QUANTUM HARMONIC OSCILLATOR

Many authors pull the definitions of the raising and lowering (or ladder) operators out of their butt with no attempt at motivation. This is pointed out nicely in [4] by Eli along with one justification based on factoring the Hamiltonian.

In [12] is a small exception to the usual presentation. In that text, these operators are defined as usual with no motivation. However, after the utility of these operators has been shown, the raising and lowering operators show up in a context that does provide that missing motivation as a side effect. It doesn't look like the author was trying to provide a motivation, but it can be interpreted that way.

When seeking the time evolution of Heisenberg-picture position and momentum operators, we will see that those solutions can be trivially expressed using the raising and lowering operators. No special tools nor black magic is required to find the structure of these operators. Unfortunately, we must first switch to both the Heisenberg picture representation of the position and momentum operators, and also employ the Heisenberg equations of motion. Neither of these last two fit into standard narrative of most introductory quantum mechanics treatments.

We will also see that these raising and lowering "operators" could also be introduced in classical mechanics, provided we were attempting to solve the SHO system using the Hamiltonian equations of motion.

I'll outline this route to finding the structure of the ladder operators below. Because these are encountered trying to solve the time evolution problem, I'll first show a simpler way to solve that problem. Because that simpler method depends a bit on lucky observation and is somewhat unstructured, I'll then outline a more structured procedure that leads to the ladder operators directly, also providing the solution to the time evolution problem as a side effect.

The starting point is the Heisenberg equations of motion. For a time independent Hamiltonian H, and a Heisenberg operator $A^{(H)}$, those equations are

$$\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}\left[A^{(H)}, H\right]. \tag{2.115}$$

Here the Heisenberg operator $A^{(H)}$ is related to the Schrödinger operator $A^{(S)}$ by

$$A^{(H)} = U^\dagger A^{(S)} U, \tag{2.116}$$

where U is the time evolution operator. For this discussion, we need only know that U commutes with H, and do not need to know the specific structure of that operator. In particular, the Heisenberg equations of motion take the form

$$\begin{aligned}\frac{dA^{(H)}}{dt} &= \frac{1}{i\hbar}\left[A^{(H)}, H\right] \\ &= \frac{1}{i\hbar}\left[U^\dagger A^{(S)} U, H\right] \\ &= \frac{1}{i\hbar}\left(U^\dagger A^{(S)} U H - H U^\dagger A^{(S)} U\right) \\ &= \frac{1}{i\hbar}\left(U^\dagger A^{(S)} H U - U^\dagger H A^{(S)} U\right) \\ &= \frac{1}{i\hbar} U^\dagger \left[A^{(S)}, H\right] U.\end{aligned} \tag{2.117}$$

The Hamiltonian for the harmonic oscillator, with Schrödinger-picture position and momentum operators x, p is

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2, \tag{2.118}$$

so the equations of motions are

$$
\begin{aligned}
\frac{dx^{(H)}}{dt} &= \frac{1}{i\hbar} U^\dagger \left[x, H \right] U \\
&= \frac{1}{i\hbar} U^\dagger \left[x, \frac{p^2}{2m} \right] U \\
&= \frac{1}{2mi\hbar} U^\dagger \left(i\hbar \frac{\partial p^2}{\partial p} \right) U \\
&= \frac{1}{m} U^\dagger p U \\
&= \frac{1}{m} p^{(H)},
\end{aligned}
\tag{2.119}
$$

and

$$
\begin{aligned}
\frac{dp^{(H)}}{dt} &= \frac{1}{i\hbar} U^\dagger \left[p, H \right] U \\
&= \frac{1}{i\hbar} U^\dagger \left[p, \frac{1}{2} m\omega^2 x^2 \right] U \\
&= \frac{m\omega^2}{2i\hbar} U^\dagger \left(-i\hbar \frac{\partial x^2}{\partial x} \right) U \\
&= -m\omega^2 U^\dagger x U \\
&= -m\omega^2 x^{(H)}.
\end{aligned}
\tag{2.120}
$$

In the Heisenberg picture the equations of motion are precisely those of classical Hamiltonian mechanics, except that we are dealing with operators instead of scalars

$$
\begin{aligned}
\frac{dp^{(H)}}{dt} &= -m\omega^2 x^{(H)} \\
\frac{dx^{(H)}}{dt} &= \frac{1}{m} p^{(H)}.
\end{aligned}
\tag{2.121}
$$

In the text the ladder operators are used to simplify the solution of these coupled equations, since they can decouple them. That's not really required since we can solve them directly in matrix form with little work

$$
\frac{d}{dt} \begin{bmatrix} p^{(H)} \\ x^{(H)} \end{bmatrix} = \begin{bmatrix} 0 & -m\omega^2 \\ \frac{1}{m} & 0 \end{bmatrix} \begin{bmatrix} p^{(H)} \\ x^{(H)} \end{bmatrix},
\tag{2.122}
$$

or, with length scaled variables

$$
\begin{aligned}
\frac{d}{dt}\begin{bmatrix} \frac{p^{(H)}}{m\omega} \\ x^{(H)} \end{bmatrix} &= \begin{bmatrix} 0 & -\omega \\ \omega & 0 \end{bmatrix}\begin{bmatrix} \frac{p^{(H)}}{m\omega} \\ x^{(H)} \end{bmatrix} \\
&= -i\omega \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} \frac{p^{(H)}}{m\omega} \\ x^{(H)} \end{bmatrix} \\
&= -i\omega\sigma_y \begin{bmatrix} \frac{p^{(H)}}{m\omega} \\ x^{(H)} \end{bmatrix}.
\end{aligned} \tag{2.123}
$$

Writing $y = \begin{bmatrix} \frac{p^{(H)}}{m\omega} \\ x^{(H)} \end{bmatrix}$, the solution can then be written immediately as

$$
\begin{aligned}
y(t) &= \exp\left(-i\omega\sigma_y t\right) y(0) \\
&= \left(\cos(\omega t)\, I - i\sigma_y \sin(\omega t)\right) y(0) \\
&= \begin{bmatrix} \cos(\omega t) & \sin(\omega t) \\ -\sin(\omega t) & \cos(\omega t) \end{bmatrix} y(0),
\end{aligned} \tag{2.124}
$$

or

$$
\begin{aligned}
\frac{p^{(H)}(t)}{m\omega} &= \cos(\omega t)\, \frac{p^{(H)}(0)}{m\omega} + \sin(\omega t)\, x^{(H)}(0) \\
x^{(H)}(t) &= -\sin(\omega t)\, \frac{p^{(H)}(0)}{m\omega} + \cos(\omega t)\, x^{(H)}(0).
\end{aligned} \tag{2.125}
$$

This solution depends on being lucky enough to recognize that the matrix has a Pauli matrix as a factor (which squares to unity, and allows the exponential to be evaluated easily.)

If we hadn't been that observant, then the first tool we'd have used instead would have been to diagonalize the matrix. For such diagonalization, it's natural to work in completely dimensionless variables. Such a non-dimensionalisation can be had by defining

$$
x_0 = \sqrt{\frac{\hbar}{m\omega}}, \tag{2.126}
$$

and dividing the working (operator) variables through by those values. Let $z = \frac{1}{x_0} y$, and $\tau = \omega t$ so that the equations of motion are

$$
\frac{dz}{d\tau} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} z. \tag{2.127}
$$

This matrix can be diagonalized as

$$
\begin{aligned}
A &= \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \\
&= V \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} V^{-1},
\end{aligned}
\tag{2.128}
$$

where

$$
V = \frac{1}{\sqrt{2}} \begin{bmatrix} i & -i \\ 1 & 1 \end{bmatrix}. \tag{2.129}
$$

The equations of motion can now be written

$$
\frac{d}{d\tau}\left(V^{-1}z\right) = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} \left(V^{-1}z\right). \tag{2.130}
$$

This final change of variables $V^{-1}z$ decouples the system as desired. Expanding that gives

$$
\begin{aligned}
V^{-1}z &= \frac{1}{\sqrt{2}} \begin{bmatrix} -i & 1 \\ i & 1 \end{bmatrix} \begin{bmatrix} \frac{p^{(H)}}{x_0 m\omega} \\ \frac{x^{(H)}}{x_0} \end{bmatrix} \\
&= \frac{1}{\sqrt{2}x_0} \begin{bmatrix} -i\frac{p^{(H)}}{m\omega} + x^{(H)} \\ i\frac{p^{(H)}}{m\omega} + x^{(H)} \end{bmatrix} \\
&= \begin{bmatrix} a^\dagger \\ a \end{bmatrix},
\end{aligned}
\tag{2.131}
$$

where

$$
\begin{aligned}
a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}} \left(-i\frac{p^{(H)}}{m\omega} + x^{(H)}\right) \\
a &= \sqrt{\frac{m\omega}{2\hbar}} \left(i\frac{p^{(H)}}{m\omega} + x^{(H)}\right).
\end{aligned}
\tag{2.132}
$$

Lo and behold, we have the standard form of the raising and lowering operators, and can write the system equations as

$$
\begin{aligned}
\frac{da^\dagger}{dt} &= i\omega a^\dagger \\
\frac{da}{dt} &= -i\omega a.
\end{aligned}
\tag{2.133}
$$

It is actually a bit fluky that this matched exactly, since we could have chosen eigenvectors that differ by constant phase factors, like

$$V = \frac{1}{\sqrt{2}} \begin{bmatrix} ie^{i\phi} & -ie^{i\psi} \\ 1e^{i\phi} & e^{i\psi} \end{bmatrix}, \tag{2.134}$$

so

$$\begin{aligned} V^{-1} z &= \frac{e^{-i(\phi+\psi)}}{\sqrt{2}} \begin{bmatrix} -ie^{i\psi} & e^{i\psi} \\ ie^{i\phi} & e^{i\phi} \end{bmatrix} \begin{bmatrix} \frac{p^{(H)}}{x_0 m\omega} \\ \frac{x^{(H)}}{x_0} \end{bmatrix} \\ &= \frac{1}{\sqrt{2} x_0} \begin{bmatrix} -ie^{i\phi} \frac{p^{(H)}}{m\omega} + e^{i\phi} x^{(H)} \\ ie^{i\psi} \frac{p^{(H)}}{m\omega} + e^{i\psi} x^{(H)} \end{bmatrix} \\ &= \begin{bmatrix} e^{i\phi} a^\dagger \\ e^{i\psi} a \end{bmatrix}. \end{aligned} \tag{2.135}$$

To make the resulting pairs of operators Hermitian conjugates, we'd want to constrain those constant phase factors by setting $\phi = -\psi$. If we were only interested in solving the time evolution problem no such additional constraints are required.

The raising and lowering operators are seen to naturally occur when seeking the solution of the Heisenberg equations of motion. This is found using the standard technique of non-dimensionalisation and then seeking a change of basis that diagonalizes the system matrix. Because the Heisenberg equations of motion are identical to the classical Hamiltonian equations of motion in this case, what we call the raising and lowering operators in quantum mechanics could also be utilized in the classical simple harmonic oscillator problem. However, in a classical context we wouldn't have a justification to call this more than a change of basis.

2.11 CONSTANT MAGNETIC SOLENOID FIELD

In [11] the following vector potential

$$\mathbf{A} = \frac{B\rho_a^2}{2\rho} \hat{\boldsymbol{\phi}}, \tag{2.136}$$

is introduced in a discussion on the Aharonov-Bohm effect, for configurations where the interior field of a solenoid is either a constant $\mathbf{B}$ or zero.

I wasn't able to make sense of this since the field I was calculating was zero for all $\rho \neq 0$

$$
\begin{aligned}
\mathbf{B} &= \boldsymbol{\nabla} \times \mathbf{A} \\
&= \left(\hat{\boldsymbol{\rho}} \partial_\rho + \hat{\mathbf{z}} \partial_z + \frac{\hat{\boldsymbol{\phi}}}{\rho} \partial_\phi \right) \times \frac{B \rho_a^2}{2\rho} \hat{\boldsymbol{\phi}} \\
&= \left(\hat{\boldsymbol{\rho}} \partial_\rho + \frac{\hat{\boldsymbol{\phi}}}{\rho} \partial_\phi \right) \times \frac{B \rho_a^2}{2\rho} \hat{\boldsymbol{\phi}} \\
&= \frac{B \rho_a^2}{2} \hat{\boldsymbol{\rho}} \times \hat{\boldsymbol{\phi}} \partial_\rho \left(\frac{1}{\rho} \right) + \frac{B \rho_a^2}{2\rho} \frac{\hat{\boldsymbol{\phi}}}{\rho} \times \partial_\phi \hat{\boldsymbol{\phi}} \\
&= \frac{B \rho_a^2}{2\rho^2} \left(-\hat{\mathbf{z}} + \hat{\boldsymbol{\phi}} \times \partial_\phi \hat{\boldsymbol{\phi}} \right).
\end{aligned}
\tag{2.137}
$$

Note that the ρ partial requires that $\rho \neq 0$. To expand the cross product in the second term let $j = \mathbf{e}_1 \mathbf{e}_2$, and expand using a Geometric Algebra representation of the unit vector

$$
\begin{aligned}
\hat{\boldsymbol{\phi}} \times \partial_\phi \hat{\boldsymbol{\phi}} &= \mathbf{e}_2 e^{j\phi} \times \left(\mathbf{e}_2 \mathbf{e}_1 \mathbf{e}_2 e^{j\phi} \right) \\
&= -\mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3 \left\langle \mathbf{e}_2 e^{j\phi} (-\mathbf{e}_1) e^{j\phi} \right\rangle_2 \\
&= \mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3 \mathbf{e}_2 \mathbf{e}_1 \\
&= \mathbf{e}_3 \\
&= \hat{\mathbf{z}}.
\end{aligned}
\tag{2.138}
$$

So, provided $\rho \neq 0$, $\mathbf{B} = 0$.

The errata [10] provides the clarification, showing that a $\rho > \rho_a$ constraint is required for this potential to produce the desired results. Continuity at $\rho = \rho_a$ means that in the interior (or at least on the boundary) we must have one of

$$
\mathbf{A} = \frac{B \rho_a}{2} \hat{\boldsymbol{\phi}},
\tag{2.139}
$$

or

$$
\mathbf{A} = \frac{B \rho}{2} \hat{\boldsymbol{\phi}}.
\tag{2.140}
$$

The first doesn't work, but the second does

$$
\begin{aligned}
\mathbf{B} &= \boldsymbol{\nabla} \times \mathbf{A} \\
&= \left(\hat{\boldsymbol{\rho}} \partial_\rho + \hat{\mathbf{z}} \partial_z + \frac{\hat{\boldsymbol{\phi}}}{\rho} \partial_\phi \right) \times \frac{B \rho}{2} \hat{\boldsymbol{\phi}} \\
&= \frac{B}{2} \hat{\boldsymbol{\rho}} \times \hat{\boldsymbol{\phi}} + \frac{B \rho}{2} \frac{\hat{\boldsymbol{\phi}}}{\rho} \times \partial_\phi \hat{\boldsymbol{\phi}} \\
&= B \hat{\mathbf{z}}.
\end{aligned}
\tag{2.141}
$$

So the vector potential that we want for a constant $B\hat{\mathbf{z}}$ field in the interior $\rho < \rho_a$ of a cylindrical space, we need

$$\mathbf{A} = \begin{cases} \frac{B\rho_a^2}{2\rho}\hat{\boldsymbol{\phi}} & \text{if } \rho \geq \rho_a \\ \frac{B\rho}{2}\hat{\boldsymbol{\phi}} & \text{if } \rho < \rho_a. \end{cases} \tag{2.142}$$

An example of the magnitude of potential is graphed in fig. 2.11.

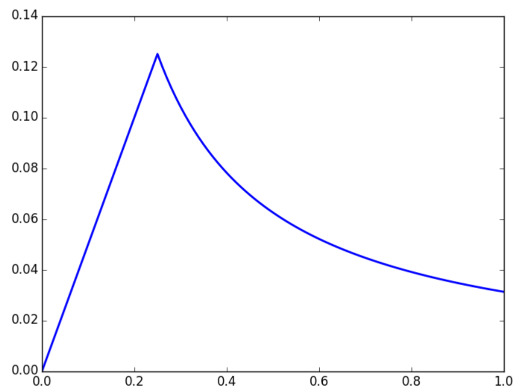

Figure 2.11: Vector potential for constant field in cylindrical region.

2.12 LAGRANGIAN FOR MAGNETIC PORTION OF LORENTZ FORCE

In [11] it is claimed in an Aharonov-Bohm discussion that a Lagrangian modification to include electromagnetism is

$$\mathcal{L} \rightarrow \mathcal{L} + \frac{e}{c}\mathbf{v} \cdot \mathbf{A}. \tag{2.143}$$

That can't be the full Lagrangian since there is no ϕ term, so what exactly do we get?

If you have somehow, like I did, forgot the exact form of the Euler-Lagrange equations (i.e. where do the dots go), then the derivation of those equations can come to your rescue. The starting point is the action

$$S = \int \mathcal{L}(x, \dot{x}, t)dt, \tag{2.144}$$

where the end points of the integral are fixed, and we assume we have no variation at the end points. The variational calculation is

$$
\begin{aligned}
\delta S &= \int \delta \mathcal{L}(x, \dot{x}, t) dt \\
&= \int \left(\frac{\partial \mathcal{L}}{\partial x} \delta x + \frac{\partial \mathcal{L}}{\partial \dot{x}} \delta \dot{x} \right) dt \\
&= \int \left(\frac{\partial \mathcal{L}}{\partial x} \delta x + \frac{\partial \mathcal{L}}{\partial \dot{x}} \delta \frac{dx}{dt} \right) dt \\
&= \int \left(\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{x}} \right) \right) \delta x dt + \delta x \frac{\partial \mathcal{L}}{\partial \dot{x}} .
\end{aligned}
\tag{2.145}
$$

The boundary term is killed after evaluation at the end points where the variation is zero. For the result to hold for all variations δx, we must have

$$
\boxed{\frac{\partial \mathcal{L}}{\partial x} = \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{x}} \right).}
\tag{2.146}
$$

Now lets apply this to the Lagrangian at hand. For the position derivative we have

$$
\frac{\partial \mathcal{L}}{\partial x_i} = \frac{e}{c} v_j \frac{\partial A_j}{\partial x_i} .
\tag{2.147}
$$

For the canonical momentum term, assuming $\mathbf{A} = \mathbf{A}(\mathbf{x})$ we have

$$
\begin{aligned}
\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}_i} &= \frac{d}{dt} \left(m \dot{x}_i + \frac{e}{c} A_i \right) \\
&= m \ddot{x}_i + \frac{e}{c} \frac{d A_i}{dt} \\
&= m \ddot{x}_i + \frac{e}{c} \frac{\partial A_i}{\partial x_j} \frac{d x_j}{dt} .
\end{aligned}
\tag{2.148}
$$

Assembling the results, we've got

$$
\begin{aligned}
0 &= \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}_i} - \frac{\partial \mathcal{L}}{\partial x_i} \\
&= m \ddot{x}_i + \frac{e}{c} \frac{\partial A_i}{\partial x_j} \frac{d x_j}{dt} - \frac{e}{c} v_j \frac{\partial A_j}{\partial x_i} ,
\end{aligned}
\tag{2.149}
$$

or

$$
\begin{aligned}
m \ddot{x}_i &= \frac{e}{c} v_j \frac{\partial A_j}{\partial x_i} - \frac{e}{c} \frac{\partial A_i}{\partial x_j} v_j \\
&= \frac{e}{c} v_j \left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j} \right) \\
&= \frac{e}{c} v_j B_k \epsilon_{ijk} .
\end{aligned}
\tag{2.150}
$$

In vector form that is

$$\boxed{m\ddot{\mathbf{x}} = \frac{e}{c}\mathbf{v} \times \mathbf{B}.} \tag{2.151}$$

So, we get the magnetic term of the Lorentz force. Also note that this shows the Lagrangian (and the end result), was not in SI units. The $1/c$ term would have to be dropped for SI.

2.13 PROBLEMS

Exercise 2.1 Lorentz force from classical electrodynamic Hamiltonian.

Given the classical Hamiltonian

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + q\phi. \tag{2.152}$$

apply the Hamiltonian equations of motion

$$\begin{aligned}\frac{d\mathbf{p}}{dt} &= -\frac{\partial H}{\partial \mathbf{q}} \\ \frac{d\mathbf{q}}{dt} &= \frac{\partial H}{\partial \mathbf{p}},\end{aligned} \tag{2.153}$$

to show that this is the Hamiltonian that describes the Lorentz force equation, and to find the velocity in terms of the canonical momentum and vector potential.

Answer for Exercise 2.1

The particle velocity follows easily

$$\begin{aligned}\mathbf{v} &= \frac{d\mathbf{r}}{dt} \\ &= \frac{\partial H}{\partial \mathbf{p}} \\ &= \frac{1}{m}(\mathbf{p} - q\mathbf{A}).\end{aligned} \tag{2.154}$$

For the Lorentz force we can proceed in the coordinate representation

$$\begin{aligned}\frac{dp_k}{dt} &= -\frac{\partial H}{\partial x_k} \\ &= -\frac{2}{2m}(p_m - qA_m)\frac{\partial}{\partial x_k}(p_m - qA_m) - q\frac{\partial \phi}{\partial x_k} \\ &= qv_m\frac{\partial A_m}{\partial x_k} - q\frac{\partial \phi}{\partial x_k},\end{aligned} \tag{2.155}$$

We also have

$$\begin{aligned}\frac{dp_k}{dt} &= \frac{d}{dt}(mx_k + qA_k) \\ &= m\frac{d^2x_k}{dt^2} + q\frac{\partial A_k}{\partial x_m}\frac{dx_m}{dt} + q\frac{\partial A_k}{\partial t}.\end{aligned} \tag{2.156}$$

Putting these together we've got

$$\begin{aligned}m\frac{d^2x_k}{dt^2} &= qv_m\frac{\partial A_m}{\partial x_k} - q\frac{\partial \phi}{\partial x_k}, -q\frac{\partial A_k}{\partial x_m}\frac{dx_m}{dt} - q\frac{\partial A_k}{\partial t} \\ &= qv_m\left(\frac{\partial A_m}{\partial x_k} - \frac{\partial A_k}{\partial x_m}\right) + qE_k \\ &= qv_m\epsilon_{kms}B_s + qE_k,\end{aligned} \tag{2.157}$$

or

$$\begin{aligned}m\frac{d^2\mathbf{x}}{dt^2} &= q\mathbf{e}_k v_m\epsilon_{kms}B_s + qE_k \\ &= q\mathbf{v}\times\mathbf{B} + q\mathbf{E}.\end{aligned} \tag{2.158}$$

Exercise 2.2 Show gauge invariance of the magnetic and electric fields.

After the gauge transformation of eq. (2.60) show that the electric and magnetic fields are unaltered.

Answer for Exercise 2.2

For the magnetic field the transformed field is

$$\begin{aligned}\mathbf{B}' &= \boldsymbol{\nabla}\times(\mathbf{A} + \boldsymbol{\nabla}\chi) \\ &= \boldsymbol{\nabla}\times\mathbf{A} + \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\chi) \\ &= \boldsymbol{\nabla}\times\mathbf{A} \\ &= \mathbf{B}.\end{aligned} \tag{2.159}$$

$$\begin{aligned}\mathbf{E}' &= -\frac{\partial \mathbf{A}'}{\partial t} - \boldsymbol{\nabla}\phi' \\ &= -\frac{\partial}{\partial t}(\mathbf{A} + \boldsymbol{\nabla}\chi) - \boldsymbol{\nabla}\left(\phi - \frac{\partial \chi}{\partial t}\right) \\ &= -\frac{\partial \mathbf{A}}{\partial t} - \boldsymbol{\nabla}\phi \\ &= \mathbf{E}.\end{aligned} \tag{2.160}$$

Exercise 2.3 Gauge transformation.

Show that after a transformation of position and momentum of the following form

$$
\begin{aligned}
\hat{\mathbf{r}}' &= \hat{\mathbf{r}} \\
\hat{\mathbf{p}}' &= \hat{\mathbf{p}} - q\boldsymbol{\nabla}\chi(\mathbf{r})
\end{aligned}
\tag{2.161}
$$

all the commutators have the expected values.

Answer for Exercise 2.3

The position commutators don't need consideration. Of interest is the momentum-position commutators

$$
\begin{aligned}
\left[\hat{p}'_k, \hat{x}'_k\right] &= \left[\hat{p}_k - q\partial_k\chi, \hat{x}_k\right] \\
&= \left[\hat{p}_k, \hat{x}_k\right] - q\left[\partial_k\chi, \hat{x}_k\right] \\
&= \left[\hat{p}_k, \hat{x}_k\right],
\end{aligned}
\tag{2.162}
$$

and the momentum commutators

$$
\begin{aligned}
\left[\hat{p}'_k, \hat{p}'_j\right] &= \left[\hat{p}_k - q\partial_k\chi, \hat{p}_j - q\partial_j\chi\right] \\
&= \left[\hat{p}_k, \hat{p}_j\right] - q\left(\left[\partial_k\chi, \hat{p}_j\right] + \left[\hat{p}_k, \partial_j\chi\right]\right).
\end{aligned}
\tag{2.163}
$$

That last sum of commutators is

$$
\begin{aligned}
\left[\partial_k\chi, \hat{p}_j\right] + \left[\hat{p}_k, \partial_j\chi\right] &= -i\hbar\left(\frac{\partial(\partial_j\chi)}{\partial k} - \frac{\partial(\partial_k\chi)}{\partial j}\right) \\
&= 0.
\end{aligned}
\tag{2.164}
$$

We've shown that

$$
\begin{aligned}
\left[\hat{p}'_k, \hat{x}'_k\right] &= \left[\hat{p}_k, \hat{x}_k\right] \\
\left[\hat{p}'_k, \hat{p}'_j\right] &= \left[\hat{p}_k, \hat{p}_j\right].
\end{aligned}
\tag{2.165}
$$

All the other commutators clearly have the desired transformation properties.

Exercise 2.4 Heisenberg picture spin precession. ([11] *pr. 2.1*)

For the spin Hamiltonian

$$
\begin{aligned}
H &= -\frac{eB}{mc}S_z \\
&= \omega S_z,
\end{aligned}
\tag{2.166}
$$

express and solve the Heisenberg equations of motion for $S_x(t)$, $S_y(t)$, and $S_z(t)$.

Answer for Exercise 2.4

The equations of motion are of the form

$$\begin{aligned}
\frac{dS_i^{\mathrm{H}}}{dt} &= \frac{1}{i\hbar}\left[S_i^{\mathrm{H}}, H\right] \\
&= \frac{1}{i\hbar}\left[U^\dagger S_i U, H\right] \\
&= \frac{1}{i\hbar}\left(U^\dagger S_i U H - H U^\dagger S_i U\right) \\
&= \frac{1}{i\hbar} U^\dagger \left(S_i H - H S_i\right) U \\
&= \frac{\omega}{i\hbar} U^\dagger \left[S_i, S_z\right] U.
\end{aligned} \tag{2.167}$$

These are

$$\begin{aligned}
\frac{dS_x^{\mathrm{H}}}{dt} &= -\omega U^\dagger S_y U \\
\frac{dS_y^{\mathrm{H}}}{dt} &= \omega U^\dagger S_x U \\
\frac{dS_z^{\mathrm{H}}}{dt} &= 0.
\end{aligned} \tag{2.168}$$

To completely specify these equations, we need to expand $U(t)$, which is

$$\begin{aligned}
U(t) &= e^{-iHt/\hbar} \\
&= e^{-i\omega S_z t/\hbar} \\
&= e^{-i\omega \sigma_z t/2} \\
&= \cos(\omega t/2) - i\sigma_z \sin(\omega t/2) \\
&= \begin{bmatrix} \cos(\omega t/2) - i\sin(\omega t/2) & 0 \\ 0 & \cos(\omega t/2) + i\sin(\omega t/2) \end{bmatrix} \\
&= \begin{bmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2} \end{bmatrix}.
\end{aligned} \tag{2.169}$$

The equations of motion can now be written out in full. To do so seems a bit silly since we also know that $S_x^{\mathrm{H}} = U^\dagger S_x U, S_y^{\mathrm{H}} U^\dagger S_x U$. However, if that is temporarily forgotten, we can show that the Heisenberg equations of motion can be solved for these too.

$$
\begin{aligned}
U^\dagger S_x U &= \frac{\hbar}{2}\begin{bmatrix} e^{i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2}\end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0\end{bmatrix}\begin{bmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2}\end{bmatrix} \\
&= \frac{\hbar}{2}\begin{bmatrix} 0 & e^{i\omega t/2} \\ e^{-i\omega t/2} & 0\end{bmatrix}\begin{bmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2}\end{bmatrix} \\
&= \frac{\hbar}{2}\begin{bmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0\end{bmatrix},
\end{aligned} \tag{2.170}
$$

and

$$
\begin{aligned}
U^\dagger S_y U &= \frac{\hbar}{2}\begin{bmatrix} e^{i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2}\end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0\end{bmatrix}\begin{bmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2}\end{bmatrix} \\
&= \frac{i\hbar}{2}\begin{bmatrix} 0 & -e^{i\omega t/2} \\ e^{-i\omega t/2} & 0\end{bmatrix}\begin{bmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2}\end{bmatrix} \\
&= \frac{i\hbar}{2}\begin{bmatrix} 0 & -e^{i\omega t} \\ e^{-i\omega t} & 0\end{bmatrix}.
\end{aligned} \tag{2.171}
$$

The equations of motion are now fully specified

$$
\begin{aligned}
\frac{dS_x^{\mathrm{H}}}{dt} &= -\frac{i\hbar\omega}{2}\begin{bmatrix} 0 & -e^{i\omega t} \\ e^{-i\omega t} & 0\end{bmatrix} \\
\frac{dS_y^{\mathrm{H}}}{dt} &= \frac{\hbar\omega}{2}\begin{bmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0\end{bmatrix} \\
\frac{dS_z^{\mathrm{H}}}{dt} &= 0.
\end{aligned} \tag{2.172}
$$

Integration gives

$$
\begin{aligned}
S_x^{\mathrm{H}} &= \frac{\hbar}{2}\begin{bmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0\end{bmatrix} + C \\
S_y^{\mathrm{H}} &= \frac{\hbar}{2}\begin{bmatrix} 0 & -ie^{i\omega t} \\ ie^{-i\omega t} & 0\end{bmatrix} + C \\
S_z^{\mathrm{H}} &= C.
\end{aligned} \tag{2.173}
$$

The integration constants are fixed by the boundary condition $S_i^{\mathrm{H}}(0) = S_i$, so

$$
\begin{aligned}
S_x^{\mathrm{H}} &= \frac{\hbar}{2} \begin{bmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{bmatrix} \\
S_y^{\mathrm{H}} &= \frac{i\hbar}{2} \begin{bmatrix} 0 & -e^{i\omega t} \\ e^{-i\omega t} & 0 \end{bmatrix} \\
S_z^{\mathrm{H}} &= S_z.
\end{aligned}
\tag{2.174}
$$

Observe that these integrated values $S_x^{\mathrm{H}}, S_y^{\mathrm{H}}$ match eq. (2.170), and eq. (2.171) as expected.

Exercise 2.5 Dynamics of non-Hermitian Hamiltonian. (*[11] pr. 2.2*)

Revisiting an earlier Hamiltonian, but assuming it was entered incorrectly as

$$
H = H_{11} \left|1\right\rangle \left\langle 1\right| + H_{22} \left|2\right\rangle \left\langle 2\right| + H_{12} \left|1\right\rangle \left\langle 2\right|. \tag{2.175}
$$

What principle is now violated? Illustrate your point explicitly by attempting to solve the most general time-dependent problem using an illegal Hamiltonian of this kind. You may assume that $H_{11} = H_{22}$ for simplicity.

Answer for Exercise 2.5

In matrix form this Hamiltonian is

$$
\begin{aligned}
H &= \begin{bmatrix} \left\langle 1\right| H \left|1\right\rangle & \left\langle 1\right| H \left|2\right\rangle \\ \left\langle 2\right| H \left|1\right\rangle & \left\langle 2\right| H \left|2\right\rangle \end{bmatrix} \\
&= \begin{bmatrix} H_{11} & H_{12} \\ 0 & H_{22} \end{bmatrix}.
\end{aligned}
\tag{2.176}
$$

This is not a Hermitian operator. What is the physical implication of this non-Hermicity? Consider the simpler case where $H_{11} = H_{22}$. Such a Hamiltonian has the form

$$
H = \begin{bmatrix} a & b \\ 0 & a \end{bmatrix}. \tag{2.177}
$$

This has only one unique eigenvector ($(1, 0)$, but we can still solve the time evolution equation

$$
i\hbar \frac{\partial U}{\partial t} = HU, \tag{2.178}
$$

since for constant H, we have

$$
U = e^{-iHt/\hbar}. \tag{2.179}
$$

To exponentiate, note that we have

$$\begin{bmatrix} a & b \\ 0 & a \end{bmatrix}^n = \begin{bmatrix} a^n & na^{n-1}b \\ 0 & a^n \end{bmatrix}. \tag{2.180}$$

To prove the induction, the $n = 2$ case follows easily

$$\begin{bmatrix} a & b \\ 0 & a \end{bmatrix}\begin{bmatrix} a & b \\ 0 & a \end{bmatrix} = \begin{bmatrix} a^2 & 2ab \\ 0 & a^2 \end{bmatrix}, \tag{2.181}$$

as does the general case

$$\begin{bmatrix} a^n & na^{n-1}b \\ 0 & a^n \end{bmatrix}\begin{bmatrix} a & b \\ 0 & a \end{bmatrix} = \begin{bmatrix} a^{n+1} & (n+1)a^n b \\ 0 & a^{n+1} \end{bmatrix}. \tag{2.182}$$

The exponential sum is thus

$$e^{H\tau} = \begin{bmatrix} e^{a\tau} & 0 + \frac{b\tau}{1!} + \frac{2ab\tau^2}{2!} + \frac{3a^2b\tau^3}{3!} + \cdots \\ 0 & e^{a\tau} \end{bmatrix}. \tag{2.183}$$

That sum simplifies to

$$\begin{aligned} &\frac{b\tau}{0!} + \frac{ab\tau^2}{1!} + \frac{a^2b\tau^3}{2!} + \cdots \\ &\quad = b\tau\left(1 + \frac{a\tau}{1!} + \frac{(a\tau)^2}{2!} + \cdots\right) \\ &\quad = b\tau e^{a\tau}. \end{aligned} \tag{2.184}$$

The exponential is thus

$$\begin{aligned} e^{H\tau} &= \begin{bmatrix} e^{a\tau} & b\tau e^{a\tau} \\ 0 & e^{a\tau} \end{bmatrix} \\ &= \begin{bmatrix} 1 & b\tau \\ 0 & 1 \end{bmatrix} e^{a\tau}. \end{aligned} \tag{2.185}$$

In particular

$$\begin{aligned} U &= e^{-iHt/\hbar} \\ &= \begin{bmatrix} 1 & -ibt/\hbar \\ 0 & 1 \end{bmatrix} e^{-iat/\hbar}. \end{aligned} \tag{2.186}$$

We can verify that this is a solution to eq. (2.178). The left hand side is

$$
\begin{aligned}
i\hbar\frac{\partial U}{\partial t} &= i\hbar \begin{bmatrix} -ia/\hbar & -ib/\hbar + (-ibt/\hbar)(-ia/\hbar) \\ 0 & -ia/\hbar \end{bmatrix} e^{-iat/\hbar} \\
&= \begin{bmatrix} a & b - iabt/\hbar \\ 0 & a \end{bmatrix} e^{-iat/\hbar},
\end{aligned}
\tag{2.187}
$$

and for the right hand side

$$
\begin{aligned}
HU &= \begin{bmatrix} a & b \\ 0 & a \end{bmatrix} \begin{bmatrix} 1 & -ibt/\hbar \\ 0 & 1 \end{bmatrix} e^{-iat/\hbar} \\
&= \begin{bmatrix} a & b - iabt/\hbar \\ 0 & a \end{bmatrix} e^{-iat/\hbar} \\
&= i\hbar\frac{\partial U}{\partial t}. \qquad \square
\end{aligned}
\tag{2.188}
$$

While the Schrödinger is satisfied, we don't have the unitary inversion physical property that is desired for the time evolution operator U. Namely

$$
\begin{aligned}
U^\dagger U &= \begin{bmatrix} 1 & 0 \\ ibt/\hbar & 1 \end{bmatrix} e^{iat/\hbar} \begin{bmatrix} 1 & -ibt/\hbar \\ 0 & 1 \end{bmatrix} e^{-iat/\hbar} \\
&= \begin{bmatrix} 1 & -ibt/\hbar \\ ibt/\hbar & (bt)^2/\hbar^2 \end{bmatrix} \ne I.
\end{aligned}
\tag{2.189}
$$

We required $U^\dagger U = I$ for the time evolution operator, but don't have that property for this non-Hermitian Hamiltonian.

Exercise 2.6 Time evolution of spin half probability and dispersion. ([11] pr. 2.3)

A spin 1/2 system $\mathbf{S}\cdot\hat{\mathbf{n}}$, with $\hat{\mathbf{n}} = \sin\beta\hat{\mathbf{x}} + \cos\beta\hat{\mathbf{z}}$, is in state with eigenvalue $\hbar/2$, acted on by a magnetic field of strength B in the $+z$ direction.

a. If S_x is measured at time t, what is the probability of getting $+\hbar/2$?

b. Evaluate the dispersion in S_x as a function of t, that is,

$$
\left\langle (S_x - \langle S_x \rangle)^2 \right\rangle.
\tag{2.190}
$$

c. Check your answers for $\beta \rightarrow 0, \pi/2$ to see if they make sense.

Answer for Exercise 2.6

Part a. The spin operator in matrix form is

$$\begin{aligned}
S \cdot \hat{\mathbf{n}} &= \frac{\hbar}{2} (\sigma_z \cos\beta + \sigma_x \sin\beta) \\
&= \frac{\hbar}{2} \left(\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \cos\beta + \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \sin\beta \right) \\
&= \frac{\hbar}{2} \begin{bmatrix} \cos\beta & \sin\beta \\ \sin\beta & -\cos\beta \end{bmatrix}.
\end{aligned} \tag{2.191}$$

The $|S \cdot \hat{\mathbf{n}}; +\rangle$ eigenstate is found from

$$(S \cdot \hat{\mathbf{n}} - \hbar/2) \begin{bmatrix} a \\ b \end{bmatrix} = 0, \tag{2.192}$$

or

$$\begin{aligned}
0 &= (\cos\beta - 1)\, a + \sin\beta b \\
&= \left(-2\sin^2(\beta/2)\right) a + 2\sin(\beta/2)\cos(\beta/2) b \\
&= (-\sin(\beta/2))\, a + \cos(\beta/2) b,
\end{aligned} \tag{2.193}$$

or

$$|S \cdot \hat{\mathbf{n}}; +\rangle = \begin{bmatrix} \cos(\beta/2) \\ \sin(\beta/2) \end{bmatrix}. \tag{2.194}$$

The Hamiltonian is

$$H = -\frac{eB}{mc} S_z = -\frac{eB\hbar}{2mc} \sigma_z, \tag{2.195}$$

so the time evolution operator is

$$\begin{aligned}
U &= e^{-iHt/\hbar} \\
&= e^{\frac{ieBt}{2mc}\sigma_z}.
\end{aligned} \tag{2.196}$$

Let $\omega = eB/(2mc)$, so

$$\begin{aligned}
U &= e^{i\sigma_z \omega t} \\
&= \cos(\omega t) + i\sigma_z \sin(\omega t) \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \cos(\omega t) + i \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \sin(\omega t) \\
&= \begin{bmatrix} e^{i\omega t} & 0 \\ 0 & e^{-i\omega t} \end{bmatrix}.
\end{aligned} \tag{2.197}$$

The time evolution of the initial state is

$$
\begin{aligned}
|S \cdot \hat{\mathbf{n}}; +\rangle (t) &= U \, |S \cdot \hat{\mathbf{n}}; +\rangle (0) \\
&= \begin{bmatrix} e^{i\omega t} & 0 \\ 0 & e^{-i\omega t} \end{bmatrix} \begin{bmatrix} \cos(\beta/2) \\ \sin(\beta/2) \end{bmatrix} \\
&= \begin{bmatrix} \cos(\beta/2) e^{i\omega t} \\ \sin(\beta/2) e^{-i\omega t} \end{bmatrix}.
\end{aligned} \tag{2.198}
$$

The probability of finding the state in $|S \cdot \hat{\mathbf{x}}; +\rangle$ at time t (i.e. measuring S_x and finding $\hbar/2$) is

$$
\begin{aligned}
|\langle S \cdot \hat{\mathbf{x}}; + | S \cdot \hat{\mathbf{n}}; +\rangle|^2 &= \left| \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} \cos(\beta/2) e^{i\omega t} \\ \sin(\beta/2) e^{-i\omega t} \end{bmatrix} \right|^2 \\
&= \frac{1}{2} \left| \cos(\beta/2) e^{i\omega t} + \sin(\beta/2) e^{-i\omega t} \right|^2 \\
&= \frac{1}{2} \left(1 + 2 \cos(\beta/2) \sin(\beta/2) \cos(2\omega t) \right) \\
&= \frac{1}{2} \left(1 + \sin(\beta) \cos(2\omega t) \right).
\end{aligned} \tag{2.199}
$$

Part b. To calculate the dispersion first note that

$$
\begin{aligned}
S_x^2 &= \left(\frac{\hbar}{2} \right)^2 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}^2 \\
&= \left(\frac{\hbar}{2} \right)^2,
\end{aligned} \tag{2.200}
$$

so only the first order expectation is non-trivial to calculate. That is

$$
\begin{aligned}
\langle S_x \rangle &= \frac{\hbar}{2} \begin{bmatrix} \cos(\beta/2) e^{-i\omega t} & \sin(\beta/2) e^{i\omega t} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \cos(\beta/2) e^{i\omega t} \\ \sin(\beta/2) e^{-i\omega t} \end{bmatrix} \\
&= \frac{\hbar}{2} \begin{bmatrix} \cos(\beta/2) e^{-i\omega t} & \sin(\beta/2) e^{i\omega t} \end{bmatrix} \begin{bmatrix} \sin(\beta/2) e^{-i\omega t} \\ \cos(\beta/2) e^{i\omega t} \end{bmatrix} \\
&= \frac{\hbar}{2} \sin(\beta/2) \cos(\beta/2) \left(e^{-2i\omega t} + e^{2i\omega t} \right) \\
&= \frac{\hbar}{2} \sin\beta \cos(2\omega t).
\end{aligned} \tag{2.201}
$$

This gives

$$\boxed{\left\langle (\Delta S_x)^2 \right\rangle = \left(\frac{\hbar}{2}\right)^2 \left(1 - \sin^2\beta \cos^2(2\omega t)\right)} \tag{2.202}$$

Part c. For $\beta = 0$, $\hat{\mathbf{n}} = \hat{\mathbf{z}}$, and $\beta = \pi/2$, $\hat{\mathbf{n}} = \hat{\mathbf{x}}$. For the first case, the state is in an eigenstate of S_z, so must evolve as

$$|S \cdot \hat{\mathbf{n}}; +\rangle (t) = |S \cdot \hat{\mathbf{n}}; +\rangle (0) e^{i\omega t}. \tag{2.203}$$

The probability of finding it in state $|S \cdot \hat{\mathbf{x}}; +\rangle$ is therefore

$$\begin{aligned}
\left| \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} e^{i\omega t} \\ 0 \end{bmatrix} \right|^2 &= \frac{1}{2} \left| e^{i\omega t} \right|^2 \\
&= \frac{1}{2} \\
&= \frac{1}{2} \left(1 + \sin(0) \cos(2\omega t)\right).
\end{aligned} \tag{2.204}$$

This matches eq. (2.199) as expected.
For $\beta = \pi/2$ we have

$$\begin{aligned}
|S \cdot \hat{\mathbf{x}}; +\rangle (t) &= \frac{1}{\sqrt{2}} \begin{bmatrix} e^{i\omega t} & 0 \\ 0 & e^{-i\omega t} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\
&= \frac{1}{\sqrt{2}} \begin{bmatrix} e^{i\omega t} \\ e^{-i\omega t} \end{bmatrix}.
\end{aligned} \tag{2.205}$$

The probability for the $\hbar/2$ S_x measurement at time t is

$$\begin{aligned}
\left| \frac{1}{2} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} e^{i\omega t} \\ e^{-i\omega t} \end{bmatrix} \right|^2 &= \frac{1}{4} \left| e^{i\omega t} + e^{-i\omega t} \right|^2 \\
&= \cos^2(\omega t) \\
&= \frac{1}{2} \left(1 + \sin(\pi/2) \cos(2\omega t)\right).
\end{aligned} \tag{2.206}$$

Again, this matches the expected value.
For the dispersions, at $\beta = 0$, the dispersion is

$$\left(\frac{\hbar}{2}\right)^2 \tag{2.207}$$

This is the maximum dispersion, which makes sense since we are measuring S_x when the initial state is $|S \cdot \hat{\mathbf{z}}; +\rangle$. For $\beta = \pi/2$ the dispersion is

$$\left(\frac{\hbar}{2}\right)^2 \sin^2(2\omega t). \tag{2.208}$$

This starts off as zero dispersion (because the initial state is $|S \cdot \hat{\mathbf{x}}; +\rangle$, but then oscillates.

Exercise 2.7 Heisenberg picture position commutator. (*[11] pr. 2.5*)

Evaluate

$$[x(t), x(0)]\,, \tag{2.209}$$

for a Heisenberg picture operator $x(t)$ for a free particle.

Answer for Exercise 2.7

The free particle Hamiltonian is

$$H = \frac{p^2}{2m}, \tag{2.210}$$

so the time evolution operator is

$$U(t) = e^{-ip^2 t/(2m\hbar)}. \tag{2.211}$$

The Heisenberg picture position operator is

$$
\begin{aligned}
x^{\mathrm{H}} &= U^\dagger x U \\
&= e^{ip^2 t/(2m\hbar)} x e^{-ip^2 t/(2m\hbar)} \\
&= \sum_{k=0}^\infty \frac{1}{k!} \left(\frac{ip^2 t}{2m\hbar}\right)^k x e^{-ip^2 t/(2m\hbar)} \\
&= \sum_{k=0}^\infty \frac{1}{k!} \left(\frac{it}{2m\hbar}\right)^k p^{2k} x e^{-ip^2 t/(2m\hbar)} \\
&= \sum_{k=0}^\infty \frac{1}{k!} \left(\frac{it}{2m\hbar}\right)^k \left(\left[p^{2k}, x\right] + x p^{2k}\right) e^{-ip^2 t/(2m\hbar)} \\
&= x + \sum_{k=0}^\infty \frac{1}{k!} \left(\frac{it}{2m\hbar}\right)^k \left[p^{2k}, x\right] e^{-ip^2 t/(2m\hbar)} \\
&= x + \sum_{k=0}^\infty \frac{1}{k!} \left(\frac{it}{2m\hbar}\right)^k \left(-i\hbar \frac{\partial p^{2k}}{\partial p}\right) e^{-ip^2 t/(2m\hbar)} \\
&= x + \sum_{k=0}^\infty \frac{1}{k!} \left(\frac{it}{2m\hbar}\right)^k \left(-i\hbar 2k p^{2k-1}\right) e^{-ip^2 t/(2m\hbar)} \\
&= x + -2i\hbar p \frac{it}{2m\hbar} \sum_{k=1}^\infty \frac{1}{(k-1)!} \left(\frac{it}{2m\hbar}\right)^{k-1} p^{2(k-1)} e^{-ip^2 t/(2m\hbar)} \\
&= x + t\frac{p}{m}.
\end{aligned}
\tag{2.212}
$$

This has the structure of a classical free particle $x(t) = x + vt$, but in this case x, p are operators.

The evolved position commutator is

$$
\begin{aligned}
[x(t), x(0)] &= [x + tp/m, x] \\
&= \frac{t}{m}[p, x] \\
&= -i\hbar \frac{t}{m}.
\end{aligned}
\tag{2.213}
$$

Compare this to the classical Poisson bracket

$$
\begin{aligned}
[x(t), x(0)]_{\text{classical}} &= \frac{\partial}{\partial x}(x + pt/m)\frac{\partial x}{\partial p} - \frac{\partial}{\partial p}(x + pt/m)\frac{\partial x}{\partial x} \\
&= -\frac{t}{m}.
\end{aligned}
\tag{2.214}
$$

This has the expected relation $\left[x(t), x(0)\right] = i\hbar \left[x(t), x(0)\right]_{\text{classical}}$.

Exercise 2.8 Virial theorem. (*phy1520 2015 ps2.2*)

Consider a three-dimensional Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}). \tag{2.215}$$

a. Calculate $[\mathbf{x} \cdot \mathbf{p}, H]$ and show that

$$\frac{d}{dt} \langle \mathbf{x} \cdot \mathbf{p} \rangle = \left\langle \frac{\mathbf{p}^2}{m} \right\rangle - \langle \mathbf{x} \cdot \boldsymbol{\nabla} V \rangle . \tag{2.216}$$

When the l.h.s. vanishes, the result that the r.h.s. is zero is called the quantum virial theorem.

b. Consider the 3D isotropic harmonic oscillator, and show explicitly that its eigenstates obey the virial theorem.

c. Evaluate the r.h.s. for the superposition state $|0, 0, 0\rangle + |0, 0, 2\rangle$ where the notation stands for $\left|n_x, n_y, n_z\right\rangle$ occupation numbers.

d. Under what conditions does the left-hand side vanish?

Answer for Exercise 2.8

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Exercise 2.9 A symmetric real Hamiltonian. (*[11] pr. 2.9*)

Find the time evolution for the state $|a'\rangle$ for a Hamiltonian of the form

$$H = \delta \left(\left|a'\right\rangle \left\langle a'\right| + \left|a''\right\rangle \left\langle a''\right| \right) \tag{2.217}$$

Answer for Exercise 2.9

This Hamiltonian has the matrix representation

$$H = \begin{bmatrix} 0 & \delta \\ \delta & 0 \end{bmatrix}, \tag{2.218}$$

which has a characteristic equation of

$$\lambda^2 - \delta^2 = 0, \tag{2.219}$$

so the energy eigenvalues are $\pm\delta$.
The diagonal basis states are respectively

$$|\pm\delta\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} \pm 1 \\ 1 \end{bmatrix}. \tag{2.220}$$

The time evolution operator is

$$\begin{aligned}
U &= e^{-iHt/\hbar} \\
&= e^{-i\delta t/\hbar} |+\delta\rangle \langle +\delta| + e^{i\delta t/\hbar} |-\delta\rangle \langle -\delta| \\
&= \frac{e^{-i\delta t/\hbar}}{2} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{e^{i\delta t/\hbar}}{2} \begin{bmatrix} -1 & 1 \end{bmatrix} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \\
&= \frac{e^{-i\delta t/\hbar}}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \frac{e^{i\delta t/\hbar}}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \\
&= \begin{bmatrix} \cos(\delta t/\hbar) & -i\sin(\delta t/\hbar) \\ -i\sin(\delta t/\hbar) & \cos(\delta t/\hbar) \end{bmatrix}.
\end{aligned} \tag{2.221}$$

The desired time evolution in the original basis is

$$\begin{aligned}
\left|a', t\right\rangle &= e^{-iHt/\hbar} \left|a', 0\right\rangle \\
&= \begin{bmatrix} \cos(\delta t/\hbar) & -i\sin(\delta t/\hbar) \\ -i\sin(\delta t/\hbar) & \cos(\delta t/\hbar) \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\
&= \begin{bmatrix} \cos(\delta t/\hbar) \\ -i\sin(\delta t/\hbar) \end{bmatrix} \\
&= \cos(\delta t/\hbar) \left|a', 0\right\rangle - i\sin(\delta t/\hbar) \left|a'', 0\right\rangle.
\end{aligned} \tag{2.222}$$

This evolution has the same structure as left circularly polarized light.
The probability of finding the system in state $|a''\rangle$ given an initial state of $|a', 0\rangle$ is

$$\begin{aligned}
P &= \left|\left\langle a'' \middle| a', t\right\rangle\right|^2 \\
&= \sin^2(\delta t/\hbar).
\end{aligned} \tag{2.223}$$

Exercise 2.10 SHO translation operator expectation. (*[11] pr. 2.12*)

Using the Heisenberg picture evaluate the expectation of the position operator $\langle x \rangle$ with respect to the initial time state

$$|\alpha, 0\rangle = e^{-ip_0 a/\hbar} |0\rangle, \tag{2.224}$$

where p_0 is the initial time position operator, and a is a constant with dimensions of position.

Answer for Exercise 2.10

Recall that the Heisenberg picture position operator expands to

$$\begin{aligned} x^{\mathrm{H}}(t) &= U^\dagger x U \\ &= x_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t), \end{aligned} \tag{2.225}$$

so the expectation of the position operator is

$$\begin{aligned} \langle x \rangle &= \langle 0| e^{ip_0 a/\hbar} \left(x_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t) \right) e^{-ip_0 a/\hbar} |0\rangle \\ &= \langle 0| \left(e^{ip_0 a/\hbar} x_0 \cos(\omega t) e^{-ip_0 a/\hbar} \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t) \right) |0\rangle . \end{aligned} \tag{2.226}$$

The exponential sandwich above can be expanded using the Baker-Campbell-Hausdorff [15] formula

$$\begin{aligned} e^{ip_0 a/\hbar} x_0 e^{-ip_0 a/\hbar} &= x_0 + \frac{ia}{\hbar} [p_0, x_0] + \frac{1}{2!} \left(\frac{ia}{\hbar} \right)^2 [p_0, [p_0, x_0]] + \cdots \\ &= x_0 + \frac{ia}{\hbar} (-i\hbar) + \frac{1}{2!} \left(\frac{ia}{\hbar} \right)^2 [p_0, -i\hbar] + \cdots \\ &= x_0 + a. \end{aligned} \tag{2.227}$$

The position expectation with respect to this translated state is

$$\begin{aligned} \langle x \rangle &= \langle 0| \left((x_0 + a) \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t) \right) |0\rangle \\ &= a \cos(\omega t). \end{aligned} \tag{2.228}$$

The final simplification above follows from $\langle n| x |n\rangle = \langle n| p |n\rangle = 0$.

Exercise 2.11 Expectations for SHO Hamiltonian, and virial theorem. (*[11] pr. 2.14*)

a. For a 1D SHO, compute $\langle m| x |n\rangle$, $\langle m| x^2 |n\rangle$, $\langle m| p |n\rangle$, $\langle m| p^2 |n\rangle$ and $\langle m| \{x, p\} |n\rangle$.

b. Verify the virial theorem is satisfied for energy eigenstates.

Answer for Exercise 2.11

Part a. Using

$$
\begin{aligned}
x &= \frac{x_0}{\sqrt{2}}\left(a + a^\dagger\right) \\
p &= \frac{i\hbar}{x_0\sqrt{2}}\left(a^\dagger - a\right) \\
a(t) &= a(0)e^{-i\omega t} \\
a(0)\left|n\right\rangle &= \sqrt{n}\left|n-1\right\rangle \\
a^\dagger(0)\left|n\right\rangle &= \sqrt{n+1}\left|n+1\right\rangle \\
x_0^2 &= \frac{\hbar}{\omega m},
\end{aligned}
\tag{2.229}
$$

we have

$$
\begin{aligned}
\left\langle m\right| x \left|n\right\rangle &= \frac{x_0}{\sqrt{2}}\left\langle m\right|\left(a + a^\dagger\right)\left|n\right\rangle \\
&= \frac{x_0}{\sqrt{2}}\left\langle m\right|\left(e^{-i\omega t}\sqrt{n}\left|n-1\right\rangle + e^{i\omega t}\sqrt{n+1}\left|n+1\right\rangle\right) \\
&= \frac{x_0}{\sqrt{2}}\left(\delta_{m,n-1}e^{-i\omega t}\sqrt{n} + \delta_{m,n+1}e^{i\omega t}\sqrt{n+1}\right),
\end{aligned}
\tag{2.230}
$$

$$
\begin{aligned}
\left\langle m\right| x^2 \left|n\right\rangle &= \frac{x_0^2}{2}\left\langle m\right|\left(a + a^\dagger\right)^2\left|n\right\rangle \\
&= \frac{x_0^2}{2}\left(e^{i\omega t}\sqrt{m}\left\langle m-1\right| + e^{-i\omega t}\sqrt{m+1}\left\langle m+1\right|\right)\left(e^{-i\omega t}\sqrt{n}\left|n-1\right\rangle + e^{i\omega t}\sqrt{n+1}\left|n+1\right\rangle\right) \\
&= \frac{x_0^2}{2}\left(\delta_{m+1,n+1}\sqrt{(m+1)(n+1)}\right. \\
&\quad \left. + \delta_{m+1,n-1}\sqrt{(m+1)n}e^{-2i\omega t} + \delta_{m-1,n+1}\sqrt{m(n+1)}e^{2i\omega t} + \delta_{m-1,n-1}\sqrt{mn}\right),
\end{aligned}
\tag{2.231}
$$

$$
\begin{aligned}
\left\langle m\right| p \left|n\right\rangle &= \frac{i\hbar}{\sqrt{2}x_0}\left\langle m\right|\left(a^\dagger - a\right)\left|n\right\rangle \\
&= \frac{i\hbar}{\sqrt{2}x_0}\left\langle m\right|\left(e^{i\omega t}\sqrt{n+1}\left|n+1\right\rangle - e^{-i\omega t}\sqrt{n}\left|n-1\right\rangle\right) \\
&= \frac{i\hbar}{\sqrt{2}x_0}\left(\delta_{m,n+1}e^{i\omega t}\sqrt{n+1} - \delta_{m,n-1}e^{-i\omega t}\sqrt{n}\right),
\end{aligned}
\tag{2.232}
$$

$$
\begin{aligned}
\langle m| p^2 |n\rangle &= \frac{\hbar^2}{2x_0^2} |m\rangle \left(a - a^\dagger\right)\left(a^\dagger - a\right)|n\rangle \\
&= \frac{\hbar^2}{2x_0^2}\left(-e^{-i\omega t}\sqrt{m+1}\,\langle m+1| + e^{i\omega t}\sqrt{m}\,\langle m-1|\right)\left(e^{i\omega t}\sqrt{n+1}\,|n+1\rangle - e^{-i\omega t}\sqrt{n}\,|n-1\rangle\right) \\
&= \frac{\hbar^2}{2x_0^2}\left(\delta_{m+1,n+1}\sqrt{(m+1)(n+1)}\right. \\
&\left. + \delta_{m+1,n-1}\sqrt{(m+1)n}e^{-2i\omega t} + \delta_{m-1,n+1}\sqrt{m(n+1)}e^{2i\omega t} + \delta_{m-1,n-1}\sqrt{mn}\right).
\end{aligned}
\tag{2.233}
$$

For the anticommutator $\{x, p\}$, we have

$$
\begin{aligned}
\{x, p\} &= \frac{i\hbar}{2}\left(\left(ae^{-i\omega t} + a^\dagger e^{i\omega t}\right)\left(a^\dagger e^{i\omega t} - ae^{-i\omega t}\right) - \left(a^\dagger e^{i\omega t} - ae^{-i\omega t}\right)\left(ae^{-i\omega t} + a^\dagger e^{i\omega t}\right)\right) \\
&= \frac{i\hbar}{2}\left(-a^2e^{-2i\omega t} + (a^\dagger)^2e^{2i\omega t} + aa^\dagger - a^\dagger a + a^2e^{-2i\omega t} - (a^\dagger)^2e^{2i\omega t} - a^\dagger a + aa^\dagger\right) \\
&= i\hbar\left(aa^\dagger - a^\dagger a\right),
\end{aligned}
\tag{2.234}
$$

so

$$
\begin{aligned}
\langle m| \{x, p\} |n\rangle &= i\hbar\,\langle m|\left(aa^\dagger - a^\dagger a\right)|n\rangle \\
&= i\hbar\,\langle m|\left(\sqrt{(n+1)^2}\,|n\rangle - \sqrt{n^2}\,|n\rangle\right) \\
&= i\hbar\,\langle m|(2n+1)|n\rangle.
\end{aligned}
\tag{2.235}
$$

Part b. For the SHO, the virial theorem requires $\left\langle p^2/m\right\rangle = \left\langle m\omega x^2\right\rangle$. That momentum expectation with respect to the eigenstate $|n\rangle$ is

$$
\left\langle p^2/m\right\rangle = \frac{\hbar^2}{2x_0^2 m}\left(\sqrt{(n+1)(n+1)} + \sqrt{nn}\right) = \frac{\hbar^2 m\omega}{2\hbar m}(2n+1) = \hbar\omega\left(n + \frac{1}{2}\right).
\tag{2.236}
$$

For the position expectation we've got

$$
\begin{aligned}
\left\langle m\omega x^2\right\rangle &= \frac{m\omega^2 x_0^2}{2}\left(\sqrt{(n+1)(n+1)} + \sqrt{nn}\right) \\
&= \frac{m\omega^2\hbar}{2m\omega}\left(\sqrt{(n+1)(n+1)} + \sqrt{nn}\right) \\
&= \frac{\omega\hbar}{2}(2n+1) \\
&= \omega\hbar\left(n + \frac{1}{2}\right).
\end{aligned}
\tag{2.237}
$$

This shows that the virial theorem holds for the SHO Hamiltonian for eigenstates.

Exercise 2.12 Momentum space representation of Schrödinger equation. ([11] pr. 2.15)

Using

$$\langle x' | p' \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ip'x'/\hbar}, \tag{2.238}$$

show that

$$\langle p' | x | \alpha \rangle = i\hbar \frac{\partial}{\partial p'} \langle p' | \alpha \rangle . \tag{2.239}$$

Use this to find the momentum space representation of the Schrödinger equation for the one dimensional SHO and the energy eigenfunctions in their momentum representation.

Answer for Exercise 2.12

To expand the matrix element, introduce both momentum and position space identity operators

$$\begin{aligned}
\langle p' | x | \alpha \rangle &= \int dx' dp'' \langle p' | x' \rangle \langle x' | x | p'' \rangle \langle p'' | \alpha \rangle \\
&= \int dx' dp'' \langle p' | x' \rangle x' \langle x' | p'' \rangle \langle p'' | \alpha \rangle \\
&= \frac{1}{2\pi\hbar} \int dx' dp'' e^{-ip'x'/\hbar} x' e^{ip''x'/\hbar} \langle p'' | \alpha \rangle \\
&= \frac{1}{2\pi\hbar} \int dx' dp'' x' e^{i(p''-p')x'/\hbar} \langle p'' | \alpha \rangle \\
&= \frac{1}{2\pi\hbar} \int dx' dp'' \frac{d}{dp''} \left(\frac{-i\hbar^{i(p''-p')x'/\hbar}}{e} \right) \langle p'' | \alpha \rangle \\
&= i\hbar \int dp'' \left(\frac{1}{2\pi\hbar} \int dx' e^{i(p''-p')x'/\hbar} \right) \frac{d}{dp''} \langle p'' | \alpha \rangle \\
&= i\hbar \int dp'' \delta(p'' - p') \frac{d}{dp''} \langle p'' | \alpha \rangle \\
&= i\hbar \frac{d}{dp'} \langle p' | \alpha \rangle . \qquad \square
\end{aligned} \tag{2.240}$$

Schrödinger's equation for a time dependent state $|\alpha\rangle = U(t) |\alpha, 0\rangle$ is

$$i\hbar \frac{\partial}{\partial t} |\alpha\rangle = H |\alpha\rangle , \tag{2.241}$$

with the momentum representation

$$i\hbar \frac{\partial}{\partial t} \langle p' | \alpha \rangle = \langle p' | H | \alpha \rangle . \tag{2.242}$$

Expansion of the Hamiltonian matrix element for a strictly spatial dependent potential $V(x)$ gives

$$\begin{aligned}\langle p'\right| H \left|\alpha\rangle &= \langle p'\right| \left(\frac{p^2}{2m} + V(x)\right) \left|\alpha\rangle\\ &= \frac{(p')^2}{2m} + \langle p'\right| V(x) \left|\alpha\rangle .\end{aligned} \tag{2.243}$$

Assuming a Taylor representation of the potential $V(x) = \sum c_k x^k$, we want to calculate

$$\langle p'| V(x) |\alpha\rangle = \sum c_k \langle p'| x^k |\alpha\rangle . \tag{2.244}$$

With $|\alpha\rangle = |p''\rangle$ eq. (2.239) provides the $k = 1$ term

$$\begin{aligned}\langle p'| x |p''\rangle &= i\hbar \frac{d}{dp'} \langle p'|p''\rangle\\ &= i\hbar \frac{d}{dp'} \delta(p' - p''),\end{aligned} \tag{2.245}$$

where it is implied here that the derivative is operating on not just the delta function, but on all else that follows.

Using this the higher powers of $\langle p'| x^k |\alpha\rangle$ can be found easily. For example for $k = 2$ we have

$$\begin{aligned}\langle p'| x^2 |\alpha\rangle &= \int dp'' \langle p'| x |p''\rangle \langle p''| x |\alpha\rangle\\ &= \int dp'' i\hbar \frac{d}{dp'} \delta(p' - p'') i\hbar \frac{d}{dp''} \langle p''|\alpha\rangle\\ &= (i\hbar)^2 \frac{d^2}{d(p')^2} \langle p'|\alpha\rangle .\end{aligned} \tag{2.246}$$

This means that the potential matrix element is

$$\begin{aligned}\langle p'| V(x) |\alpha\rangle &= \sum c_k \left(i\hbar \frac{d}{dp'}\right)^k \langle p'|\alpha\rangle\\ &= V\left(i\hbar \frac{d}{dp'}\right).\end{aligned} \tag{2.247}$$

Writing $\Psi_\alpha(p') = \langle p'|\alpha\rangle$, the momentum space representation of Schrödinger's equation for a position dependent potential is

$$\boxed{i\hbar \frac{\partial}{\partial t} \Psi_\alpha(p') = \left(\frac{(p')^2}{2m} + V\left(i\hbar\partial/\partial p'\right)\right) \Psi_\alpha(p').} \tag{2.248}$$

For the SHO Hamiltonian the potential is $V(x) = (1/2)m\omega^2 x^2$, so the Schrödinger equation is

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Psi_\alpha(p') &= \left(\frac{(p')^2}{2m} - \frac{1}{2}m\omega^2\hbar^2\frac{\partial^2}{\partial(p')^2}\right)\Psi_\alpha(p') \\ &= \frac{1}{2m}\left((p')^2 - m^2\omega^2\hbar^2\frac{\partial^2}{\partial(p')^2}\right)\Psi_\alpha(p'). \end{aligned} \tag{2.249}$$

To determine the wave functions, let's non-dimensionalize this and compare to the position space Schrödinger equation. Let

$$p_0^2 = m\omega\hbar, \tag{2.250}$$

so

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Psi_\alpha(p') &= \frac{p_0^2}{2m}\left(\left(\frac{p'}{p_0}\right)^2 - \frac{\partial^2}{\partial(p'/p_0)^2}\right)\Psi_\alpha(p') \\ &= \frac{\omega\hbar}{2}\left(-\frac{\partial^2}{\partial(p'/p_0)^2} + \left(\frac{p'}{p_0}\right)^2\right)\Psi_\alpha(p'). \end{aligned} \tag{2.251}$$

Compare this to the position space equation with $x_0^2 = m\omega/\hbar$,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Psi_\alpha(x') &= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial(x')^2} + \frac{1}{2}m\omega^2(x')^2\right)\Psi_\alpha(x') \\ &= \frac{\hbar^2}{2m}\left(-\frac{\partial^2}{\partial(x')^2} + \frac{m^2\omega^2}{\hbar^2}(x')^2\right)\Psi_\alpha(x') \\ &= \frac{\hbar^2 x_0^2}{2m}\left(-\frac{\partial^2}{\partial(x'/x_0)^2} + \left(\frac{x'}{x_0}\right)^2\right)\Psi_\alpha(x') \\ &= \frac{\hbar\omega}{2}\left(-\frac{\partial^2}{\partial(x'/x_0)^2} + \left(\frac{x'}{x_0}\right)^2\right)\Psi_\alpha(x'). \end{aligned} \tag{2.252}$$

It's clear that there is a straightforward duality relationship between the respective wave functions. Since

$$\langle x' | n \rangle = \frac{1}{\pi^{1/4}\sqrt{2^n n!}\, x_0^{n+1/2}}\left(x' - x_0^2\frac{d}{dx'}\right)^n \exp\left(-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right), \tag{2.253}$$

the momentum space wave functions are

$$\langle p' | n \rangle = \frac{1}{\pi^{1/4}\sqrt{2^n n!}\, p_0^{n+1/2}}\left(p' - p_0^2\frac{d}{dp'}\right)^n \exp\left(-\frac{1}{2}\left(\frac{p'}{p_0}\right)^2\right). \tag{2.254}$$

Exercise 2.13 **Correlation function.** (*phy1520 2015 ps2.3*)

Consider $\langle x(0)x(t)\rangle$ and $\langle p(0)p(t)\rangle$ where operators are in the Heisenberg representation. These are called correlation functions. Evaluate this for the 1D harmonic oscillator in an energy eigenstate $|n\rangle$.

Answer for Exercise 2.13

PROBLEM SET RELATED MATERIAL REDACTED IN THIS DOCUMENT.PLEASE FEEL FREE TO EMAIL ME FOR THE FULL VERSION IF YOU AREN'T TAKING PHY1520. [redacted]. END-REDACTION

Exercise 2.14 **1D SHO linear superposition that maximizes expectation.** (*[11] pr. 2.17*)

For a 1D SHO

a. Construct a linear combination of $|0\rangle, |1\rangle$ that maximizes $\langle x\rangle$ without using wave functions.
b. How does this state evolve with time?
c. Evaluate $\langle x\rangle$ using the Schrödinger picture.
d. Evaluate $\langle x\rangle$ using the Heisenberg picture.
e. Evaluate $\left\langle (\Delta x)^2\right\rangle$.

Answer for Exercise 2.14

Part a. Forming

$$|\psi\rangle = \frac{|0\rangle + \sigma\,|1\rangle}{\sqrt{1 + |\sigma|^2}} \tag{2.255}$$

the position expectation is

$$\langle\psi|\, x\,|\psi\rangle = \frac{1}{1 + |\sigma|^2}\left(\langle 0| + \sigma^*\langle 1|\right)\frac{x_0}{\sqrt{2}}\left(a^\dagger + a\right)\left(|0\rangle + \sigma\,|1\rangle\right). \tag{2.256}$$

Evaluating the action of the operators on the kets, we've got

$$\left(a^\dagger + a\right)(|0\rangle + \sigma |1\rangle) = |1\rangle + \sqrt{2}\sigma |2\rangle + \sigma |0\rangle . \tag{2.257}$$

The $|2\rangle$ term is killed by the bras, leaving

$$\begin{aligned} \langle x \rangle &= \frac{1}{1 + |\sigma|^2} \frac{x_0}{\sqrt{2}} (\sigma + \sigma^*) \\ &= \frac{\sqrt{2} x_0 \operatorname{Re} \sigma}{1 + |\sigma|^2}. \end{aligned} \tag{2.258}$$

Any imaginary component in σ will reduce the expectation, so we are constrained to picking a real value.

The derivative of

$$f(\sigma) = \frac{\sigma}{1 + \sigma^2}, \tag{2.259}$$

is

$$f'(\sigma) = \frac{1 - \sigma^2}{(1 + \sigma^2)^2}. \tag{2.260}$$

That has zeros at $\sigma = \pm 1$. The second derivative is

$$f''(\sigma) = \frac{-2\sigma(3 - \sigma^2)}{(1 + \sigma^2)^3}. \tag{2.261}$$

That will be negative (maximum for the extreme value) at $\sigma = 1$, so the linear superposition of these first two energy eigenkets that maximizes the position expectation is

$$\psi = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) . \tag{2.262}$$

That maximized position expectation is

$$\langle x \rangle = \frac{x_0}{\sqrt{2}}. \tag{2.263}$$

Part b. The time evolution is given by

$$\begin{aligned} |\Psi(t)\rangle &= e^{-iHt/\hbar} \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \\ &= \frac{1}{\sqrt{2}} \left(e^{-i(0+1/2)\hbar\omega t/\hbar} |0\rangle + e^{-i(1+1/2)\hbar\omega t/\hbar} |1\rangle \right) \\ &= \frac{1}{\sqrt{2}} \left(e^{-i\omega t/2} |0\rangle + e^{-3i\omega t/2} |1\rangle \right). \end{aligned} \tag{2.264}$$

Part c. The position expectation in the Schrödinger representation is

$$\begin{aligned}\langle x(t)\rangle &= \frac{1}{2}\left(e^{i\omega t/2}\langle 0| + e^{3i\omega t/2}\langle 1|\right)\frac{x_0}{\sqrt{2}}\left(a^\dagger + a\right)\left(e^{-i\omega t/2}|0\rangle + e^{-3i\omega t/2}|1\rangle\right)\\ &= \frac{x_0}{2\sqrt{2}}\left(e^{i\omega t/2}\langle 0| + e^{3i\omega t/2}\langle 1|\right)\left(e^{-i\omega t/2}|1\rangle + e^{-3i\omega t/2}\sqrt{2}|2\rangle + e^{-3i\omega t/2}|0\rangle\right)\\ &= \frac{x_0}{\sqrt{2}}\cos(\omega t).\end{aligned} \tag{2.265}$$

Part d.

$$\begin{aligned}\langle x(t)\rangle &= \frac{1}{2}\left(\langle 0| + \langle 1|\right)\frac{x_0}{\sqrt{2}}\left(a^\dagger e^{i\omega t} + ae^{-i\omega t}\right)\left(|0\rangle + |1\rangle\right)\\ &= \frac{x_0}{2\sqrt{2}}\left(\langle 0| + \langle 1|\right)\left(e^{i\omega t}|1\rangle + \sqrt{2}e^{i\omega t}|2\rangle + e^{-i\omega t}|0\rangle\right)\\ &= \frac{x_0}{\sqrt{2}}\cos(\omega t),\end{aligned} \tag{2.266}$$

matching the calculation using the Schrödinger picture.

Part e. Let's use the Heisenberg picture for the uncertainty calculation. Using the calculation above we have

$$\begin{aligned}\left\langle x^2\right\rangle &= \frac{1}{2}\frac{x_0^2}{2}\left(e^{-i\omega t}\langle 1| + \sqrt{2}e^{-i\omega t}\langle 2| + e^{i\omega t}\langle 0|\right)\left(e^{i\omega t}|1\rangle + \sqrt{2}e^{i\omega t}|2\rangle + e^{-i\omega t}|0\rangle\right)\\ &= \frac{x_0^2}{4}(1+2+1)\\ &= x_0^2.\end{aligned} \tag{2.267}$$

The uncertainty is

$$\begin{aligned}\left\langle(\Delta x)^2\right\rangle &= \left\langle x^2\right\rangle - \langle x\rangle^2\\ &= x_0^2 - \frac{x_0^2}{2}\cos^2(\omega t)\\ &= \frac{x_0^2}{2}\left(2 - \cos^2(\omega t)\right)\\ &= \frac{x_0^2}{2}\left(1 + \sin^2(\omega t)\right)\end{aligned} \tag{2.268}$$

Exercise 2.15 **Plane wave ground state expectation for 1D SHO.** ([11] pr. 2.18)

For a 1D SHO, show that

$$\langle 0| e^{ikx} |0\rangle = \exp\left(-k^2 \langle 0| x^2 |0\rangle /2\right). \tag{2.269}$$

Answer for Exercise 2.15

Despite the simple appearance of this problem, I found this quite involved to show. To do so, start with a series expansion of the expectation

$$\langle 0| e^{ikx} |0\rangle = \sum_{m=0}^{\infty} \frac{(ik)^m}{m!} \langle 0| x^m |0\rangle. \tag{2.270}$$

Let

$$X = \left(a + a^\dagger\right), \tag{2.271}$$

so that

$$x = \sqrt{\frac{\hbar}{2\omega m}} X = \frac{x_0}{\sqrt{2}} X. \tag{2.272}$$

Consider the first few values of $\langle 0| X^n |0\rangle$

$$\begin{aligned}\langle 0| X |0\rangle &= \langle 0| \left(a + a^\dagger\right) |0\rangle \\ &= \langle 0|1\rangle \\ &= 0,\end{aligned} \tag{2.273}$$

$$\begin{aligned}\langle 0| X^2 |0\rangle &= \langle 0| \left(a + a^\dagger\right)^2 |0\rangle \\ &= \langle 1|1\rangle \\ &= 1,\end{aligned} \tag{2.274}$$

$$\begin{aligned}\langle 0| X^3 |0\rangle &= \langle 0| \left(a + a^\dagger\right)^3 |0\rangle \\ &= \langle 1| \left(\sqrt{2} |2\rangle + |0\rangle\right) \\ &= 0.\end{aligned} \tag{2.275}$$

Whenever the power n in X^n is even, the braket can be split into a bra that has only contributions from odd eigenstates and a ket with even eigenstates. We conclude that $\langle 0| X^n |0\rangle = 0$ when n is odd.

Noting that $\langle 0| x^2 |0\rangle = x_0^2/2$, this leaves

$$\begin{aligned}\langle 0| e^{ikx} |0\rangle &= \sum_{m=0}^{\infty} \frac{(ik)^{2m}}{(2m)!} \langle 0| x^{2m} |0\rangle \\ &= \sum_{m=0}^{\infty} \frac{(ik)^{2m}}{(2m)!} \left(\frac{x_0^2}{2}\right)^m \langle 0| X^{2m} |0\rangle \\ &= \sum_{m=0}^{\infty} \frac{1}{(2m)!} \left(-k^2 \langle 0| x^2 |0\rangle\right)^m \langle 0| X^{2m} |0\rangle .\end{aligned} \tag{2.276}$$

This problem is now reduced to showing that

$$\frac{1}{(2m)!} \langle 0| X^{2m} |0\rangle = \frac{1}{m!\, 2^m}, \tag{2.277}$$

or

$$\begin{aligned}\langle 0| X^{2m} |0\rangle &= \frac{(2m)!}{m!\, 2^m} \\ &= \frac{(2m)(2m-1)(2m-2)\cdots(2)(1)}{2^m m!} \\ &= \frac{2^m (m)(2m-1)(m-1)(2m-3)(m-2)\cdots(2)(3)(1)(1)}{2^m m!} \\ &= (2m-1)!\,!\,,\end{aligned} \tag{2.278}$$

where $n!\,! = n(n-2)(n-4)\cdots$.

It looks like $\langle 0| X^{2m} |0\rangle$ can be expanded by inserting an identity operator and proceeding recursively, like

$$\begin{aligned}\langle 0| X^{2m} |0\rangle &= \langle 0| X^2 \left(\sum_{n=0}^{\infty} |n\rangle \langle n|\right) X^{2m-2} |0\rangle \\ &= \langle 0| X^2 \left(|0\rangle \langle 0| + |2\rangle \langle 2|\right) X^{2m-2} |0\rangle \\ &= \langle 0| X^{2m-2} |0\rangle + \langle 0| X^2 |2\rangle \langle 2| X^{2m-2} |0\rangle .\end{aligned} \tag{2.279}$$

This has made use of the observation that $\langle 0| X^2 |n\rangle = 0$ for all $n \neq 0, 2$. The remaining term includes the factor

$$\begin{aligned}\langle 0| X^2 |2\rangle &= \langle 0| \left(a + a^\dagger\right)^2 |2\rangle \\ &= \left(\langle 0| + \sqrt{2} \langle 2|\right) |2\rangle \\ &= \sqrt{2},\end{aligned} \tag{2.280}$$

Since $\sqrt{2}\,|2\rangle = \left(a^\dagger\right)^2 |0\rangle$, the expectation of interest can be written

$$\langle 0|\, X^{2m} \,|0\rangle = \langle 0|\, X^{2m-2} \,|0\rangle + \langle 0|\, a^2 X^{2m-2} \,|0\rangle\,. \tag{2.281}$$

How do we expand the second term. Let's look at how a and X commute

$$\begin{aligned} aX &= [a, X] + Xa \\ &= \left[a, a + a^\dagger\right] + Xa \\ &= \left[a, a^\dagger\right] + Xa \\ &= 1 + Xa, \end{aligned} \tag{2.282}$$

$$\begin{aligned} a^2 X &= a\,(aX) \\ &= a\,(1 + Xa) \\ &= a + aXa \\ &= a + (1 + Xa)\,a \\ &= 2a + Xa^2. \end{aligned} \tag{2.283}$$

Proceeding to expand $a^2 X^n$ we find

$$\begin{aligned} a^2X^3 &= 6X + 6X^2a + X^3a^2 \\ a^2X^4 &= 12X^2 + 8X^3a + X^4a^2 \\ a^2X^5 &= 20X^3 + 10X^4a + X^5a^2 \\ a^2X^6 &= 30X^4 + 12X^5a + X^6a^2. \end{aligned} \tag{2.284}$$

It appears that we have

$$\left[a^2X^n, X^na^2\right] = \beta_n X^{n-2} + 2nX^{n-1}a, \tag{2.285}$$

where

$$\beta_n = \beta_{n-1} + 2(n-1), \tag{2.286}$$

and $\beta_2 = 2$. Some goofing around shows that $\beta_n = n(n-1)$, so the induction hypothesis is

$$\left[a^2X^n, X^na^2\right] = n(n-1)X^{n-2} + 2nX^{n-1}a. \tag{2.287}$$

Let's check the induction

$$\begin{aligned}
a^2 X^{n+1} &= a^2 X^n X \\
&= \left(n(n-1)X^{n-2} + 2nX^{n-1}a + X^n a^2\right) X \\
&= n(n-1)X^{n-1} + 2nX^{n-1}aX + X^n a^2 X \\
&= n(n-1)X^{n-1} + 2nX^{n-1}\,(1 + Xa) + X^n \left(2a + Xa^2\right) \\
&= n(n-1)X^{n-1} + 2nX^{n-1} + 2nX^n a + 2X^n a + X^{n+1}a^2 \\
&= X^{n+1}a^2 + (2+2n)X^n a + (2n + n(n-1))\,X^{n-1} \\
&= X^{n+1}a^2 + 2(n+1)X^n a + (n+1)nX^{n-1},
\end{aligned} \tag{2.288}$$

which concludes the induction, giving

$$\langle 0| a^2 X^n |0\rangle = n(n-1)\,\langle 0| X^{n-2} |0\rangle\,, \tag{2.289}$$

and

$$\langle 0| X^{2m} |0\rangle = \langle 0| X^{2m-2} |0\rangle + (2m-2)(2m-3)\,\langle 0| X^{2m-4} |0\rangle\,. \tag{2.290}$$

Let

$$\sigma_n = \langle 0| X^n |0\rangle\,, \tag{2.291}$$

so that the recurrence relation, for $2n \geq 4$ is

$$\sigma_{2n} = \sigma_{2n-2} + (2n-2)(2n-3)\sigma_{2n-4} \tag{2.292}$$

We want to show that this simplifies to

$$\sigma_{2n} = (2n-1)!\,! \tag{2.293}$$

The first values are

$$\sigma_0 = \langle 0| X^0 |0\rangle = 1 \tag{2.294a}$$

$$\sigma_2 = \langle 0| X^2 |0\rangle = 1 \tag{2.294b}$$

which gives us the right result for the first term in the induction

$$\begin{aligned}
\sigma_4 &= \sigma_2 + 2 \times 1 \times \sigma_0 \\
&= 1 + 2 \\
&= 3!\,!
\end{aligned} \tag{2.295}$$

For the general induction term, consider

$$
\begin{aligned}
\sigma_{2n+2} &= \sigma_{2n} + 2n(2n-1)\sigma_{2n-2} \\
&= (2n-1)!! + 2n(2n-1)(2n-3)!! \\
&= (2n+1)(2n-1)!! \\
&= (2n+1)!!,
\end{aligned}
\tag{2.296}
$$

which completes the final induction. That was also the last thing required to complete the proof, so we are done!

Exercise 2.16 Relation of probability flux to momentum.

Show that the probability flux

$$
\mathbf{j}(\mathbf{x}, t) = -\frac{i\hbar}{2m}\left(\psi^* \boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\right),
\tag{2.297}
$$

is related to the momentum expectation at a given time by the integral of the flux over all space

$$
\int d^3x \mathbf{j}(\mathbf{x}, t) = \frac{\langle \mathbf{p} \rangle_t}{m}.
\tag{2.298}
$$

Answer for Exercise 2.16

This can be seen by recasting the integral in bra-ket form. Let

$$
\psi(\mathbf{x}, t) = \langle \mathbf{x} | \psi(t) \rangle,
\tag{2.299}
$$

and note that the momentum portions of the flux can be written as

$$
-i\hbar\boldsymbol{\nabla}\psi(\mathbf{x}, t) = \langle \mathbf{x} | \, \mathbf{p} \, | \psi(t) \rangle.
\tag{2.300}
$$

The current is therefore

$$
\begin{aligned}
\mathbf{j}(\mathbf{x}, t) &= \frac{1}{2m}\left(\psi^* \langle \mathbf{x} | \, \mathbf{p} \, | \psi(t) \rangle + \psi \langle \mathbf{x} | \, \mathbf{p} \, | \psi(t) \rangle^*\right) \\
&= \frac{1}{2m}\left(\langle \mathbf{x} | \psi(t) \rangle^* \langle \mathbf{x} | \, \mathbf{p} \, | \psi(t) \rangle + \langle \mathbf{x} | \psi(t) \rangle \langle \mathbf{x} | \, \mathbf{p} \, | \psi(t) \rangle^*\right) \\
&= \frac{1}{2m}\left(\langle \psi(t) | \mathbf{x} \rangle \langle \mathbf{x} | \, \mathbf{p} \, | \psi(t) \rangle + \langle \psi(t) | \, \mathbf{p} \, | \mathbf{x} \rangle \langle \mathbf{x} | \psi(t) \rangle\right).
\end{aligned}
\tag{2.301}
$$

Integrating and noting that the spatial identity is $1 = \int d^3x \, |\mathbf{x}\rangle \langle \mathbf{x}|$, we have

$$
\int d^3x \mathbf{j}(\mathbf{x}, t) = \langle \psi(t) | \, \mathbf{p} \, | \psi(t) \rangle,
\tag{2.302}
$$

This is just the expectation of $\mathbf{p}$ with respect to a specific time-instance state, demonstrating the desired relationship.

Exercise 2.17 Hermite polynomial normalization constant. ([11] *pr. 2.21*)

Derive the normalization constant c_n for the Harmonic oscillator solution

$$u_n(x) = c_n H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right) e^{-m\omega x^2/2\hbar}, \tag{2.303}$$

by deriving the orthogonality relationship using generating functions

$$g(x,t) = e^{-t^2+2tx} = \sum_{n=0}^\infty H_n(x)\frac{t^n}{n!}. \tag{2.304}$$

Start by working out the integral

$$I = \int_{-\infty}^\infty g(x,t)g(x,s)e^{-x^2}dx, \tag{2.305}$$

consider the integral twice with each side definition of the generating function.

Answer for Exercise 2.17

First using the exponential definition of the generating function

$$\begin{aligned}
\int_{-\infty}^\infty g(x,t)g(x,s)e^{-x^2}dx &= \int_{-\infty}^\infty e^{-t^2+2tx}e^{-s^2+2sx}e^{-x^2}dx \\
&= e^{-t^2-s^2}\int_{-\infty}^\infty e^{-(x^2-2tx-2sx)}dx \\
&= e^{-t^2-s^2+(s+t)^2}\int_{-\infty}^\infty e^{-(x-t-s)^2}dx \\
&= e^{2st}\int_{-\infty}^\infty e^{-u^2}du \\
&= \sqrt{\pi}e^{2st}.
\end{aligned} \tag{2.306}$$

With the Hermite polynomial definition of the generating function, this integral is

$$\begin{aligned}
\int_{-\infty}^\infty g(x,t)g(x,s)e^{-x^2}dx &= \int_{-\infty}^\infty \sum_{n=0}^\infty H_n(x)\frac{t^n}{n!}\sum_{m=0}^\infty H_m(x)\frac{s^m}{m!}e^{-x^2}dx \\
&= \sum_{n=0}^\infty \frac{t^n}{n!}\sum_{m=0}^\infty \frac{s^m}{m!}\int_{-\infty}^\infty H_n(x)H_m(x)e^{-x^2}dx.
\end{aligned} \tag{2.307}$$

Let

$$\alpha_{nm} = \int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx, \tag{2.308}$$

and equate the two expansions of this integral

$$\sqrt{\pi} \sum_{n=0}^{\infty} \frac{(2st)^n}{n!} = \sum_{n=0}^{\infty} \frac{t^n}{n!} \sum_{m=0}^{\infty} \frac{s^m}{m!} \alpha_{nm}, \tag{2.309}$$

or, after equating powers of t^n

$$\sqrt{\pi}(2s)^n = \sum_{m=0}^{\infty} \frac{s^m}{m!} \alpha_{nm}. \tag{2.310}$$

This requires α_{nm} to be zero for $n \neq m$, so

$$\sqrt{\pi} 2^n = \frac{1}{n!} \alpha_{nn}, \tag{2.311}$$

and

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx = \delta_{nm} \sqrt{\pi} 2^n n! \,. \tag{2.312}$$

The SHO normalization is fixed by

$$\begin{aligned} \int_{-\infty}^{\infty} u_n^2(x) dx &= c_n^2 \int_{-\infty}^{\infty} H_n^2(x/x_0) e^{-(x/x_0)^2} dx \\ &= c_n^2 x_0 \sqrt{\pi} 2^n n! \,, \end{aligned} \tag{2.313}$$

or

$$\begin{aligned} c_n &= \frac{1}{\sqrt{\sqrt{\pi} 2^n n! \sqrt{\frac{\hbar}{m\omega}}}} \\ &= \left(\frac{m\omega}{\hbar\pi} \right)^{1/4} 2^{-n/2} \frac{1}{\sqrt{n!}} \end{aligned} \tag{2.314}$$

Exercise 2.18 **Dirac delta function potential.** (*[11] pr. 2.24,2.25*)

Given a Dirac delta function potential

$$H = \frac{p^2}{2m} - V_0 \delta(x), \tag{2.315}$$

which vanishes after $t = 0$.

a. Solve for the bound state for $t < 0$,

b. Solve for the time evolution after that.

Answer for Exercise 2.18

Part a. This problem can be solved directly by considering the $|x| > 0$ and $x = 0$ regions separately.

For $|x| > 0$ Schrödinger's equation takes the form

$$E\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}. \tag{2.316}$$

With

$$\kappa = \frac{\sqrt{-2mE}}{\hbar}, \tag{2.317}$$

this has solutions

$$\psi = e^{\pm\kappa x}. \tag{2.318}$$

For $x > 0$ we must have

$$\psi = ae^{-\kappa x}, \tag{2.319}$$

and for $x < 0$

$$\psi = be^{\kappa x}. \tag{2.320}$$

requiring that ψ is continuous at $x = 0$ means $a = b$, or

$$\psi = \psi(0)e^{-\kappa|x|}. \tag{2.321}$$

For the $x = 0$ region, consider an interval $[-\epsilon, \epsilon]$ region around the origin. We must have

$$E\int_{-\epsilon}^{\epsilon}\psi(x)dx = \frac{-\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}dx - V_0\int_{-\epsilon}^{\epsilon}\delta(x)\psi(x)dx. \tag{2.322}$$

The RHS is zero

$$\begin{aligned} E\int_{-\epsilon}^{\epsilon}\psi(x)dx &= E\frac{e^{-\kappa(\epsilon)} - 1}{-\kappa} - E\frac{1 - e^{\kappa(-\epsilon)}}{\kappa} \\ &\rightarrow 0. \end{aligned} \tag{2.323}$$

That leaves

$$\begin{aligned} V_0\int_{-\epsilon}^{\epsilon}\delta(x)\psi(x)dx &= \frac{-\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}dx \\ &= \frac{-\hbar^2}{2m}\left.\frac{d\psi}{dx}\right|_{-\epsilon}^{\epsilon} \\ &= \frac{-\hbar^2}{2m}\psi(0)\left(-\kappa e^{-\kappa(\epsilon)} - \kappa e^{\kappa(-\epsilon)}\right). \end{aligned} \tag{2.324}$$

In the $\epsilon \to 0$ limit this gives

$$V_0 = \frac{\hbar^2 \kappa}{m}. \tag{2.325}$$

Equating relations for κ we have

$$\kappa = \frac{m V_0}{\hbar^2} = \frac{\sqrt{-2mE}}{\hbar}, \tag{2.326}$$

or

$$E = -\frac{1}{2m}\left(\frac{m V_0}{\hbar}\right)^2, \tag{2.327}$$

with

$$\psi(x, t < 0) = C \exp\left(-iEt/\hbar - \kappa|x|\right). \tag{2.328}$$

The normalization requires

$$\begin{aligned} 1 &= 2|C|^2 \int_0^\infty e^{-2\kappa x} dx \\ &= 2|C|^2 \left.\frac{e^{-2\kappa x}}{-2\kappa}\right|_0^\infty \\ &= \frac{|C|^2}{\kappa}, \end{aligned} \tag{2.329}$$

so

$$\boxed{\psi(x, t < 0) = \sqrt{\kappa} \exp\left(-iEt/\hbar - \kappa|x|\right).} \tag{2.330}$$

There is only one bound state for such a potential.

Part b. After turning off the potential, any plane wave

$$\psi(x, t) = e^{ikx - iE(k)t/\hbar}, \tag{2.331}$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}, \tag{2.332}$$

is a solution. In particular, at $t = 0$, the wave packet

$$\psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} A(k) dk, \tag{2.333}$$

is a solution. To solve for $A(k)$, we require

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} A(k) dk = \sqrt{\kappa} e^{-\kappa |x|}, \tag{2.334}$$

or

$$\boxed{A(k) = \sqrt{\frac{\kappa}{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} e^{-\kappa |x|} dx = \sqrt{\frac{2}{\pi}} \frac{\kappa^{3/2}}{\kappa^2 + k^2}.} \tag{2.335}$$

The initial time state established by the delta function potential evolves as

$$\boxed{\psi(x, t > 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx - i\hbar k^2 t/2m} A(k) dk.} \tag{2.336}$$

In terms of m, V_0 that is

$$\psi(x, t > 0) = \frac{(mV_0)^{3/2}}{\pi \hbar} \int_{-\infty}^{\infty} \frac{e^{ikx - i\hbar k^2 t/2m}}{k^2 \hbar^2 + m^2 V_0^2 / \hbar^2} dk. \tag{2.337}$$

This integral resists an attempt to evaluate with Mathematica.

Exercise 2.19 Free particle propagator. ([11] pr. 2.31)

Derive the free particle propagator in one and three dimensions.

Answer for Exercise 2.19

I found the description in the text confusing, so let's start from scratch with the definition of the propagator. This is the kernel of the spatial convolution integral that encodes time evolution, and can be expressed by expanding a general time state with two sets of identity operators. Let the position relative state at time t, relative to an initial time t_0 be given by $\langle \mathbf{x} | \alpha, t; t_0 \rangle$, and expand this in terms of a complete basis of energy eigenstates $|a'\rangle$ and the time evolution operator

$$
\begin{aligned}
\langle \mathbf{x}'' | \alpha, t; t_0 \rangle &= \langle \mathbf{x}'' | \, U \, |\alpha, t_0 \rangle \\
&= \langle \mathbf{x}'' | \, e^{-iH(t-t_0)/\hbar} \, |\alpha, t_0 \rangle \\
&= \langle \mathbf{x}'' | \, e^{-iH(t-t_0)/\hbar} \left(\sum_{a'} |a'\rangle \langle a'| \right) |\alpha, t_0 \rangle \\
&= \langle \mathbf{x}'' | \sum_{a'} e^{-iE_{a'}(t-t_0)/\hbar} \, |a'\rangle \langle a' | \alpha, t_0 \rangle \\
&= \langle \mathbf{x}'' | \sum_{a'} e^{-iE_{a'}(t-t_0)/\hbar} \, |a'\rangle \langle a' | \left(\int d^3\mathbf{x}' \, |\mathbf{x}'\rangle \langle \mathbf{x}'| \right) |\alpha, t_0 \rangle \\
&= \int d^3\mathbf{x}' \left(\langle \mathbf{x}'' | \sum_{a'} e^{-iE_{a'}(t-t_0)/\hbar} \, |a'\rangle \langle a' | \mathbf{x}' \rangle \right) \langle \mathbf{x}' | \alpha, t_0 \rangle \\
&= \int d^3\mathbf{x}' \, K(\mathbf{x}'', t; \mathbf{x}', t_0) \, \langle \mathbf{x}' | \alpha, t_0 \rangle ,
\end{aligned}
\tag{2.338}
$$

where

$$
K(\mathbf{x}'', t; \mathbf{x}', t_0) = \sum_{a'} \langle \mathbf{x}'' | a' \rangle \langle a' | \mathbf{x}' \rangle \, e^{-iE_{a'}(t-t_0)/\hbar}, \tag{2.339}
$$

the propagator, is the kernel of the convolution integral that takes the state $|\alpha, t_0\rangle$ to state $|\alpha, t; t_0\rangle$. Evaluating this over the momentum states (where integration and not plain summation is required), we have

$$
\begin{aligned}
K(\mathbf{x}'', t; \mathbf{x}', t_0) &= \int d^3\mathbf{p}' \, \langle \mathbf{x}'' | \mathbf{p}' \rangle \langle \mathbf{p}' | \mathbf{x}' \rangle \, e^{-iE_{\mathbf{p}'}(t-t_0)/\hbar} \\
&= \int d^3\mathbf{p}' \, \langle \mathbf{x}'' | \mathbf{p}' \rangle \langle \mathbf{p}' | \mathbf{x}' \rangle \exp\left(-i \frac{(\mathbf{p}')^2 (t - t_0)}{2m\hbar} \right) \\
&= \int d^3\mathbf{p}' \, \frac{e^{i\mathbf{x}'' \cdot \mathbf{p}'/\hbar}}{(\sqrt{2\pi\hbar})^3} \frac{e^{-i\mathbf{x}' \cdot \mathbf{p}'/\hbar}}{(\sqrt{2\pi\hbar})^3} \exp\left(-i \frac{(\mathbf{p}')^2 (t - t_0)}{2m\hbar} \right) \\
&= \frac{1}{(2\pi\hbar)^3} \int d^3\mathbf{p}' \, e^{i(\mathbf{x}'' - \mathbf{x}') \cdot \mathbf{p}'/\hbar} \exp\left(-i \frac{(\mathbf{p}')^2 (t - t_0)}{2m\hbar} \right) \\
&= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp'_1 e^{i(x''_1 - x'_1)p'_1/\hbar} \exp\left(-i \frac{(p'_1)^2 (t - t_0)}{2m\hbar} \right) \times \\
&\quad \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp'_2 e^{i(x''_2 - x'_2)p'_2/\hbar} \exp\left(-i \frac{(p'_2)^2 (t - t_0)}{2m\hbar} \right) \times \\
&\quad \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp'_3 e^{i(x''_3 - x'_3)p'_3/\hbar} \exp\left(-i \frac{(p'_3)^2 (t - t_0)}{2m\hbar} \right)
\end{aligned}
\tag{2.340}
$$

With $a = (t - t_0)/2m\hbar$, each of these three integral factors is of the form

$$
\begin{aligned}
\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp e^{i\Delta x p/\hbar} \exp\left(-iap^2\right) &= \frac{1}{2\pi\hbar\sqrt{a}}\int_{-\infty}^{\infty} du e^{i\Delta x u/(\sqrt{a}\hbar)} \exp\left(-iu^2\right) \\
&= \frac{1}{2\pi\hbar\sqrt{a}}\int_{-\infty}^{\infty} du e^{i\Delta x u/(\sqrt{a}\hbar)} \exp\left(-i(u - \Delta x/(2\sqrt{a}\hbar))^2 + i(\Delta x/(2\sqrt{a}\hbar))^2\right) \\
&= \frac{1}{2\pi\hbar\sqrt{a}} \exp\left(\frac{i(\Delta x)^2 2m\hbar}{4(t-t_0)\hbar^2}\right)\int_{-\infty}^{\infty} dz e^{-iz^2} \\
&= \sqrt{\frac{-i\pi 2m\hbar}{4\pi^2\hbar^2(t-t_0)}} \exp\left(\frac{i(\Delta x)^2 m}{2(t-t_0)\hbar}\right) \\
&= \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}} \exp\left(\frac{i(\Delta x)^2 m}{2(t-t_0)\hbar}\right).
\end{aligned}
\tag{2.341}
$$

Note that the integral above has value $\sqrt{-i\pi}$ which can be found by integrating over the contour of fig. 2.12, letting $R \to \infty$.

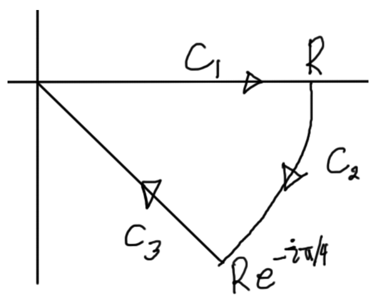

Figure 2.12: Integration contour for $\int e^{-iz^2}$.

Multiplying out each of the spatial direction factors gives the propagator in its closed form

$$
\boxed{K(\mathbf{x}'', t; \mathbf{x}', t_0) = \left(\sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\right)^3 \exp\left(\frac{i(\mathbf{x}'' - \mathbf{x}')^2 m}{2(t-t_0)\hbar}\right).}
\tag{2.342}
$$

In one or two dimensions the exponential power 3 need only be adjusted appropriately.

Exercise 2.20 Partition function and ground state energy. ([11] pr. 2.32)

Define the partition function as

$$
Z = \int d^3x' \, K(\mathbf{x}', t; \mathbf{x}', 0)\Big|_{\beta = it/\hbar},
\tag{2.343}
$$

Show that the ground state energy is given by

$$
-\frac{1}{Z}\frac{\partial Z}{\partial \beta}, \qquad \beta \to \infty.
\tag{2.344}
$$

Answer for Exercise 2.20

The propagator evaluated at the same point is

$$\begin{aligned}
K(\mathbf{x}', t; \mathbf{x}', 0) &= \sum_{a'} \langle \mathbf{x}' | a' \rangle \, | a' \rangle \, \mathbf{x}' \exp\left(-\frac{i E_{a'} t}{\hbar} \right) \\
&= \sum_{a'} \left| \langle \mathbf{x}' | a' \rangle \right|^2 \exp\left(-\frac{i E_{a'} t}{\hbar} \right) \\
&= \sum_{a'} \left| \langle \mathbf{x}' | a' \rangle \right|^2 \exp\left(-E_{a'} \beta \right).
\end{aligned} \tag{2.345}$$

The derivative is

$$\frac{\partial Z}{\partial \beta} = -\int d^3 x' \sum_{a'} E_{a'} \left| \langle \mathbf{x}' | a' \rangle \right|^2 \exp\left(-E_{a'} \beta \right). \tag{2.346}$$

In the $\beta \rightarrow \infty$ this sum will be dominated by the term with the lowest value of $E_{a'}$. Suppose that state is $a' = 0$, then

$$\begin{aligned}
\lim_{\beta \rightarrow \infty} -\frac{1}{Z} \frac{\partial Z}{\partial \beta} &= \frac{\int d^3 x' E_0 |\langle \mathbf{x}' | 0 \rangle|^2 \exp\left(-E_0 \beta \right)}{\int d^3 x' |\langle \mathbf{x}' | 0 \rangle|^2 \exp\left(-E_0 \beta \right)} \\
&= E_0.
\end{aligned} \tag{2.347}$$

This this stat mech like result seems very striking and profound, and makes me want to go off and study the QM formulation of stat mech that I recall seeing in [9], but not covered back in phy452.

Exercise 2.21 Momentum space free particle propagator. (*[11] pr. 2.33*)

Derive the free particle propagator in momentum space.

Answer for Exercise 2.21

The momentum space propagator follows in the same fashion as the spatial propagator

$$
\begin{aligned}
\langle \mathbf{p}'' | \alpha, t; t_0 \rangle &= \langle \mathbf{p}'' | U | \alpha, t_0 \rangle \\
&= \langle \mathbf{p}'' | e^{-iH(t-t_0)/\hbar} | \alpha, t_0 \rangle \\
&= \langle \mathbf{p}'' | e^{-iH(t-t_0)/\hbar} \left(\sum_{a'} | a' \rangle \langle a' | \right) | \alpha, t_0 \rangle \\
&= \langle \mathbf{p}'' | \sum_{a'} e^{-iE_{a'}(t-t_0)/\hbar} | a' \rangle \langle a' | \alpha, t_0 \rangle \\
&= \langle \mathbf{p}'' | \sum_{a'} e^{-iE_{a'}(t-t_0)/\hbar} | a' \rangle \langle a' | \left(\int d^3\mathbf{p}' | \mathbf{p}' \rangle \langle \mathbf{p}' | \right) | \alpha, t_0 \rangle \\
&= \int d^3\mathbf{p}' \left(\langle \mathbf{p}'' | \sum_{a'} e^{-iE_{a'}(t-t_0)/\hbar} | a' \rangle \langle a' | \mathbf{p}' \rangle \right) \langle \mathbf{p}' | \alpha, t_0 \rangle \\
&= \int d^3\mathbf{p}' K(\mathbf{p}'', t; \mathbf{p}', t_0) \langle \mathbf{p}' | \alpha, t_0 \rangle ,
\end{aligned}
\tag{2.348}
$$

so

$$
K(\mathbf{p}'', t; \mathbf{p}', t_0) = \sum_{a'} \langle \mathbf{p}'' | a' \rangle \langle a' | \mathbf{p}' \rangle e^{-iE_{a'}(t-t_0)/\hbar}. \tag{2.349}
$$

For the free particle Hamiltonian, this can be evaluated over a momentum space basis

$$
\begin{aligned}
K(\mathbf{p}'', t; \mathbf{p}', t_0) &= \int d^3\mathbf{p}''' \langle \mathbf{p}'' | \mathbf{p}''' \rangle \langle \mathbf{p}''' | \mathbf{p}' \rangle e^{-iE_{\mathbf{p}'''}(t-t_0)/\hbar} \\
&= \int d^3\mathbf{p}''' \langle \mathbf{p}'' | \mathbf{p}''' \rangle \delta(\mathbf{p}''' - \mathbf{p}') \exp\left(-i \frac{(\mathbf{p}''')^2 (t - t_0)}{2m\hbar} \right) \\
&= \langle \mathbf{p}'' | \mathbf{p}' \rangle \exp\left(-i \frac{(\mathbf{p}')^2 (t - t_0)}{2m\hbar} \right)
\end{aligned}
\tag{2.350}
$$

or

$$
\boxed{K(\mathbf{p}'', t; \mathbf{p}', t_0) = \delta(\mathbf{p}'' - \mathbf{p}') \exp\left(-i \frac{(\mathbf{p}')^2 (t - t_0)}{2m\hbar} \right).} \tag{2.351}
$$

This is what we expect since the time evolution is given by just this exponential factor

$$
\langle \mathbf{p}' | \alpha, t_0; t \rangle = \langle \mathbf{p}' | \exp\left(-i \frac{(\mathbf{p}')^2 (t - t_0)}{2m\hbar} \right) | \alpha, t_0 \rangle = \exp\left(-i \frac{(\mathbf{p}')^2 (t - t_0)}{2m\hbar} \right) \langle \mathbf{p}' | \alpha, t_0 \rangle . \tag{2.352}
$$

Exercise 2.22 **Gauge transformation of free particle Hamiltonian.** (*[11] pr. 37(a)*)

Given a gauge transformation of the free particle Hamiltonian to

$$H = \frac{1}{2m}\boldsymbol{\Pi}\cdot\boldsymbol{\Pi} + e\phi, \tag{2.353}$$

where

$$\boldsymbol{\Pi} = \mathbf{p} - \frac{e}{c}\mathbf{A}, \tag{2.354}$$

calculate $m d\mathbf{x}/dt$, $[\Pi_i, \Pi_j]$, and $m d^2\mathbf{x}/dt^2$, where $\mathbf{x}$ is the Heisenberg picture position operator, and the fields are functions only of position $\phi = \phi(\mathbf{x}), \mathbf{A} = \mathbf{A}(\mathbf{x})$.

Answer for Exercise 2.22

The final results for these calculations are found in [11], but seem worth deriving to exercise our commutator muscles.

Heisenberg picture velocity operator The first order of business is the Heisenberg picture velocity operator, but first note

$$\begin{aligned}\boldsymbol{\Pi}\cdot\boldsymbol{\Pi} &= \left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\cdot\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\\ &= \mathbf{p}^2 - \frac{e}{c}\left(\mathbf{A}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{A}\right) + \frac{e^2}{c^2}\mathbf{A}^2.\end{aligned} \tag{2.355}$$

The time evolution of the Heisenberg picture position operator is therefore

$$\begin{aligned}\frac{d\mathbf{x}}{dt} &= \frac{1}{i\hbar}\left[\mathbf{x}, H\right]\\ &= \frac{1}{i\hbar 2m}\left[\mathbf{x}, \boldsymbol{\Pi}^2\right]\\ &= \frac{1}{i\hbar 2m}\left[\mathbf{x}, \mathbf{p}^2 - \frac{e}{c}\left(\mathbf{A}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{A}\right) + \frac{e^2}{c^2}\mathbf{A}^2\right]\\ &= \frac{1}{i\hbar 2m}\left(\left[\mathbf{x}, \mathbf{p}^2\right] - \frac{e}{c}\left[\mathbf{x}, \mathbf{A}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{A}\right]\right).\end{aligned} \tag{2.356}$$

For the $\mathbf{p}^2$ commutator we have

$$\begin{aligned}\left[x_r, \mathbf{p}^2\right] &= i\hbar\frac{\partial \mathbf{p}^2}{\partial p_r}\\ &= 2i\hbar p_r,\end{aligned} \tag{2.357}$$

or

$$\left[\mathbf{x}, \mathbf{p}^2\right] = 2i\hbar\mathbf{p}. \tag{2.358}$$

Computing the remaining commutator, we've got

$$\begin{aligned}
\left[x_r, \mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}\right] &= x_r p_s A_s - p_s A_s x_r \\
&\quad + x_r A_s p_s - A_s p_s x_r \\
&= \left(\left[x_r, p_s\right] + p_s x_r\right) A_s - p_s A_s x_r \\
&\quad + x_r A_s p_s - A_s \left(\left[p_s, x_r\right] + x_r p_s\right) \\
&= \left[x_r, p_s\right] A_s + \cancel{p_s A_s x_r - p_s A_s x_r} \\
&\quad + \cancel{x_r A_s p_s - x_r A_s p_s} + A_s \left[x_r, p_s\right] \\
&= 2i\hbar\delta_{rs} A_s \\
&= 2i\hbar A_r,
\end{aligned} \tag{2.359}$$

so

$$\left[\mathbf{x}, \mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}\right] = 2i\hbar\mathbf{A}. \tag{2.360}$$

Assembling these results gives

$$\boxed{\frac{d\mathbf{x}}{dt} = \frac{1}{m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right) = \frac{1}{m}\boldsymbol{\Pi},} \tag{2.361}$$

as asserted in the text.

Kinetic Momentum commutators

$$\begin{aligned}
\left[\Pi_r, \Pi_s\right] &= \left[p_r - eA_r/c, p_s - eA_s/c\right] \\
&= \cancel{\left[p_r, p_s\right]} - \frac{e}{c}\left(\left[p_r, A_s\right] + \left[A_r, p_s\right]\right) + \frac{e^2}{c^2}\cancel{\left[A_r, A_s\right]} \\
&= -\frac{e}{c}\left((-i\hbar)\frac{\partial A_s}{\partial x_r} + (i\hbar)\frac{\partial A_r}{\partial x_s}\right) \\
&= -\frac{ie\hbar}{c}\left(-\frac{\partial A_s}{\partial x_r} + \frac{\partial A_r}{\partial x_s}\right) \\
&= -\frac{ie\hbar}{c}\epsilon_{tsr} B_t,
\end{aligned} \tag{2.362}$$

or

$$\boxed{\left[\Pi_r, \Pi_s\right] = \frac{ie\hbar}{c}\epsilon_{rst} B_t.} \tag{2.363}$$

Quantum Lorentz force For the force equation we have

$$\begin{aligned} m\frac{d^2\mathbf{x}}{dt^2} &= \frac{d\boldsymbol{\Pi}}{dt} \\ &= \frac{1}{i\hbar}\left[\boldsymbol{\Pi}, H\right] \\ &= \frac{1}{i\hbar 2m}\left[\boldsymbol{\Pi}, \boldsymbol{\Pi}^2\right] + \frac{1}{i\hbar}\left[\boldsymbol{\Pi}, e\phi\right]. \end{aligned} \tag{2.364}$$

For the ϕ commutator consider one component

$$\begin{aligned} \left[\Pi_r, e\phi\right] &= e\left[p_r - \frac{e}{c}A_r, \phi\right] \\ &= e\left[p_r, \phi\right] \\ &= e(-i\hbar)\frac{\partial\phi}{\partial x_r}, \end{aligned} \tag{2.365}$$

or

$$\frac{1}{i\hbar}\left[\boldsymbol{\Pi}, e\phi\right] = -e\boldsymbol{\nabla}\phi = e\mathbf{E}. \tag{2.366}$$

For the $\boldsymbol{\Pi}^2$ commutator I initially did this the hard way (it took four notebook pages, plus two for a false start.) Realizing that I didn't use eq. (2.363) for that expansion was the clue to doing this more expediently.

Considering a single component

$$\begin{aligned} \left[\Pi_r, \boldsymbol{\Pi}^2\right] &= \left[\Pi_r, \Pi_s\Pi_s\right] \\ &= \Pi_r\Pi_s\Pi_s - \Pi_s\Pi_s\Pi_r \\ &= \left(\left[\Pi_r, \Pi_s\right] + \cancel{\Pi_s\Pi_r}\right)\Pi_s - \Pi_s\left(\left[\Pi_s, \Pi_r\right] + \cancel{\Pi_r\Pi_s}\right) \\ &= i\hbar\frac{e}{c}\epsilon_{rst}\left(B_t\Pi_s + \Pi_s B_t\right), \end{aligned} \tag{2.367}$$

or

$$\begin{aligned} \frac{1}{i\hbar 2m}\left[\boldsymbol{\Pi}, \boldsymbol{\Pi}^2\right] &= \frac{e}{2mc}\epsilon_{rst}\mathbf{e}_r\left(B_t\Pi_s + \Pi_s B_t\right) \\ &= \frac{e}{2mc}\left(\boldsymbol{\Pi}\times\mathbf{B} - \mathbf{B}\times\boldsymbol{\Pi}\right). \end{aligned} \tag{2.368}$$

Putting all the pieces together we've got the quantum equivalent of the Lorentz force equation

$$\boxed{m\frac{d^2\mathbf{x}}{dt^2} = e\mathbf{E} + \frac{e}{2c}\left(\frac{d\mathbf{x}}{dt}\times\mathbf{B} - \mathbf{B}\times\frac{d\mathbf{x}}{dt}\right).} \tag{2.369}$$

While this looks equivalent to the classical result, all the vectors here are Heisenberg picture operators dependent on position.

Exercise 2.23 Gauge transformed probability current. ([11] *pr. 2.37 (b)*)

a. For the gauge transformed Schrödinger equation

$$\frac{1}{2m}\boldsymbol{\Pi}(\mathbf{x}) \cdot \boldsymbol{\Pi}(\mathbf{x})\psi(\mathbf{x}, t) + e\phi(\mathbf{x})\psi(\mathbf{x}, t) = i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x}, t), \tag{2.370}$$

where

$$\boldsymbol{\Pi}(\mathbf{x}) = -i\hbar\boldsymbol{\nabla} - \frac{e}{c}\mathbf{A}(\mathbf{x}), \tag{2.371}$$

find the probability current defined by

$$\frac{\partial\psi}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{j}. \tag{2.372}$$

b. Once obtained, let use a $\psi = \sqrt{\rho}e^{iS/\hbar}$ wavefunction representation, and find the corresponding form for the probability current.

c. Evaluate $\int d^3x\mathbf{j}$.

Answer for Exercise 2.23

Part a. Equation eq. (2.370) and its conjugate are

$$\begin{aligned}\frac{1}{2m}\boldsymbol{\Pi} \cdot \boldsymbol{\Pi}\psi + e\phi\psi &= i\hbar\frac{\partial\psi}{\partial t} \\ \frac{1}{2m}\boldsymbol{\Pi}^* \cdot \boldsymbol{\Pi}^*\psi^* + e\phi\psi^* &= -i\hbar\frac{\partial\psi^*}{\partial t}\end{aligned} \tag{2.373}$$

which can be used immediately in a chain rule expansion of the probability time derivative

$$\begin{aligned}i\hbar\frac{\partial\rho}{\partial t} &= i\hbar\psi^*\frac{\partial\psi}{\partial t} + i\hbar\psi\frac{\partial\psi^*}{\partial t} \\ &= \psi^*\left(\frac{1}{2m}\boldsymbol{\Pi} \cdot \boldsymbol{\Pi}\psi + e\phi\psi\right) - \psi\left(\frac{1}{2m}\boldsymbol{\Pi}^* \cdot \boldsymbol{\Pi}^*\psi^* + e\phi\psi^*\right) \\ &= \frac{1}{2m}\left(\psi^*\boldsymbol{\Pi} \cdot \boldsymbol{\Pi}\psi - \psi\boldsymbol{\Pi}^* \cdot \boldsymbol{\Pi}^*\psi^*\right).\end{aligned} \tag{2.374}$$

We have a difference of conjugates, so can get away with expanding just the first term

$$\begin{aligned}\psi^*\boldsymbol{\Pi} \cdot \boldsymbol{\Pi}\psi &= \psi^*\psi \\ &= \psi^*\left(-i\hbar\boldsymbol{\nabla} - \frac{e}{c}\mathbf{A}\right) \cdot \left(-i\hbar\boldsymbol{\nabla} - \frac{e}{c}\mathbf{A}\right)\psi \\ &= \psi^*\left(-\hbar^2\boldsymbol{\nabla}^2 + \frac{i\hbar e}{c}\left(\mathbf{A} \cdot \boldsymbol{\nabla} + \boldsymbol{\nabla} \cdot \mathbf{A}\right) + \frac{e^2}{c^2}\mathbf{A}^2\right)\psi.\end{aligned} \tag{2.375}$$

Note that in the directional derivative terms, the gradient operates on everything to its right, including $\mathbf{A}$. Also note that the last term has no imaginary component, so it will not contribute to the difference of conjugates.

This gives

$$\begin{aligned}\psi^*\mathbf{\Pi}\cdot\mathbf{\Pi}\psi - \psi\mathbf{\Pi}^*\cdot\mathbf{\Pi}^*\psi^* &= \psi^*\left(-\hbar^2\boldsymbol{\nabla}^2\psi + \frac{i\hbar e}{c}\left(\mathbf{A}\cdot\boldsymbol{\nabla}\psi + \boldsymbol{\nabla}\cdot(\mathbf{A}\psi)\right)\right)\\ &\quad - \psi\left(-\hbar^2\boldsymbol{\nabla}^2\psi^* - \frac{i\hbar e}{c}\left(\mathbf{A}\cdot\boldsymbol{\nabla}\psi^* + \boldsymbol{\nabla}\cdot(\mathbf{A}\psi^*)\right)\right)\\ &= -\hbar^2\left(\psi^*\boldsymbol{\nabla}^2\psi - \psi\boldsymbol{\nabla}^2\psi^*\right)\\ &\quad + \frac{i\hbar e}{c}\left(\psi^*\mathbf{A}\cdot\boldsymbol{\nabla}\psi + \psi^*\boldsymbol{\nabla}\cdot(\mathbf{A}\psi) + \psi\mathbf{A}\cdot\boldsymbol{\nabla}\psi^* + \psi\boldsymbol{\nabla}\cdot(\mathbf{A}\psi^*)\right)\end{aligned} \tag{2.376}$$

The first term is recognized as a divergence

$$\begin{aligned}\boldsymbol{\nabla}\cdot(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*) &= \psi^*\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\psi + \boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\psi^* - \psi\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\psi^* - \boldsymbol{\nabla}\psi^*\cdot\boldsymbol{\nabla}\psi\\ &= \psi^*\boldsymbol{\nabla}^2\psi - \psi\boldsymbol{\nabla}^2\psi^*.\end{aligned} \tag{2.377}$$

The second term can also be factored into a divergence operation

$$\begin{aligned}&\psi^*\mathbf{A}\cdot\boldsymbol{\nabla}\psi + \psi^*\boldsymbol{\nabla}\cdot(\mathbf{A}\psi) + \psi\mathbf{A}\cdot\boldsymbol{\nabla}\psi^* + \psi\boldsymbol{\nabla}\cdot(\mathbf{A}\psi^*)\\ &\qquad = \left(\psi^*\mathbf{A}\cdot\boldsymbol{\nabla}\psi + \psi\boldsymbol{\nabla}\cdot(\mathbf{A}\psi^*)\right) + \left(\psi\mathbf{A}\cdot\boldsymbol{\nabla}\psi^* + \psi^*\boldsymbol{\nabla}\cdot(\mathbf{A}\psi)\right)\\ &\qquad = 2\boldsymbol{\nabla}\cdot\left(\mathbf{A}\psi\psi^*\right)\end{aligned} \tag{2.378}$$

Putting all the pieces back together we have

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= \frac{1}{2mi\hbar}\left(\psi^*\mathbf{\Pi}\cdot\mathbf{\Pi}\psi - \psi\mathbf{\Pi}^*\cdot\mathbf{\Pi}^*\psi^*\right)\\ &= \boldsymbol{\nabla}\cdot\frac{1}{2mi\hbar}\left(-\hbar^2\left(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\right) + \frac{i\hbar e}{c}2\mathbf{A}\psi\psi^*\right)\\ &= \boldsymbol{\nabla}\cdot\left(\frac{i\hbar}{2m}\left(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\right) + \frac{e}{mc}\mathbf{A}\psi\psi^*\right).\end{aligned} \tag{2.379}$$

From eq. (2.372), the probability current must be

$$\mathbf{j} = \frac{\hbar}{2im}\left(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\right) - \frac{e}{mc}\mathbf{A}\psi\psi^*, \tag{2.380}$$

or

$$\boxed{\mathbf{j} = \frac{\hbar}{m}\,\mathrm{Im}\left(\psi^*\boldsymbol{\nabla}\psi\right) - \frac{e}{mc}\mathbf{A}\psi\psi^*.} \tag{2.381}$$

Part b. To find the $\psi = \sqrt{\rho} e^{iS/\hbar}$ form of the current, note that

$$\boldsymbol{\nabla}\psi = e^{iS/\hbar}\boldsymbol{\nabla}\sqrt{\rho} + \sqrt{\rho}e^{iS/\hbar}\boldsymbol{\nabla}(iS/\hbar), \tag{2.382}$$

so

$$\psi^*\boldsymbol{\nabla}\psi = \sqrt{\rho}\boldsymbol{\nabla}\sqrt{\rho} + \frac{i\rho}{\hbar}\boldsymbol{\nabla}S. \tag{2.383}$$

Discarding the real part of this product, we have

$$\mathbf{j} = \frac{\hbar}{m}\rho\boldsymbol{\nabla}S - \frac{e}{mc}\mathbf{A}\rho, \tag{2.384}$$

or

$$\boxed{\mathbf{j} = \frac{\rho}{m}\left(\boldsymbol{\nabla}S - \frac{e}{c}\mathbf{A}\right).} \tag{2.385}$$

Part c. Finally, note that

$$-i\hbar\boldsymbol{\nabla}\psi = \langle\mathbf{x}|\,\mathbf{p}\,|\psi\rangle, \tag{2.386}$$

so

$$\mathbf{j} = \frac{\hbar}{m}\operatorname{Im}\left(\langle\Psi|\mathbf{x}\rangle\left(\frac{i}{\hbar}\right)\langle\mathbf{x}|\,\mathbf{p}\,|\psi\rangle\right) - \frac{e}{mc}\mathbf{A}\,\langle\psi|\mathbf{x}\rangle\,\langle\mathbf{x}|\psi\rangle\,. \tag{2.387}$$

Integrating over all space to eliminate the identity operators, this is

$$\begin{aligned}\int d^3x\mathbf{j} &= \frac{1}{m}\operatorname{Im}\left(i\,\langle\Psi|\,\mathbf{p}\,|\psi\rangle\right) - \frac{e}{mc}\mathbf{A}\,\langle\psi|\psi\rangle \\ &= \frac{1}{m}\,\langle\psi|\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)|\psi\rangle \\ &= \frac{1}{m}\,\langle\boldsymbol{\Pi}\rangle\,.\end{aligned} \tag{2.388}$$

Exercise 2.24 Coherent States. (*phy1520 2015 ps2.1, and [11] pr. 2.19(c)*)

Consider the harmonic oscillator Hamiltonian $H = p^2/2m + m\omega^2x^2/2$. Define the coherent state $|z\rangle$ as the eigenfunction of the annihilation operator, via $a\,|z\rangle = z\,|z\rangle$, where a is the oscillator annihilation operator and z is some complex number which characterizes the coherent state.

a. Expanding $|z\rangle$ in terms of oscillator energy eigenstates $|n\rangle$, show that $|z\rangle = Ce^{za^\dagger}\,|0\rangle$. Find the normalization constant C.

b. Calculate the overlap $\langle z|z'\rangle$ for normalized coherent states $|z\rangle$.

c. Using the wavefunction $|z\rangle$, compute $\langle x\rangle, \langle p\rangle, \left\langle x^2\right\rangle$, and $\left\langle p^2\right\rangle$ by defining x, p in terms of $a, a^\dagger$.

d. The time evolution of any observed quantity in quantum mechanics can be described in two ways:

 (a) Schrödinger: the wavefunction evolves as $|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle$ and the operator A is time-independent, or

 (b) Heisenberg: the wavefunction is fixed to its value at $t = 0$, say $|\psi\rangle$, and operators evolve as $A(t) = e^{iHt/\hbar}Ae^{-iHt/\hbar}$.

 Show that both prescriptions yield the same result for any matrix elements or measured quantities.

e. Using the Heisenberg picture, compute the time evolution of $\langle x(t)\rangle, \langle p(t)\rangle, \left\langle x^2(t)\right\rangle$, and $\left\langle p^2(t)\right\rangle$ in the coherent state $|z\rangle$. Comment on connections to classical dynamics of the oscillator in phase space.

f. Show that $|f(n)|^2$ for a coherent state written as

$$|z\rangle = \sum_{n=0}^{\infty} f(n)|n\rangle \tag{2.389}$$

 has the form of a Poisson distribution, and find the most probable value of n, and thus the most probable energy.

Answer for Exercise 2.24

PROBLEM SET RELATED MATERIAL REDACTED IN THIS DOCUMENT.PLEASE FEEL FREE TO EMAIL ME FOR THE FULL VERSION IF YOU AREN'T TAKING PHY1520. [redacted]. END-REDACTION

Exercise 2.25 Aharonov Bohm effect. (*phy1520 2015 ps3.1*)

a. Consider Young's double slit experiment with electrons, having a monoenergetic source of electrons hitting a double slit with slit spacing d, with the electrons then landing on a screen at a distance D away from the double slit. For electrons with energy E, find the de Broglie wavelength λ, and hence the spacing between the fringes on the screen. You can ignore the drop in intensity as the electron beam 'spreads' when it travels from the slits to the screen (recall that the slits act as effective point sources), so just take phase changes into account along the travel path.

b. Next, imagine a thin solenoidal flux Φ being placed between the two slits, so that electron paths which encircle the flux once will pick up an Aharonov Bohm phase $e\Phi/\hbar c$. Compute the resulting shift in the interference pattern on the screen. Show that when the flux Φ is increased from $0 \rightarrow hc/e$, the interference pattern shifts by exactly one fringe, so the new pattern appears the same as the old. This is the same flux periodicity we saw in class for the energy levels versus flux for a particle on a ring.

Answer for Exercise 2.25

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Exercise 2.26 Landau Levels - Symmetric gauge. (*phy1520 2015 ps3.2*)

Consider a charged particle moving in two dimensions (xy-plane) in a uniform magnetic field $B_0\hat{\mathbf{z}}$ perpendicular to the plane. Let us work in a different gauge from the Landau gauge we discussed in class, namely, let us set

$$\mathbf{A} = \frac{B_0}{2}\left(x\hat{\mathbf{y}} - y\hat{\mathbf{x}}\right), \tag{2.390}$$

where (x, y) denotes the particle position. This is called the 'symmetric gauge'.

In this gauge,

a. work out the energy spectrum, and the eigenfunctions, and

b. provide a crude counting of the number of states per energy level (i.e., the degeneracy) for an electron on a disk of radius R.

Answer for Exercise 2.26

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Exercise 2.27 **Aharonov Bohm effect.** ([11] *pr. 2.28, phy1520 2015 ps3.3*)

Consider an electron confined to the interior of a finite hollow cylinder with its axis being $\hat{\mathbf{z}}$. Let the inner and outer walls of the cylinder be at radial coordinates ρ_a and $\rho_b > \rho_a$ respectively. Let the cylinder have its top and bottom ends at $z = 0, L$.

a. Find the eigenstates for a particle confined to this cylinder (ignore normalization), and show that its energies are given by

$$E_{lmn} = \frac{\hbar^2}{2m}\left(k_{mn}^2 + \left(\frac{\pi l}{L}\right)^2\right) \qquad (l = 1, 2, 3, \cdots; m = 0, 1, 2, \cdots) \tag{2.391}$$

where k_{mn} is the nth root of the equation

$$J_m(k_{mn}\rho_b)N_m(k_{mn}\rho_a) - N_m(k_{mn}\rho_b)J_m(k_{mn}\rho_a) = 0. \tag{2.392}$$

b. Repeat this problem with a uniform magnetic field $B\hat{\mathbf{z}}$ which is confined to the region $0 < \rho < \rho_a$ (i.e., only in the hollow part of the cylinder).

c. Show that there is a periodicity of the energy levels with the field, with the period being such that $\pi\rho_a^2 B = 2\pi N\hbar c/e$.

Answer for Exercise 2.27

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Exercise 2.28 Two spin time evolution. (*midterm pr. 1.iii*)

Compute the time evolution of a two particle state

$$\psi = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \tag{2.393}$$

under the action of the Hamiltonian

$$H = -BS_{z,1} + 2BS_{x,2} = \frac{\hbar B}{2} \left(-\sigma_{z,1} + 2\sigma_{x,2} \right). \tag{2.394}$$

Answer for Exercise 2.28

We have to know the action of the Hamiltonian on all the states

$$\begin{aligned}
H |\uparrow\uparrow\rangle &= \frac{B\hbar}{2} \left(- |\uparrow\uparrow\rangle + 2 |\uparrow\downarrow\rangle \right) \\
H |\uparrow\downarrow\rangle &= \frac{B\hbar}{2} \left(- |\uparrow\downarrow\rangle + 2 |\uparrow\uparrow\rangle \right) \\
H |\downarrow\uparrow\rangle &= \frac{B\hbar}{2} \left(|\downarrow\uparrow\rangle + 2 |\downarrow\downarrow\rangle \right) \\
H |\downarrow\downarrow\rangle &= \frac{B\hbar}{2} \left(|\downarrow\downarrow\rangle + 2 |\downarrow\uparrow\rangle \right)
\end{aligned} \tag{2.395}$$

With respect to the basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, the matrix of the Hamiltonian is

$$H = \frac{\hbar B}{2} \begin{bmatrix} -1 & 2 & 0 & 0 \\ 2 & -1 & 0 & 0 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 2 & 1 \end{bmatrix} \tag{2.396}$$

Utilizing the block diagonal form (and ignoring the $\hbar B/2$ factor for now), the characteristic equation is

$$\begin{aligned}
0 &= \begin{vmatrix} -1-\lambda & 2 \\ 2 & -1-\lambda \end{vmatrix} \begin{vmatrix} 1-\lambda & 2 \\ 2 & 1-\lambda \end{vmatrix} \\
&= \left((1+\lambda)^2 - 4 \right) \left((1-\lambda)^2 - 4 \right).
\end{aligned} \tag{2.397}$$

This has solutions

$$1 \pm \lambda = \pm 2, \tag{2.398}$$

or, with the $\hbar B/2$ factors put back in

$$\lambda = \pm\hbar B/2, \pm 3\hbar B/2. \tag{2.399}$$

I was thinking that we needed to compute the time evolution operator

$$U = e^{-iHt/\hbar}, \tag{2.400}$$

but we actually only need the eigenvectors, and the inverse relations. We can find the eigenvectors by inspection in each case from

$$\begin{aligned}
H - (1)\frac{\hbar B}{2} &= \frac{\hbar B}{2}\begin{bmatrix} -2 & 2 & 0 & 0 \\ 2 & -2 & 0 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 2 & 0 \end{bmatrix} \\
H - (-1)\frac{\hbar B}{2} &= \frac{\hbar B}{2}\begin{bmatrix} 0 & 2 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 2 & 2 \end{bmatrix} \\
H - (3)\frac{\hbar B}{2} &= \frac{\hbar B}{2}\begin{bmatrix} -4 & 2 & 0 & 0 \\ 2 & -4 & 0 & 0 \\ 0 & 0 & -2 & 2 \\ 0 & 0 & 2 & -2 \end{bmatrix} \\
H - (-3)\frac{\hbar B}{2} &= \frac{\hbar B}{2}\begin{bmatrix} 2 & 2 & 0 & 0 \\ 2 & 2 & 0 & 0 \\ 0 & 0 & 4 & 2 \\ 0 & 0 & 2 & 1 \end{bmatrix}.
\end{aligned} \tag{2.401}$$

The eigenkets are

$$
\begin{aligned}
|1\rangle &= \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\\0\\0\end{bmatrix}\\
|-1\rangle &= \frac{1}{\sqrt{2}}\begin{bmatrix}0\\0\\1\\-1\end{bmatrix}\\
|3\rangle &= \frac{1}{\sqrt{2}}\begin{bmatrix}0\\0\\1\\1\end{bmatrix}\\
|-3\rangle &= \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\\0\\0\end{bmatrix},
\end{aligned}
\tag{2.402}
$$

or

$$
\begin{aligned}
\sqrt{2}\,|1\rangle &= |\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle\\
\sqrt{2}\,|-1\rangle &= |\downarrow\uparrow\rangle - |\downarrow\downarrow\rangle\\
\sqrt{2}\,|3\rangle &= |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle\\
\sqrt{2}\,|-3\rangle &= |\uparrow\uparrow\rangle - |\uparrow\downarrow\rangle\,.
\end{aligned}
\tag{2.403}
$$

We can invert these

$$
\begin{aligned}
|\uparrow\uparrow\rangle &= \frac{1}{\sqrt{2}}\left(|1\rangle + |-3\rangle\right)\\
|\uparrow\downarrow\rangle &= \frac{1}{\sqrt{2}}\left(|1\rangle - |-3\rangle\right)\\
|\downarrow\uparrow\rangle &= \frac{1}{\sqrt{2}}\left(|3\rangle + |-1\rangle\right)\\
|\downarrow\downarrow\rangle &= \frac{1}{\sqrt{2}}\left(|3\rangle - |-1\rangle\right)
\end{aligned}
\tag{2.404}
$$

The original state of interest can now be expressed in terms of the eigenkets

$$\psi = \frac{1}{2} \left(|1\rangle - |{-3}\rangle - |3\rangle - |{-1}\rangle \right) \tag{2.405}$$

The time evolution of this ket is

$$\begin{aligned}
\psi(t) &= \frac{1}{2} \left(e^{-iBt/2} |1\rangle - e^{3iBt/2} |{-3}\rangle - e^{-3iBt/2} |3\rangle - e^{iBt/2} |{-1}\rangle \right) \\
&= \frac{1}{2\sqrt{2}} \Big(e^{-iBt/2} \left(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle \right) - e^{3iBt/2} \left(|\uparrow\uparrow\rangle - |\uparrow\downarrow\rangle \right) \\
&\quad - e^{-3iBt/2} \left(|\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle \right) - e^{iBt/2} \left(|\downarrow\uparrow\rangle - |\downarrow\downarrow\rangle \right) \Big) \\
&= \frac{1}{2\sqrt{2}} \Big(\left(e^{-iBt/2} - e^{3iBt/2} \right) |\uparrow\uparrow\rangle + \left(e^{-iBt/2} + e^{3iBt/2} \right) |\uparrow\downarrow\rangle \\
&\quad - \left(e^{-3iBt/2} + e^{iBt/2} \right) |\downarrow\uparrow\rangle + \left(e^{iBt/2} - e^{-3iBt/2} \right) |\downarrow\downarrow\rangle \Big) \\
&= \frac{1}{2\sqrt{2}} \Big(e^{iBt/2} \left(e^{-2iBt/2} - e^{2iBt/2} \right) |\uparrow\uparrow\rangle + e^{iBt/2} \left(e^{-2iBt/2} + e^{2iBt/2} \right) |\uparrow\downarrow\rangle \\
&\quad - e^{-iBt/2} \left(e^{-2iBt/2} + e^{2iBt/2} \right) |\downarrow\uparrow\rangle + e^{-iBt/2} \left(e^{2iBt/2} - e^{-2iBt/2} \right) |\downarrow\downarrow\rangle \Big) \\
&= \frac{1}{\sqrt{2}} \left(i \sin(Bt) \left(e^{-iBt/2} |\downarrow\downarrow\rangle - e^{iBt/2} |\uparrow\uparrow\rangle \right) + \cos(Bt) \left(e^{iBt/2} |\uparrow\downarrow\rangle - e^{-iBt/2} |\downarrow\uparrow\rangle \right) \right)
\end{aligned} \tag{2.406}$$

Note that this returns to the original state when $t = \frac{2\pi n}{B}, n \in \mathbb{Z}$. I think I've got it right this time (although I got a slightly different answer on paper before typing it up.)

Exercise 2.29 Particle in uniform electric and magnetic fields. (*2015 midterm p2*)

Find the energy eigenvalues and states for a charged particle moving the in the x, y plane in a uniform magnetic field $B\hat{\mathbf{z}}$ and a uniform electric field $E\hat{\mathbf{y}}$.

Answer for Exercise 2.29

The Hamiltonian for such a problem has the form

$$H = \frac{(p_x - qA_x/c)^2}{2m} + \frac{(p_y - qA_y/c)^2}{2m} + q\phi, \tag{2.407}$$

where $\mathbf{A}, \phi$ are the potentials for the electromagnetic field. Since we don't want a time dependent electric potential, our only choice is

$$E\hat{\mathbf{y}} = -\boldsymbol{\nabla}\phi = -\boldsymbol{\nabla}(-Ey). \tag{2.408}$$

We have many choices for the magnetic field, but it will have to be of the form $\mathbf{A} = B(-ay, bx, 0)$, for example $a = b = 1/2$. The Hamiltonian becomes

$$H = \frac{(p_x + qBay/c)^2}{2m} + \frac{(p_y - qBbx/c)^2}{2m} - qEy, \tag{2.409}$$

We seek a wave function that makes this separable. If we try $\psi = e^{iky}\phi(x)$ we get

$$\frac{H\psi}{e^{iky}} = \left(\frac{(p_x + qBay/c)^2}{2m} + \frac{(\hbar k - qBbx/c)^2}{2m} - qEy\right)\phi(x), \tag{2.410}$$

and if we try $\psi = e^{iky}\phi(x)$ we get

$$\frac{H\psi}{e^{ikx}} = \left(\frac{(\hbar k + qBay/c)^2}{2m} + \frac{(p_y - qBbx/c)^2}{2m} - qEy\right)\phi(y). \tag{2.411}$$

The latter is separable if we set $b = 0$, which requires $a = 1$, leaving an eigenvalue equation for $\phi(y)$

$$\begin{aligned}
H' &= \frac{(\hbar k + qBy/c)^2}{2m} + \frac{p_y^2}{2m} - qEy \\
&= \frac{p_y^2}{2m} - (qE - \hbar kqB/mc)\, y + \frac{1}{2m}\left(\frac{qBy}{c}\right)^2 + \frac{(\hbar k)^2}{2m} \\
&= \frac{p_y^2}{2m} + \frac{1}{2m}\left(\frac{qB}{c}\right)^2\left(-\frac{2}{m}\left(\frac{mc}{qB}\right)^2 (qE - \hbar kqB/mc)\, y + y^2\right) + \frac{(\hbar k)^2}{2m} \\
&= \frac{p_y^2}{2m} + \frac{1}{2}m\left(\frac{qB}{mc}\right)^2\left(y - \frac{1}{m}\left(\frac{mc}{qB}\right)^2 (qE - \hbar kqB/mc)\right)^2 - \frac{1}{2m}\left(\frac{mc}{qB}\right)^2 (qE - \hbar kqB/mc)^2 + \frac{(\hbar k)^2}{2m}.
\end{aligned} \tag{2.412}$$

Let

$$\begin{aligned}
\omega &= \frac{qB}{mc} \\
y_0 &= \frac{1}{m\omega^2}\,(qE - \hbar k\omega) \\
E_0 &= \frac{(\hbar k)^2}{2m} - \frac{1}{2}m\omega^2 y_0^2,
\end{aligned} \tag{2.413}$$

leaving

$$H' = \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2(y - y_0)^2 + E_0. \tag{2.414}$$

The energy eigenvalues are therefore

$$E = \hbar\omega\left(n + \frac{1}{2}\right) + E_0, \tag{2.415}$$

and the eigenfunctions are

$$\psi = e^{ikx}\phi_n(y - y_0), \tag{2.416}$$

where $\phi_n(y)$ is the n-th Harmonic oscillator wavefunction.

3 DIRAC EQUATION IN 1D

3.1 CONSTRUCTION OF THE DIRAC EQUATION

Schrödinger Derivation Recall that a "derivation" of the Schrödinger equation can be associated with the following equivalences

$$E \leftrightarrow \hbar\omega \leftrightarrow i\hbar\frac{\partial}{\partial t} \tag{3.1}$$

$$p \leftrightarrow \hbar k \leftrightarrow -i\hbar\frac{\partial}{\partial t} \tag{3.2}$$

so that the classical energy relationship

$$E = \frac{p^2}{2m} \tag{3.3}$$

takes the form

$$i\hbar\frac{\partial}{\partial t} = -\frac{\hbar^2}{2m}. \tag{3.4}$$

How do we do this in a relativistic context where the energy momentum relationship is

$$\begin{aligned} E &= \sqrt{p^2c^2 + m^2c^4} \\ &\approx mc^2 + \frac{p^2}{2m} + \cdots \end{aligned} \tag{3.5}$$

where m is the rest mass and c is the speed of light.

Attempt I

$$E = mc^2 + \frac{p^2}{2m} + (...)p^4 + (...)p^6 + \cdots \tag{3.6}$$

First order in time, but infinite order in space $\partial/\partial x$. Useless.

Attempt II

$$E^2 = p^2c^2 + m^2c^4. \tag{3.7}$$

This gives

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2} = -\hbar^2c^2\frac{\partial^2\psi}{\partial x^2} + m^2c^4\psi. \tag{3.8}$$

This is the Klein-Gordon equation, which is second order in time.

Attempt III Suppose that we have the matrix

$$\begin{bmatrix} pc & mc^2 \\ mc^2 & -pc \end{bmatrix}, \tag{3.9}$$

or

$$\begin{bmatrix} mc^2 & ipc \\ -ipc & -mc^2 \end{bmatrix}, \tag{3.10}$$

These both happen to have eigenvalues $\lambda_\pm = \pm\sqrt{p^2c^2}$. For those familiar with the Dirac matrices, this amounts to a choice for different representations of the gamma matrices.

Working with eq. (3.9), which has some nicer features than other possible representations, we seek a state

$$\boldsymbol{\psi} = \begin{bmatrix} \psi_1(x,t) \\ \psi_2(x,t) \end{bmatrix}, \tag{3.11}$$

where we aim to write down an equation for this composite state.

$$i\hbar\frac{\partial\boldsymbol{\psi}}{\partial t} = \mathbf{H}\boldsymbol{\psi} \tag{3.12}$$

Assuming the matrix is the Hamiltonian, multiplying that with the composite state gives

$$\begin{aligned} \begin{bmatrix} i\hbar\frac{\partial\psi_1}{\partial t} \\ i\hbar\frac{\partial\psi_1}{\partial t} \end{bmatrix} &= \begin{bmatrix} \hat{p}c & mc^2 \\ mc^2 & -\hat{p}c \end{bmatrix}\begin{bmatrix} \psi_1(x,t) \\ \psi_2(x,t) \end{bmatrix} \\ &= \begin{bmatrix} \hat{p}c\psi_1 + mc^2\psi_2 \\ mc^2\psi_1 - \hat{p}c\psi_2 \end{bmatrix}. \end{aligned} \tag{3.13}$$

What happens when we square this

$$
\begin{aligned}
\left(i\hbar\frac{\partial}{\partial t}\right)^2 \boldsymbol{\psi} &= \mathbf{H}\mathbf{H}\boldsymbol{\psi} \\
&= \begin{bmatrix} \hat{p}c & mc^2 \\ mc^2 & -\hat{p}c \end{bmatrix} \begin{bmatrix} \hat{p}c & mc^2 \\ mc^2 & -\hat{p}c \end{bmatrix} \boldsymbol{\psi} \\
&= \begin{bmatrix} \hat{p}^2c^2 + m^2c^4 & 0 \\ 0 & \hat{p}^2c^2 + m^2c^4 \end{bmatrix}
\end{aligned}
\tag{3.14}
$$

$$
-\hbar^2 \frac{\partial^2}{\partial t^2} \boldsymbol{\psi} = \left(\hat{p}^2c^2 + m^2c^4\right) \mathbf{1}\boldsymbol{\psi},
\tag{3.15}
$$

or more exactly

$$
-\hbar^2 \frac{\partial^2}{\partial t^2} \psi_{1,2} = \left(\hat{p}^2c^2 + m^2c^4\right) \psi_{1,2}.
\tag{3.16}
$$

This recovers the Klein Gordon equation for each of the wave functions ψ_1, ψ_2.

3.2 PLANE WAVE SOLUTION

Instead of squaring the operators, lets try to solve the first order equation. To do so we'll want to diagonalize $\mathbf{H}$.

Before doing that, let's write out the Hamiltonian in an alternate but useful form

$$
\begin{aligned}
\mathbf{H} &= \hat{p}c \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + mc^2 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\
&= \hat{p}c\hat{\sigma}_z + mc^2\hat{\sigma}_x.
\end{aligned}
\tag{3.17}
$$

We have two types of operators in the mix here. We have matrix operators that act on the wave function matrices, as well as derivative operators that act on the components of those matrices.

We have

$$
\hat{\sigma}_z \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} \psi_1 \\ -\psi_2 \end{bmatrix},
\tag{3.18}
$$

and

$$
\hat{\sigma}_x \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} \psi_2 \\ \psi_1 \end{bmatrix}.
\tag{3.19}
$$

Because the derivative actions of $\hat{p}$ and the matrix operators are independent, we see that these operators commute. For example

$$\begin{aligned}\hat{\sigma}_z \hat{p} \begin{bmatrix}\psi_1 \\ \psi_2\end{bmatrix} &= \hat{\sigma}_z \begin{bmatrix}-i\hbar \frac{\partial \psi_1}{\partial x} \\ -i\hbar \frac{\partial \psi_2}{\partial x}\end{bmatrix} \\ &= \begin{bmatrix}-i\hbar \frac{\partial \psi_1}{\partial x} \\ i\hbar \frac{\partial \psi_2}{\partial x}\end{bmatrix} \\ &= \hat{p}\hat{\sigma}_z \begin{bmatrix}\psi_1 \\ \psi_2\end{bmatrix}.\end{aligned} \tag{3.20}$$

Diagonalizing it Suppose the wave function matrix has the structure

$$\boldsymbol{\psi} = \begin{bmatrix}f_+ \\ f_-\end{bmatrix} e^{ikx}. \tag{3.21}$$

We'll plug this into the Schrödinger equation and see what we get.

Where we left off

$$-i\hbar \frac{\partial}{\partial t} \begin{bmatrix}\psi_1 \\ \psi_2\end{bmatrix} = \begin{bmatrix}-i\hbar c \frac{\partial}{\partial x} & mc^2 \\ mc^2 & i\hbar c \frac{\partial}{\partial x}\end{bmatrix}. \tag{3.22}$$

With a potential this would be

$$-i\hbar \frac{\partial}{\partial t} \begin{bmatrix}\psi_1 \\ \psi_2\end{bmatrix} = \begin{bmatrix}-i\hbar c \frac{\partial}{\partial x} + V(x) & mc^2 \\ mc^2 & i\hbar c \frac{\partial}{\partial x} + V(x)\end{bmatrix}. \tag{3.23}$$

This means that the potential is raising the energy eigenvalue of the system.

Free Particle Assuming a form

$$\begin{bmatrix}\psi_1(x,t) \\ \psi_2(x,t)\end{bmatrix} = e^{ikx} \begin{bmatrix}f_1(t) \\ f_2(t)\end{bmatrix}, \tag{3.24}$$

and plugging back into the Dirac equation we have

$$-i\hbar \frac{\partial}{\partial t} \begin{bmatrix}f_1 \\ f_2\end{bmatrix} = \begin{bmatrix}k\hbar c & mc^2 \\ mc^2 & -\hbar kc\end{bmatrix} \begin{bmatrix}f_1 \\ f_2\end{bmatrix}. \tag{3.25}$$

We can use a diagonalizing rotation

$$
\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} \cos\theta_k & -\sin\theta_k \\ \sin\theta_k & \cos\theta_k \end{bmatrix} \begin{bmatrix} f_+ \\ f_- \end{bmatrix}. \tag{3.26}
$$

Plugging this in reduces the system to the form

$$
-i\hbar \frac{\partial}{\partial t} \begin{bmatrix} f_+ \\ f_- \end{bmatrix} = \begin{bmatrix} E_k & 0 \\ 0 & -E_k \end{bmatrix} \begin{bmatrix} f_+ \\ f_- \end{bmatrix}. \tag{3.27}
$$

Where the rotation angle is found to be given by

$$
\begin{aligned}
\sin(2\theta_k) &= \frac{mc^2}{\sqrt{(\hbar kc)^2 + m^2c^4}} \\
\cos(2\theta_k) &= \frac{\hbar kc}{\sqrt{(\hbar kc)^2 + m^2c^4}} \\
E_k &= \sqrt{(\hbar kc)^2 + m^2c^4}
\end{aligned} \tag{3.28}
$$

3.3 DIRAC SEA AND PAIR CREATION

See fig. 3.1 for a sketch of energy vs momentum. The asymptotes are the limiting cases when $mc^2 \to 0$. The + branch is what we usually associate with particles. What about the other energy states. For Fermions Dirac argued that the lower energy states could be thought of as “filled up”, using the Pauli principle to leave only the positive energy states available. This was called the “Dirac Sea”. This isn’t a good solution, and won’t work for example for Bosons.

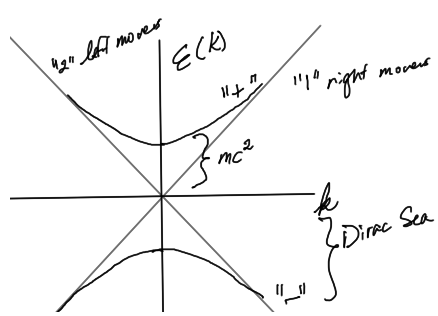

Figure 3.1: Dirac equation solution space.

Another way to rationalize this is to employ ideas from solid state theory. For example consider a semiconductor with a valence and conduction band as sketched in fig. 3.2.

A photon can excite an electron from the valence band to the conduction band, leaving all the valence band states filled except for one (a hole). For an electron we can use almost the same picture, as sketched in fig. 3.3.

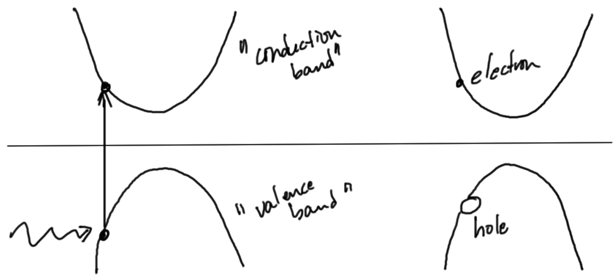

Figure 3.2: Solid state valence and conduction band transition.

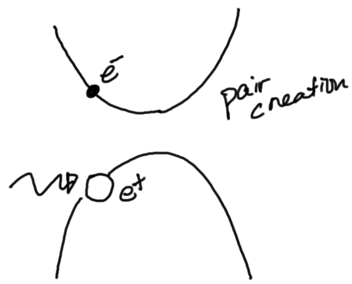

Figure 3.3: Pair creation.

A photon with energy $E_k - (-E_k)$ can create a positron-electron pair from the vacuum, where the energy of the electron and positron pair is E_k. At high enough energies, we can see this pair creation occur.

3.4 ZITTERBEWEGUNG

If a particle is created at a non-eigenstate such as one on the asymptotes, then oscillations between the positive and negative branches are possible as sketched in fig. 3.4.

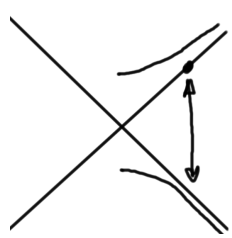

Figure 3.4: Zitterbewegung oscillation.

Only “vertical" oscillations between the positive and negative locations on these branches is possible since those are the points that match the particle momentum. Examining this will be the aim of one of the problem set problems.

3.5 PROBABILITY AND CURRENT DENSITY

If we define a probability density

$$\rho(x, t) = |\psi_1|^2 + |\psi_2|^2, \tag{3.29}$$

does this satisfy a probability conservation relation

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0, \tag{3.30}$$

where j is the probability current. Plugging in the density, we have

$$\frac{\partial \rho}{\partial t} = \frac{\partial \psi_1^*}{\partial t}\psi_1 + \psi_1^*\frac{\partial \psi_1}{\partial t} + \frac{\partial \psi_2^*}{\partial t}\psi_2 + \psi_2^*\frac{\partial \psi_2}{\partial t}. \tag{3.31}$$

It turns out that the probability current has the form

$$j(x, t) = c\left(\psi_1^*\psi_1 - \psi_2^*\psi_2\right). \tag{3.32}$$

Here the speed of light c is the slope of the line in the plots above. We can think of this current density as right movers minus the left movers. Any state that is given can be thought of as a combination of right moving and left moving states, neither of which are eigenstates of the free particle Hamiltonian.

3.6 POTENTIAL STEP

The next logical thing to think about, as in non-relativistic quantum mechanics, is to think about what occurs when the particle hits a potential step, as in fig. 3.5.

The approach is the same. We write down the wave functions for the $V = 0$ region (I), and the higher potential region (II).

The eigenstates are found on the solid lines above the asymptotes on the right hand movers side as sketched in fig. 3.6. The right and left moving designations are based on the phase velocity $\partial E/\partial k$ (approaching $\pm c$ on the top-right and top-left quadrants respectively).

For $k > 0$, an eigenstate for the incident wave is

$$\boldsymbol{\psi}_{\text{inc}}(x) = \begin{bmatrix} \cos\theta_k \\ \sin\theta_k \end{bmatrix} e^{ikx}, \tag{3.33}$$

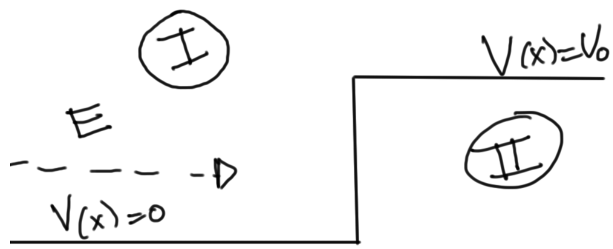

Figure 3.5: Reflection off a potential barrier.

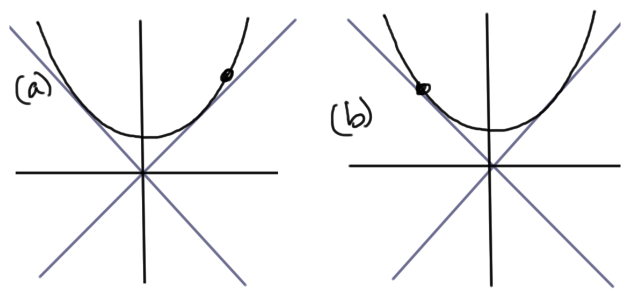

Figure 3.6: Right movers and left movers.

For the reflected wave function, we pick a function on the left moving side of the positive energy branch.

$$\psi_{\text{ref}}(x) = \begin{bmatrix} ? \\ ? \end{bmatrix} e^{-ikx}, \tag{3.34}$$

We'll go through this in more detail next time.

3.7 DIRAC SCATTERING OFF A POTENTIAL STEP

For the non-relativistic case we have

$$\begin{aligned} E < V_0 &\implies T = 0, R = 1 \\ E > V_0 &\implies T > 0, R < 1. \end{aligned} \tag{3.35}$$

What happens for a relativistic 1D particle?
Referring to fig. 3.7.

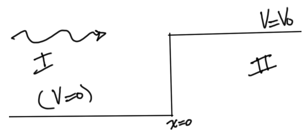

Figure 3.7: Potential step.

the region I Hamiltonian is

$$H = \begin{bmatrix} \hat{p}c & mc^2 \\ mc^2 & -\hat{p}c \end{bmatrix}, \tag{3.36}$$

for which the solution is

$$\Phi = e^{ik_1 x} \begin{bmatrix} \cos\theta_1 \\ \sin\theta_1 \end{bmatrix}, \tag{3.37}$$

where

$$\begin{aligned} \cos 2\theta_1 &= \frac{\hbar c k_1}{E_{k_1}} \\ \sin 2\theta_1 &= \frac{mc^2}{E_{k_1}} \end{aligned} \tag{3.38}$$

To consider the $k_1 < 0$ case, note that

$$\begin{aligned} \cos^2\theta_1 - \sin^2\theta_1 &= \cos 2\theta_1 \\ 2\sin\theta_1\cos\theta_1 &= \sin 2\theta_1 \end{aligned} \tag{3.39}$$

so after flipping the signs on all the k_1 terms we find for the reflected wave

$$\Phi = e^{-ik_1 x} \begin{bmatrix} \sin\theta_1 \\ \cos\theta_1 \end{bmatrix}. \tag{3.40}$$

FIXME: this reasoning doesn't entirely make sense to me. Make sense of this by trying this solution as was done for the form of the incident wave solution.

The region I wave has the form

$$\Phi_I = A e^{ik_1 x} \begin{bmatrix} \cos\theta_1 \\ \sin\theta_1 \end{bmatrix} + B e^{-ik_1 x} \begin{bmatrix} \sin\theta_1 \\ \cos\theta_1 \end{bmatrix}. \tag{3.41}$$

By the time we are done we want to have computed the reflection coefficient

$$R = \frac{|B|^2}{|A|^2}. \tag{3.42}$$

The region I energy is

$$E = \sqrt{\left(mc^2\right)^2 + \left(\hbar c k_1\right)^2}. \tag{3.43}$$

We must have

$$E = \sqrt{\left(mc^2\right)^2 + \left(\hbar c k_2\right)^2} + V_0 = \sqrt{\left(mc^2\right)^2 + \left(\hbar c k_1\right)^2}, \tag{3.44}$$

so

$$\begin{aligned} \left(\hbar c k_2\right)^2 &= \left(E - V_0\right)^2 - \left(mc^2\right)^2 \\ &= \underbrace{\boxed{\left(E - V_0 + mc^2\right)}}_{r_1}\underbrace{\boxed{\left(E - V_0 - mc^2\right)}}_{r_2}. \end{aligned} \tag{3.45}$$

The r_1 and r_2 branches are sketched in fig. 3.8.

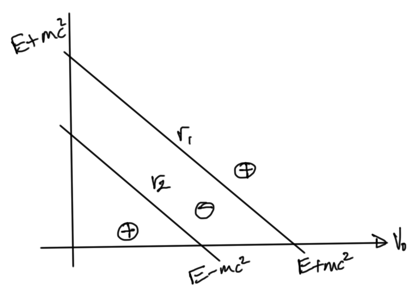

Figure 3.8: Energy signs.

For low energies, we have a set of potentials for which we will have propagation, despite having a potential barrier. For still higher values of the potential barrier the product $r_1 r_2$ will be negative, so the solutions will be decaying. Finally, for even higher energies, there will again be propagation.

The non-relativistic case is sketched in fig. 3.9.

For the relativistic case we must consider three different cases, sketched in fig. 3.10, fig. 3.11, and fig. 3.12 respectively. For the low potential energy, a particle with positive group velocity (what we've called right moving) can be matched to an equal energy portion of the potential

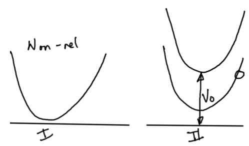

Figure 3.9: Effects of increasing potential for non-relativistic case.

shifted parabola in region II. This is a case where we have transmission, but no antiparticle creation. There will be an energy region where the region II wave function has only a dissipative term, since there is no region of either of the region II parabolic branches available at the incident energy. When the potential is shifted still higher so that $V_0 > E + mc^2$, a positive group velocity in region I with a given energy can be matched to an antiparticle branch in the region II parabolic energy curve.

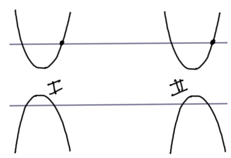

Figure 3.10: Low potential energy.

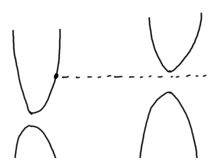

Figure 3.11: High enough potential energy for no propagation.

Boundary value conditions We want to ensure that the current across the barrier is conserved (no particles are lost), as sketched in fig. 3.13.

Recall that given a wave function

$$\Psi = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}, \tag{3.46}$$

the density and currents are respectively

$$\begin{aligned} \rho &= \psi_1^* \psi_1 + \psi_2^* \psi_2 \\ j &= \psi_1^* \psi_1 - \psi_2^* \psi_2 \end{aligned} \tag{3.47}$$

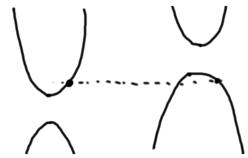

Figure 3.12: High potential energy.

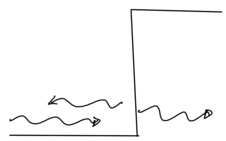

Figure 3.13: Transmitted, reflected and incident components.

Matching boundary value conditions requires

1. For both the relativistic and non-relativistic cases we must have

$$\Psi_{\mathrm{L}} = \Psi_{\mathrm{R}}, \qquad \text{at } x = 0. \tag{3.48}$$

2. For the non-relativistic case we want

$$\int_{-\epsilon}^{\epsilon} -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} = \cancel{\int_{-\epsilon}^{\epsilon} (E - V(x))\,\Psi(x)} \tag{3.49}$$

$$-\frac{\hbar^2}{2m}\left(\left.\frac{\partial \Psi}{\partial x}\right|_{\mathrm{R}} - \left.\frac{\partial \Psi}{\partial x}\right|_{\mathrm{L}}\right) = 0. \tag{3.50}$$

We have to match

For the relativistic case

$$-i\hbar\sigma_z \int_{-\epsilon}^{\epsilon} \frac{\partial \Psi}{\partial x} + \cancel{mc^2\sigma_x \int_{-\epsilon}^{\epsilon} \psi} = \cancel{\int_{-\epsilon}^{\epsilon} (E - V_0)\,\psi}, \tag{3.51}$$

so

$$-i\hbar c\sigma_z\left(\psi(\epsilon) - \psi(-\epsilon)\right) = -i\hbar c\sigma_z\left(\psi_{\mathrm{R}} - \psi_{\mathrm{L}}\right). \tag{3.52}$$

so we must match

$$\sigma_z \psi_{\mathrm{R}} = \sigma_z \psi_{\mathrm{L}}. \tag{3.53}$$

It appears that things are simpler, because we only have to match the wave function values at the boundary, and don't have to match the derivatives too. However, we have a two component wave function, so there are still two tasks.

Solving the system Let's look for a solution for the $E + mc^2 > V_0$ case on the right branch, as sketched in fig. 3.14.

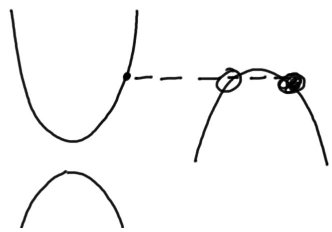

Figure 3.14: High potential region. Anti-particle transmission.

While the right branch in this case is left going, this might work out since that is an antiparticle. We could try both.

Try

$$\Psi_{II} = D e^{i k_2 x} \begin{bmatrix} -\sin\theta_2 \\ \cos\theta_2 \end{bmatrix}. \tag{3.54}$$

This is justified by

$$+E \rightarrow \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}, \tag{3.55}$$

so

$$-E \rightarrow \begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix} \tag{3.56}$$

At $x = 0$ the exponentials vanish, so equating the waves at that point means

$$\begin{bmatrix} \cos\theta_1 \\ \sin\theta_1 \end{bmatrix} + \frac{B}{A} \begin{bmatrix} \sin\theta_1 \\ \cos\theta_1 \end{bmatrix} = \frac{D}{A} \begin{bmatrix} -\sin\theta_2 \\ \cos\theta_2 \end{bmatrix}. \tag{3.57}$$

Solving this yields

$$\frac{B}{A} = -\frac{\cos(\theta_1 - \theta_2)}{\sin(\theta_1 + \theta_2)}. \tag{3.58}$$

This yields

$$\boxed{R = \frac{1 + \cos(2\theta_1 - 2\theta_2)}{1 - \cos(2\theta_1 - 2\theta_2)}.} \tag{3.59}$$

As $V_0 \to \infty$ this simplifies to

$$R = \frac{E - \sqrt{E^2 - (mc^2)^2}}{E + \sqrt{E^2 - (mc^2)^2}}. \tag{3.60}$$

Filling in the details for these results part of problem set 4.

3.8 PROBLEMS

Exercise 3.1 Calculate the right going diagonalization.

a. Prove eq. (3.28).

Answer for Exercise 3.1

Part a. To determine the relations for θ_k we have to solve

$$\begin{bmatrix} E_k & 0 \\ 0 & -E_k \end{bmatrix} = R^{-1} H R. \tag{3.61}$$

Working with $\hbar = c = 1$ temporarily, and $C = \cos\theta_k, S = \sin\theta_k$, that is

$$\begin{aligned}
\begin{bmatrix} E_k & 0 \\ 0 & -E_k \end{bmatrix} &= \begin{bmatrix} C & S \\ -S & C \end{bmatrix} \begin{bmatrix} k & m \\ m & -k \end{bmatrix} \begin{bmatrix} C & -S \\ S & C \end{bmatrix} \\
&= \begin{bmatrix} C & S \\ -S & C \end{bmatrix} \begin{bmatrix} kC + mS & -kS + mC \\ mC - kS & -mS - kC \end{bmatrix} \\
&= \begin{bmatrix} kC^2 + mSC + mCS - kS^2 & -kSC + mC^2 - mS^2 - kCS \\ -kCS - mS^2 + mC^2 - kSC & kS^2 - mCS - mSC - kC^2 \end{bmatrix} \\
&= \begin{bmatrix} k\cos(2\theta_k) + m\sin(2\theta_k) & m\cos(2\theta_k) - k\sin(2\theta_k) \\ m\cos(2\theta_k) - k\sin(2\theta_k) & -k\cos(2\theta_k) - m\sin(2\theta_k) \end{bmatrix}.
\end{aligned} \tag{3.62}$$

This gives

$$
\begin{aligned}
E_k \begin{bmatrix} 1 \\ 0 \end{bmatrix} &= \begin{bmatrix} k\cos(2\theta_k) + m\sin(2\theta_k) \\ m\cos(2\theta_k) - k\sin(2\theta_k) \end{bmatrix} \\
&= \begin{bmatrix} k & m \\ m & -k \end{bmatrix} \begin{bmatrix} \cos(2\theta_k) \\ \sin(2\theta_k) \end{bmatrix}.
\end{aligned}
\tag{3.63}
$$

Adding back in the $\hbar$'s and c's this is

$$
\begin{aligned}
\begin{bmatrix} \cos(2\theta_k) \\ \sin(2\theta_k) \end{bmatrix} &= \frac{E_k}{-(\hbar kc)^2 - (mc^2)^2} \begin{bmatrix} -\hbar kc & -mc^2 \\ -mc^2 & \hbar kc \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\
&= \frac{1}{E_k} \begin{bmatrix} \hbar kc \\ mc^2 \end{bmatrix}.
\end{aligned}
\tag{3.64}
$$

Exercise 3.2 Verify the plane wave eigenstate.

a. Verify eq. (3.33).

b. Find the form of the reflected wave.

Answer for Exercise 3.2

Part a. With

$$
\begin{aligned}
H_k &= \begin{bmatrix} \hbar kc & mc^2 \\ mc^2 & -\hbar kc \end{bmatrix} \\
&= R \begin{bmatrix} E_k & 0 \\ 0 & -E_k \end{bmatrix} R^{-1},
\end{aligned}
\tag{3.65}
$$

We wish to show that

$$
H_k \begin{bmatrix} \cos\theta_k \\ \sin\theta_k \end{bmatrix} e^{ikx} = E_k \begin{bmatrix} \cos\theta_k \\ \sin\theta_k \end{bmatrix} e^{ikx}.
\tag{3.66}
$$

The LHS side expands to

$$\begin{aligned}
\begin{bmatrix} C & -S \\ S & C \end{bmatrix}\begin{bmatrix} E_k & 0 \\ 0 & -E_k \end{bmatrix}\begin{bmatrix} C & S \\ -S & C \end{bmatrix}\begin{bmatrix} C \\ S \end{bmatrix} e^{ikx} &= \begin{bmatrix} C & -S \\ S & C \end{bmatrix}\begin{bmatrix} E_k & 0 \\ 0 & -E_k \end{bmatrix}\begin{bmatrix} C^2 + S^2 \\ 0 \end{bmatrix} e^{ikx} \\
&= \begin{bmatrix} C & -S \\ S & C \end{bmatrix}\begin{bmatrix} E_k \\ 0 \end{bmatrix} e^{ikx} \\
&= E_k \begin{bmatrix} C \\ S \end{bmatrix} e^{ikx}. \qquad \square
\end{aligned} \tag{3.67}$$

Part b. For the reflected wave, let's assume that the reflected wave has the form

$$\Psi = \begin{bmatrix} \sin\theta_k \\ -\cos\theta_k \end{bmatrix} e^{-ikx}. \tag{3.68}$$

Let's verify this

$$\begin{aligned}
&\begin{bmatrix} C & -S \\ S & C \end{bmatrix}\begin{bmatrix} E_k & 0 \\ 0 & -E_k \end{bmatrix}\begin{bmatrix} C & S \\ -S & C \end{bmatrix}\begin{bmatrix} S \\ -C \end{bmatrix} e^{-ikx} \\
&= \begin{bmatrix} C & -S \\ S & C \end{bmatrix}\begin{bmatrix} E_k & 0 \\ 0 & -E_k \end{bmatrix}\begin{bmatrix} CS - SC \\ -S^2 - C^2 \end{bmatrix} e^{-ikx} \\
&= \begin{bmatrix} C & -S \\ S & C \end{bmatrix}\begin{bmatrix} 0 \\ E_k \end{bmatrix} e^{-ikx} \\
&= E_k \begin{bmatrix} -S \\ C \end{bmatrix} e^{-ikx} \\
&= -E_k \begin{bmatrix} S \\ -C \end{bmatrix} e^{-ikx}.
\end{aligned} \tag{3.69}$$

However, note that we have a different rotation angle θ_k for the forward going and reverse going waves.

For the incident wave, $k > 0$, we have

$$\tan 2\theta_k = \frac{\hbar kc}{mc^2}, \tag{3.70}$$

and for the reflected wave, $k < 0$, we have

$$\tan 2\theta_k = \frac{-\hbar kc}{mc^2}. \tag{3.71}$$

The rotation angle for both cases can therefore be expressed as

$$\theta_k = \frac{1}{2} \operatorname{atan}\left(\left|\frac{\hbar k}{mc}\right|\right). \tag{3.72}$$

Exercise 3.3 Verify the Dirac current relationship.

Prove eq. (3.32).

Answer for Exercise 3.3

The components of the Schrödinger equation are

$$\begin{aligned} -i\hbar \frac{\partial \psi_1}{\partial t} &= -i\hbar c \frac{\partial \psi_1}{\partial x} + mc^2 \psi_2 \\ -i\hbar \frac{\partial \psi_2}{\partial t} &= mc^2 \psi_1 + i\hbar c \frac{\partial \psi_2}{\partial x}, \end{aligned} \tag{3.73}$$

The conjugates of these are

$$\begin{aligned} i\hbar \frac{\partial \psi_1^*}{\partial t} &= i\hbar c \frac{\partial \psi_1^*}{\partial x} + mc^2 \psi_2^* \\ i\hbar \frac{\partial \psi_2^*}{\partial t} &= mc^2 \psi_1^* - i\hbar c \frac{\partial \psi_2^*}{\partial x}. \end{aligned} \tag{3.74}$$

This gives

$$\begin{aligned} i\hbar \frac{\partial \rho}{\partial t} = &\left(i\hbar c \frac{\partial \psi_1^*}{\partial x} + mc^2 \psi_2^* \right) \psi_1 \\ &+ \psi_1^* \left(i\hbar c \frac{\partial \psi_1}{\partial x} - mc^2 \psi_2 \right) \\ &+ \left(mc^2 \psi_1^* - i\hbar c \frac{\partial \psi_2^*}{\partial x} \right) \psi_2 \\ &+ \psi_2^* \left(-mc^2 \psi_1 - i\hbar c \frac{\partial \psi_2}{\partial x} \right). \end{aligned} \tag{3.75}$$

All the non-derivative terms cancel leaving

$$\begin{aligned} \frac{1}{c} \frac{\partial \rho}{\partial t} &= \frac{\partial \psi_1^*}{\partial x} \psi_1 + \psi_1^* \frac{\partial \psi_1}{\partial x} - \frac{\partial \psi_2^*}{\partial x} \psi_2 - \psi_2^* \frac{\partial \psi_2}{\partial x} \\ &= \frac{\partial}{\partial x} \left(\psi_1^* \psi_1 - \psi_2^* \psi_2 \right). \end{aligned} \tag{3.76}$$

Exercise 3.4 Zitterbewegung in one dimension. (*2015 ps4 p1*)

Consider the Dirac Hamiltonian $H = c\hat{p}\sigma_z + mc^2\sigma_x$. Using the Heisenberg equations of motion, derive a second order equation of motion (eom) for the velocity operator $\hat{v} = d\hat{x}/dt$. For a state

$$\Psi = \begin{bmatrix} 1 \\ 0 \end{bmatrix} e^{ikx} \tag{3.77}$$

with $k = 0$, average this eom in state Ψ to get a homogeneous second order differential equation for $\langle \hat{v} \rangle$. Using this equation of motion and the initial conditions on the velocity and its time-derivative, obtain $\langle \hat{v} \rangle (t)$ and $\langle \hat{x}(t) \rangle$. Show that these oscillate with a rapid frequency $2mc^2/h$, with the oscillation of the position having an amplitude $\hbar/mc$ which is the Compton wavelength. This 'trembling' motion is called zitterbewegung.

Answer for Exercise 3.4

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Exercise 3.5 Jackiw-Rebbi problem. (*2015 ps4 p2*)

Recall that the energy of a relativistic particle is $E(p) = \sqrt{p^2c^2 + m^2c^4}$, which is independent of the sign of m. Thus $m > 0$ and $m < 0$ lead to the same dispersion relation. Set aside for now, the physical meaning of $m < 0$. Assume $V(x) = 0$ but let us assume the mass m is a function of position $m(x)$. This leads to

$$H = \begin{bmatrix} c\hat{p} & m(x)c^2 \\ m(x)c^2 & -c\hat{p} \end{bmatrix}. \tag{3.78}$$

Let $m(x)$ be such that $m(-x) = -m(x)$, i.e., an odd function of position which changes sign at $x = 0$.

a. Show that the operator $\mathcal{P}\widehat{\mathcal{P}}_{\text{Dirac}} = \sigma_y \mathcal{P}\widehat{\mathcal{P}}$ commutes with the Hamiltonian, where

$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{3.79}$$

is the y-Pauli matrix, and $\widehat{\mathcal{P}\mathcal{P}}$ is the parity operator which sends $x \to -x$.

b. Consider the wavefunction

$$\Phi(x) = \begin{bmatrix} f(x) \\ -if(x) \end{bmatrix}, \tag{3.80}$$

where $f(-x) = f(x)$ is an even function. Show $\Phi(x)$ is an eigenstate of $\widehat{\mathcal{P}\mathcal{P}}_{\text{Dirac}}$ with eigenvalue -1.

c. Next, assuming $m(x > 0) = m_0$ and $m(x < 0) = -m_0$, where $m_0 > 0$, find $f(x)$ such that $\Phi(x)$ is an eigenstate of H with zero energy.

d. Normalize the wavefunction $\Phi(x)$.

Answer for Exercise 3.5

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Exercise 3.6 Scattering off a potential step. (*2015 ps4 p3*)

Consider the 1D Dirac Hamiltonian as

$$H = \begin{bmatrix} c\hat{p} + V(x) & mc^2 \\ mc^2 & -c\hat{p} + V(x) \end{bmatrix} \tag{3.81}$$

where the operator $\hat{p} = -i\hbar\partial/\partial x$ is the rest mass, and c is the speed of light, and with 2-component wavefunctions

$$\Psi(x,t) \equiv \begin{bmatrix} \psi_1(x,t) \\ \psi_2(x,t) \end{bmatrix} \tag{3.82}$$

such that $i\hbar\partial\Psi(x,t)/\partial t = H\Psi(x,t)$. Assuming a potential step, where $V(x<0) = 0$ and $V(x>0) = V_0$, with $V_0 > 0$ as in class, complete the details of the scattering onto the step which was done in class. Discuss the incident current, reflected current, and transmitted current for the case where the incident energy is such that $E > 0$ and $V_0 > 2mc^2$, and $E > 0$ and $V_0 < 2mc^2$. Draw pictures to illustrate the parabola and the location in momentum of the incident and reflected particles.

Answer for Exercise 3.6

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Exercise 3.7 **Alternate Dirac equation representation.** (*phy1520 2015 midterm pr. 2*)

Given an alternate representation of the Dirac equation

$$H = \begin{bmatrix} mc^2 + V_0 & c\hat{p} \\ c\hat{p} & -mc^2 + V_0 \end{bmatrix}, \tag{3.83}$$

calculate

a. the constant momentum plane wave solutions,
b. the constant momentum hyperbolic solutions,
c. the Heisenberg velocity operator $\hat{v}$, and
d. find the form of the probability density current.

Answer for Exercise 3.7

Part a. The action of the Hamiltonian on

$$\psi = e^{ikx - iEt/\hbar} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} \tag{3.84}$$

is

$$
\begin{aligned}
H\psi &= \begin{bmatrix} mc^2 + V_0 & c(-i\hbar)ik \\ c(-i\hbar)ik & -mc^2 + V_0 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} e^{ikx - iEt/\hbar} \\
&= \begin{bmatrix} mc^2 + V_0 & c\hbar k \\ c\hbar k & -mc^2 + V_0 \end{bmatrix} \psi.
\end{aligned}
\tag{3.85}
$$

Writing

$$
H_k = \begin{bmatrix} mc^2 + V_0 & c\hbar k \\ c\hbar k & -mc^2 + V_0 \end{bmatrix}
\tag{3.86}
$$

the characteristic equation is

$$
\begin{aligned}
0 &= (mc^2 + V_0 - \lambda)(-mc^2 + V_0 - \lambda) - (c\hbar k)^2 \\
&= \left((\lambda - V_0)^2 - (mc^2)^2 \right) - (c\hbar k)^2,
\end{aligned}
\tag{3.87}
$$

so

$$
\lambda = V_0 \pm \epsilon,
\tag{3.88}
$$

where

$$
\epsilon^2 = (mc^2)^2 + (c\hbar k)^2.
\tag{3.89}
$$

We've got

$$
\begin{aligned}
H - (V_0 + \epsilon) &= \begin{bmatrix} mc^2 - \epsilon & c\hbar k \\ c\hbar k & -mc^2 - \epsilon \end{bmatrix} \\
H - (V_0 - \epsilon) &= \begin{bmatrix} mc^2 + \epsilon & c\hbar k \\ c\hbar k & -mc^2 + \epsilon \end{bmatrix},
\end{aligned}
\tag{3.90}
$$

so the eigenkets are

$$
\begin{aligned}
|V_0 + \epsilon\rangle &\propto \begin{bmatrix} -c\hbar k \\ mc^2 - \epsilon \end{bmatrix} \\
|V_0 - \epsilon\rangle &\propto \begin{bmatrix} -c\hbar k \\ mc^2 + \epsilon \end{bmatrix}.
\end{aligned}
\tag{3.91}
$$

Up to an arbitrary phase for each, these are

$$\begin{aligned}
|V_0 + \epsilon\rangle &= \frac{1}{\sqrt{2\epsilon(\epsilon - mc^2)}}\begin{bmatrix} c\hbar k \\ \epsilon - mc^2 \end{bmatrix} \\
|V_0 - \epsilon\rangle &= \frac{1}{\sqrt{2\epsilon(\epsilon + mc^2)}}\begin{bmatrix} -c\hbar k \\ \epsilon + mc^2 \end{bmatrix}
\end{aligned} \tag{3.92}$$

We can now write

$$H_k = E\begin{bmatrix} V_0 + \epsilon & 0 \\ 0 & V_0 - \epsilon \end{bmatrix}E^{-1}, \tag{3.93}$$

where

$$\begin{aligned}
E &= \frac{1}{\sqrt{2\epsilon}}\begin{bmatrix} \frac{c\hbar k}{\sqrt{\epsilon - mc^2}} & -\frac{c\hbar k}{\sqrt{\epsilon + mc^2}} \\ \sqrt{\epsilon - mc^2} & \sqrt{\epsilon + mc^2} \end{bmatrix}, \qquad k > 0 \\
E &= \frac{1}{\sqrt{2\epsilon}}\begin{bmatrix} -\frac{c\hbar k}{\sqrt{\epsilon - mc^2}} & -\frac{c\hbar k}{\sqrt{\epsilon + mc^2}} \\ -\sqrt{\epsilon - mc^2} & \sqrt{\epsilon + mc^2} \end{bmatrix}, \qquad k < 0.
\end{aligned} \tag{3.94}$$

Here the signs have been adjusted to ensure the transformation matrix has a unit determinant.
Observe that there's redundancy in this matrix since $c\hbar|k|/\sqrt{\epsilon - mc^2} = \sqrt{\epsilon + mc^2}$, and $c\hbar|k|/\sqrt{\epsilon + mc^2} = \sqrt{\epsilon - mc^2}$, which allows the transformation matrix to be written in the form of a rotation matrix

$$\begin{aligned}
E &= \frac{1}{\sqrt{2\epsilon}}\begin{bmatrix} \frac{c\hbar k}{\sqrt{\epsilon - mc^2}} & -\frac{c\hbar k}{\sqrt{\epsilon + mc^2}} \\ \frac{c\hbar k}{\sqrt{\epsilon + mc^2}} & \frac{c\hbar k}{\sqrt{\epsilon - mc^2}} \end{bmatrix}, \qquad k > 0 \\
E &= \frac{1}{\sqrt{2\epsilon}}\begin{bmatrix} -\frac{c\hbar k}{\sqrt{\epsilon - mc^2}} & -\frac{c\hbar k}{\sqrt{\epsilon + mc^2}} \\ \frac{c\hbar k}{\sqrt{\epsilon + mc^2}} & -\frac{c\hbar k}{\sqrt{\epsilon - mc^2}} \end{bmatrix}, \qquad k < 0
\end{aligned} \tag{3.95}$$

With

$$\begin{aligned}
\cos\theta &= \frac{c\hbar|k|}{\sqrt{2\epsilon(\epsilon - mc^2)}} = \frac{\sqrt{\epsilon + mc^2}}{\sqrt{2\epsilon}} \\
\sin\theta &= \frac{c\hbar k}{\sqrt{2\epsilon(\epsilon + mc^2)}} = \frac{\operatorname{sgn}(k)\sqrt{\epsilon - mc^2}}{\sqrt{2\epsilon}},
\end{aligned} \tag{3.96}$$

the transformation matrix (and eigenkets) is

$$\boxed{E = \begin{bmatrix} |V_0 + \epsilon\rangle & |V_0 - \epsilon\rangle \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}.} \tag{3.97}$$

Observe that eq. (3.96) can be simplified by using double angle formulas

$$
\begin{aligned}
\cos(2\theta) &= \frac{\left(\epsilon + mc^2\right)}{2\epsilon} - \frac{\left(\epsilon - mc^2\right)}{2\epsilon} \\
&= \frac{1}{2\epsilon}\left(\epsilon + mc^2 - \epsilon + mc^2\right) \\
&= \frac{mc^2}{\epsilon},
\end{aligned}
\tag{3.98}
$$

and

$$
\begin{aligned}
\sin(2\theta) &= 2\frac{1}{2\epsilon}\operatorname{sgn}(k)\sqrt{\epsilon^2 - (mc^2)^2} \\
&= \frac{\hbar kc}{\epsilon}.
\end{aligned}
\tag{3.99}
$$

This allows all the θ dependence on $\hbar kc$ and mc^2 to be expressed as a ratio of momenta

$$
\boxed{\tan(2\theta) = \frac{\hbar k}{mc}.}
\tag{3.100}
$$

Part b. For a wave function of the form

$$
\psi = e^{kx - iEt/\hbar}\begin{bmatrix}\psi_1 \\ \psi_2\end{bmatrix},
\tag{3.101}
$$

some of the work above can be recycled if we substitute $k \rightarrow -ik$, which yields unnormalized eigenfunctions

$$
\begin{aligned}
\lvert V_0 + \epsilon\rangle &\propto \begin{bmatrix} ic\hbar k \\ mc^2 - \epsilon \end{bmatrix} \\
\lvert V_0 - \epsilon\rangle &\propto \begin{bmatrix} ic\hbar k \\ mc^2 + \epsilon \end{bmatrix},
\end{aligned}
\tag{3.102}
$$

where

$$
\epsilon^2 = (mc^2)^2 - (c\hbar k)^2.
\tag{3.103}
$$

The squared magnitude of these wavefunctions are

$$
\begin{aligned}
(c\hbar k)^2 + (mc^2 \mp \epsilon)^2 &= (c\hbar k)^2 + (mc^2)^2 + \epsilon^2 \mp 2mc^2\epsilon \\
&= (c\hbar k)^2 + (mc^2)^2 + (mc^2)^2 \mp (c\hbar k)^2 - 2mc^2\epsilon \\
&= 2(mc^2)^2 \mp 2mc^2\epsilon \\
&= 2mc^2(mc^2 \mp \epsilon),
\end{aligned}
\tag{3.104}
$$

so, up to a constant phase for each, the normalized kets are

$$
\begin{aligned}
|V_0 + \epsilon\rangle &= \frac{1}{\sqrt{2mc^2(mc^2 - \epsilon)}} \begin{bmatrix} ic\hbar k \\ mc^2 - \epsilon \end{bmatrix} \\
|V_0 - \epsilon\rangle &= \frac{1}{\sqrt{2mc^2(mc^2 + \epsilon)}} \begin{bmatrix} ic\hbar k \\ mc^2 + \epsilon \end{bmatrix},
\end{aligned}
\tag{3.105}
$$

After the $k \rightarrow -ik$ substitution, H_k is not Hermitian, so these kets aren't expected to be orthonormal, which is readily verified

$$
\begin{aligned}
\langle V_0 + \epsilon | V_0 - \epsilon\rangle &= \frac{1}{\sqrt{2mc^2(mc^2 - \epsilon)}} \frac{1}{\sqrt{2mc^2(mc^2 + \epsilon)}} \begin{bmatrix} -ic\hbar k & mc^2 - \epsilon \end{bmatrix} \begin{bmatrix} ic\hbar k \\ mc^2 + \epsilon \end{bmatrix} \\
&= \frac{2(c\hbar k)^2}{2mc^2\sqrt{(\hbar kc)^2}} \\
&= \operatorname{sgn}(k)\frac{\hbar k}{mc}.
\end{aligned}
\tag{3.106}
$$

Part c.

$$
\begin{aligned}
\hat{v} &= \frac{1}{i\hbar}[\hat{x}, H] \\
&= \frac{1}{i\hbar}\left[\hat{x}, mc^2\sigma_z + V_0 + c\hat{p}\sigma_x\right] \\
&= \frac{c\sigma_x}{i\hbar}[\hat{x}, \hat{p}] \\
&= c\sigma_x.
\end{aligned}
\tag{3.107}
$$

Part d. Acting against a completely general wavefunction the Hamiltonian action $H\psi$ is

$$
\begin{aligned}
i\hbar\frac{\partial\psi}{\partial t} &= mc^2\sigma_z\psi + V_0\psi + c\hat{p}\sigma_x\psi \\
&= mc^2\sigma_z\psi + V_0\psi - i\hbar c\sigma_x\frac{\partial\psi}{\partial x}.
\end{aligned}
\tag{3.108}
$$

Conversely, the conjugate $(H\psi)^\dagger$ is

$$-i\hbar\frac{\partial\psi^\dagger}{\partial t} = mc^2\psi^\dagger\sigma_z + V_0\psi^\dagger + i\hbar c\frac{\partial\psi^\dagger}{\partial x}\sigma_x. \tag{3.109}$$

These give

$$\begin{aligned} i\hbar\psi^\dagger\frac{\partial\psi}{\partial t} &= mc^2\psi^\dagger\sigma_z\psi + V_0\psi^\dagger\psi - i\hbar c\psi^\dagger\sigma_x\frac{\partial\psi}{\partial x} \\ -i\hbar\frac{\partial\psi^\dagger}{\partial t}\psi &= mc^2\psi^\dagger\sigma_z\psi + V_0\psi^\dagger\psi + i\hbar c\frac{\partial\psi^\dagger}{\partial x}\sigma_x\psi. \end{aligned} \tag{3.110}$$

Taking differences

$$\psi^\dagger\frac{\partial\psi}{\partial t} + \frac{\partial\psi^\dagger}{\partial t}\psi = -c\psi^\dagger\sigma_x\frac{\partial\psi}{\partial x} - c\frac{\partial\psi^\dagger}{\partial x}\sigma_x\psi, \tag{3.111}$$

or

$$0 = \frac{\partial}{\partial t}\left(\psi^\dagger\psi\right) + \frac{\partial}{\partial x}\left(c\psi^\dagger\sigma_x\psi\right). \tag{3.112}$$

The probability current still has the usual form $\rho = \psi^\dagger\psi = \psi_1^*\psi_1 + \psi_2^*\psi_2$, but the probability current with this representation of the Dirac Hamiltonian is

$$\begin{aligned} j &= c\psi^\dagger\sigma_x\psi \\ &= c\begin{bmatrix}\psi_1^* & \psi_2^*\end{bmatrix}\begin{bmatrix}\psi_2 \\ \psi_1\end{bmatrix} \\ &= c\left(\psi_1^*\psi_2 + \psi_2^*\psi_1\right). \end{aligned} \tag{3.113}$$

4 SYMMETRIES IN QUANTUM MECHANICS

4.1 SYMMETRY IN CLASSICAL MECHANICS

In a classical context considering a Hamiltonian

$$H(q_i, p_i), \tag{4.1}$$

a symmetry means that certain q_i don't appear. In that case the rate of change of one of the generalized momenta is zero

$$\frac{dp_k}{dt} = -\frac{\partial H}{\partial q_k} = 0, \tag{4.2}$$

so p_k is a constant of motion. This simplifies the problem by reducing the number of degrees of freedom. Another aspect of such a symmetry is that it relates trajectories. For example, assuming a rotational symmetry as in fig. 4.1.

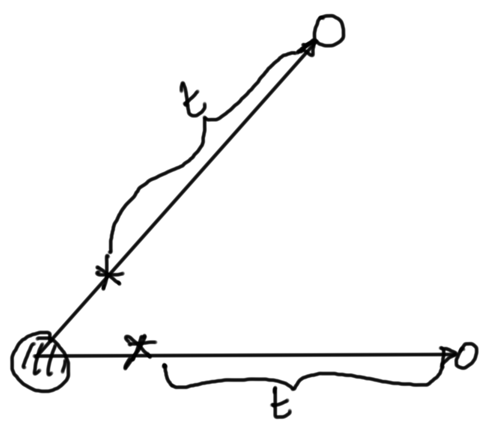


Figure 4.1: Trajectory under rotational symmetry.

the trajectory of a particle after rotation is related by rotation to the trajectory of the unrotated particle.

4.2 SYMMETRY IN QUANTUM MECHANICS

Suppose that we have a symmetry operation that takes states from

$$|\psi\rangle \rightarrow |U\psi\rangle \tag{4.3}$$

$$|\phi\rangle \rightarrow |U\phi\rangle\,, \tag{4.4}$$

we expect that

$$|\langle\psi|\phi\rangle|^2 = |\langle U\psi|U\phi\rangle|^2. \tag{4.5}$$

This won't hold true for a general operator. Two cases where this does hold true is when

- $\langle\psi|\phi\rangle = \langle U\psi|U\phi\rangle$. Here U is unitary, and the equivalence follows from

$$\langle U\psi|U\phi\rangle = \langle\psi|\, U^\dagger U\phi = \langle\psi|\, 1\phi = \langle\psi|\phi\rangle\,. \tag{4.6}$$

- $\langle\psi|\phi\rangle = \langle U\psi|U\phi\rangle^*$. Here U is anti-unitary.

Unitary case If an "observable" is not changed by a unitary operation representing a symmetry we must have

$$\begin{aligned}\langle\psi|\,\hat{A}\,|\psi\rangle &\rightarrow \langle U\psi|\,\hat{A}\,|U\psi\rangle \\ &= \langle\psi|\,U^\dagger\hat{A}U\,|\psi\rangle\,,\end{aligned} \tag{4.7}$$

so

$$U^\dagger\hat{A}U = \hat{A}, \tag{4.8}$$

or

$$\boxed{\hat{A}U = U\hat{A}.} \tag{4.9}$$

An observable that is unchanged by a unitary symmetry commutes $\left[\hat{A}, U\right]$ with the operator U for that transformation.

Symmetries of the Hamiltonian Given

$$[H, U] = 0, \tag{4.10}$$

H is invariant.
Given

$$H |\phi_n\rangle = \epsilon_n |\phi_n\rangle . \tag{4.11}$$

$$\begin{aligned} UH |\phi_n\rangle &= HU |\phi_n\rangle \\ &= \epsilon_n U |\phi_n\rangle \end{aligned} \tag{4.12}$$

Such a state

$$|\psi_n\rangle = U |\phi_n\rangle \tag{4.13}$$

is also an eigenstate with the same energy.
Suppose this process is repeated, finding other states

$$U |\psi_n\rangle = |\chi_n\rangle \tag{4.14}$$

$$U |\chi_n\rangle = |\alpha_n\rangle \tag{4.15}$$

Because such a transformation only generates states with the initial energy, this process cannot continue forever. At some point this process will enumerate a fixed size set of states. These states can be orthonormalized.

We can say that symmetry operations are generators of a group. For a set of symmetry operations we can

- Form products that lie in a closed set

$$U_1 U_2 = U_3 \tag{4.16}$$

- can define an inverse

$$U \leftrightarrow U^{-1}. \tag{4.17}$$

- obeys associative rules for multiplication

$$U_1(U_2 U_3) = (U_1 U_2)U_3. \tag{4.18}$$

- has an identity operation.

When H has a symmetry, then degenerate eigenstates form irreducible representations (which cannot be further block diagonalized).

Parity symmetry

Example 4.1: Inversion.

Given a state and a parity operation $\hat{\Pi}$, with the transformation

$$|\psi\rangle \rightarrow \hat{\Pi} |\psi\rangle \tag{4.19}$$

In one dimension, the parity operation is just inversion. In two dimensions, this is a set of flipping operations on two axes fig. 4.2.

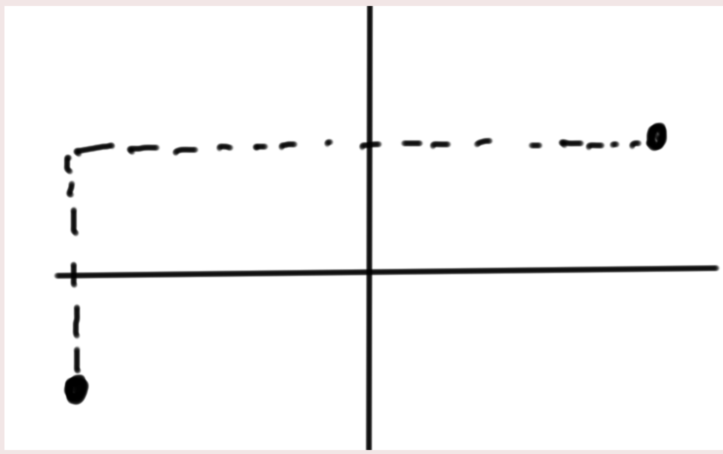


Figure 4.2: 2D parity operation.

The operational effects of this operator are

$$\begin{aligned} \hat{x} &\rightarrow -\hat{x} \\ \hat{p} &\rightarrow -\hat{p}. \end{aligned} \tag{4.20}$$

Acting again with the parity operator produces the original value, so it is its own inverse, and $\hat{\Pi}^\dagger = \hat{\Pi} = \hat{\Pi}^{-1}$. In an expectation value

$$\left\langle \hat{\Pi}\psi \right| \hat{x} \left| \hat{\Pi}\psi \right\rangle = - \langle \psi | \hat{x} | \psi \rangle . \tag{4.21}$$

This means that

$$\hat{\Pi}^\dagger \hat{x} \hat{\Pi} = -\hat{x}, \tag{4.22}$$

or

$$\hat{x}\hat{\Pi} = -\hat{\Pi}\hat{x}, \tag{4.23}$$

$$\begin{aligned}\hat{x}\hat{\Pi}\,|x_0\rangle &= -\hat{\Pi}\hat{x}\,|x_0\rangle \\ &= -\hat{\Pi}x_0\,|x_0\rangle \\ &= -x_0\hat{\Pi}\,|x_0\rangle\end{aligned} \tag{4.24}$$

so

$$\hat{\Pi}\,|x_0\rangle = |-x_0\rangle\,. \tag{4.25}$$

Acting on a wave function

$$\begin{aligned}\langle x|\,\hat{\Pi}\,|\psi\rangle &= \langle -x|\psi\rangle \\ &= \psi(-x).\end{aligned} \tag{4.26}$$

What does this mean for eigenfunctions. Eigenfunctions are supposed to form irreducible representations of the group. The group has just two elements

$$\left\{1, \hat{\Pi}\right\}, \tag{4.27}$$

where $\hat{\Pi}^2 = 1$.

Suppose we have a Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}), \tag{4.28}$$

where $V(\hat{x})$ is even, or $\left[V(\hat{x}), \hat{\Pi}\right] = 0$. The squared momentum commutes with the parity operator

$$\begin{aligned}\left[\hat{p}^2, \hat{\Pi}\right] &= \hat{p}^2\hat{\Pi} - \hat{\Pi}\hat{p}^2 \\ &= \hat{p}^2\hat{\Pi} - (\hat{\Pi}\hat{p})\hat{p} \\ &= \hat{p}^2\hat{\Pi} - (-\hat{p}\hat{\Pi})\hat{p} \\ &= \hat{p}^2\hat{\Pi} + \hat{p}(-\hat{p}\hat{\Pi}) \\ &= 0.\end{aligned} \tag{4.29}$$

Only two functions are possible in the symmetry set $\left\{\Psi(x), \hat{\Pi}\Psi(x)\right\}$, since

$$\begin{aligned}\hat{\Pi}^2\Psi(x) &= \hat{\Pi}\Psi(-x) \\ &= \Psi(x).\end{aligned} \tag{4.30}$$

This symmetry severely restricts the possible solutions, making it so there can be only one dimensional forms of this problem with solutions that are either even or odd respectively

$$\begin{aligned}\phi_e(x) &= \psi(x) + \psi(-x) \\ \phi_o(x) &= \psi(x) - \psi(-x).\end{aligned} \tag{4.31}$$

Parity (review)

$$\hat{\Pi}\hat{x}\hat{\Pi} = -\hat{x} \tag{4.32}$$

$$\hat{\Pi}\hat{p}\hat{\Pi} = -\hat{p} \tag{4.33}$$

These are polar vectors, in contrast to an axial vector such as $\mathbf{L} = \mathbf{r} \times \mathbf{p}$.

$$\hat{\Pi}^2 = 1 \tag{4.34}$$

$$\Psi(x) \rightarrow \Psi(-x) \tag{4.35}$$

If $\left[\hat{\Pi}, \hat{H}\right] = 0$ then all the eigenstates are either

- even: $\hat{\Pi}$ eigenvalue is $+1$.
- odd: $\hat{\Pi}$ eigenvalue is -1.

Note on parity in multiple dimensions A Hamiltonian can be constructed with parity symmetries in one or more directions. For example, given a potential

$$V(x, y) = ax + bx^2 + cy^2, \tag{4.36}$$

We don't have parity symmetry for $\mathbf{x} = (x, y)$, but do have parity symmetry in the y direction. Assuming a separated variables form for the wave function, say $\psi(x, y) = X(x)Y(y)$, we can't say much about X on the grounds of symmetry considerations only, but know that Y has to be either an even or odd function.

4.3 TRANSLATIONS

Define a (continuous) translation operator

$$\hat{T}_\epsilon \left|x\right\rangle = \left|x + \epsilon\right\rangle \tag{4.37}$$

The action of this operator is sketched in fig. 4.3.

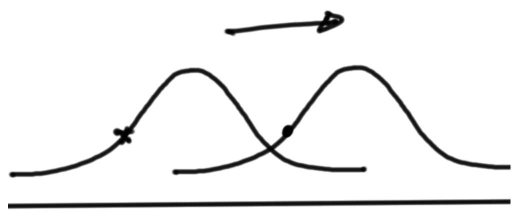


Figure 4.3: Translation operation.

This is a unitary operator

$$\hat{T}_{-\epsilon} = \hat{T}_{\epsilon}^{\dagger} = \hat{T}_{\epsilon}^{-1} \tag{4.38}$$

In a position basis, the action of this operator is

$$\begin{aligned} \langle x| \hat{T}_{\epsilon} |\psi\rangle &= \langle x - \epsilon|\psi\rangle \\ &= \psi(x - \epsilon) \end{aligned} \tag{4.39}$$

$$\Psi(x - \epsilon) \approx \Psi(x) - \epsilon \frac{\partial \Psi}{\partial x} \tag{4.40}$$

$$\langle x| \hat{T}_{\epsilon} |\Psi\rangle = \langle x|\Psi\rangle - \frac{\epsilon}{\hbar} \langle x| i\hat{p} |\Psi\rangle \tag{4.41}$$

$$\hat{T}_{\epsilon} \approx \left(1 - i\frac{\epsilon}{\hbar}\hat{p}\right) \tag{4.42}$$

A non-infinitesimal translation can be composed of many small translations, as sketched in fig. 4.4.

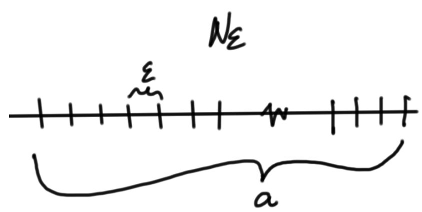


Figure 4.4: Composition of small translations.

For $\epsilon \to 0, N \to \infty, N\epsilon = a$, the total translation operator is

$$
\begin{aligned}
\hat{T}_a &= \hat{T}_\epsilon^N \\
&= \lim_{\epsilon\to 0, N\to\infty, N\epsilon=a} \left(1 - \frac{\epsilon}{\hbar}\hat{p}\right)^N \\
&= e^{-ia\hat{p}/\hbar}
\end{aligned}
\tag{4.43}
$$

The momentum $\hat{p}$ is called a "Generator" of translations. If a Hamiltonian H is translationally invariant, then

$$\left[\hat{T}_a, H\right] = 0, \qquad \forall a. \tag{4.44}$$

This means that momentum will be a good quantum number

$$[\hat{p}, H] = 0. \tag{4.45}$$

4.4 ROTATIONS

Rotations form a non-Abelian group , since the order of rotations $\hat{R}_1\hat{R}_2 \neq \hat{R}_2\hat{R}_1$.

Given a rotation acting on a ket

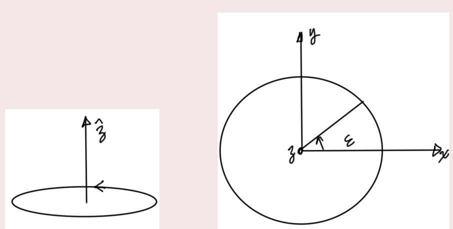
$$\hat{R}\left|\mathbf{r}\right\rangle = \left|R\mathbf{r}\right\rangle, \tag{4.46}$$

observe that the action of the rotation operator on a wave function is inverted

$$
\begin{aligned}
\langle\mathbf{r}|\,\hat{R}\,|\Psi\rangle &= \left\langle R^{-1}\mathbf{r}\right|\,|\Psi\rangle \\
&= \Psi(R^{-1}\mathbf{r}).
\end{aligned}
\tag{4.47}
$$

Example 4.2: Z axis normal rotation

Consider an infinitesimal rotation about the z-axis as sketched in fig. 4.5.



(a) (b)

Figure 4.5: Rotation about z-axis.

$$
\begin{aligned}
x' &= x - \epsilon y \\
y' &= y + \epsilon y \\
z' &= z
\end{aligned}
\tag{4.48}
$$

The rotated wave function is

$$
\begin{aligned}
\tilde{\Psi}(x, y, z) &= \Psi(x + \epsilon y, y - \epsilon x, z) \\
&= \Psi(x, y, z) + \epsilon y \underbrace{\boxed{\frac{\partial \Psi}{\partial x}}}_{i\hat{p}_x/\hbar} - \epsilon x \underbrace{\boxed{\frac{\partial \Psi}{\partial y}}}_{i\hat{p}_y/\hbar} .
\end{aligned}
\tag{4.49}
$$

The state must then transform as

$$
\left|\tilde{\Psi}\right\rangle = \left(1 + i\frac{\epsilon}{\hbar}\hat{y}\hat{p}_x - i\frac{\epsilon}{\hbar}\hat{x}\hat{p}_y\right)|\Psi\rangle . \tag{4.50}
$$

Observe that the combination $\hat{x}\hat{p}_y - \hat{y}\hat{p}_x$ is the $\hat{L}_z$ component of angular momentum $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$, so the infinitesimal rotation can be written

$$
\boxed{\hat{R}_z(\epsilon)\,|\Psi\rangle = \left(1 - i\frac{\epsilon}{\hbar}\hat{L}_z\right)|\Psi\rangle .} \tag{4.51}
$$

For a finite rotation $\epsilon \to 0, N \to \infty, \phi = \epsilon N$, the total rotation is

$$
\hat{R}_z(\phi) = \left(1 - \frac{i\epsilon}{\hbar}\hat{L}_z\right)^N , \tag{4.52}
$$

or

$$
\boxed{\hat{R}_z(\phi) = e^{-i\frac{\phi}{\hbar}\hat{L}_z}.} \tag{4.53}
$$

Note that $\left[\hat{L}_x, \hat{L}_y\right] \neq 0$.

By construction using Euler angles or any other method, a general rotation will include contributions from components of all the angular momentum operator, and will have the structure

$$
\boxed{\hat{R}_{\hat{\mathbf{n}}}(\phi) = e^{-i\frac{\phi}{\hbar}\left(\hat{\mathbf{L}}\cdot\hat{\mathbf{n}}\right)}.} \tag{4.54}
$$

Rotationally invariant $\hat{H}$. Given a rotationally invariant Hamiltonian

$$\left[\hat{R}_{\hat{\mathbf{n}}}(\phi), \hat{H}\right] = 0 \qquad \forall \hat{\mathbf{n}}, \phi, \tag{4.55}$$

then every

$$\left[\mathbf{L} \cdot \hat{\mathbf{n}}, \hat{H}\right] = 0, \tag{4.56}$$

or

$$\left[L_i, \hat{H}\right] = 0, \tag{4.57}$$

Non-Abelian implies degeneracies in the spectrum.

4.5 TIME-REVERSAL

Imagine that we have something moving along a curve at time $t = 0$, and ending up at the final position at time $t = t_f$, as sketched in fig. 4.6.

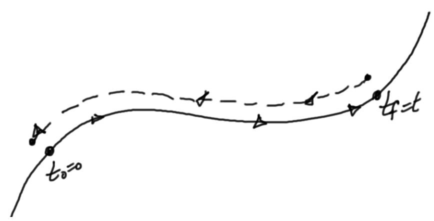


Figure 4.6: Time reversal trajectory.

Now imagine that we flip the direction of motion (i.e. flipping the velocity) and run time backwards so the final-time state becomes the initial state.

If the time reversal operator is designated $\hat{\Theta}$, with operation

$$\hat{\Theta} \left|\Psi\right\rangle = \left|\tilde{\Psi}\right\rangle, \tag{4.58}$$

so that

$$\hat{\Theta}^{-1} e^{-i\hat{H}t/\hbar} \hat{\Theta} \left|\Psi(t)\right\rangle = \left|\Psi(0)\right\rangle, \tag{4.59}$$

or

$$\hat{\Theta}^{-1} e^{-i\hat{H}t/\hbar} \hat{\Theta} \left|\Psi(0)\right\rangle = \left|\Psi(-t)\right\rangle. \tag{4.60}$$

Time reversal (cont.) Given a time reversed state

$$\left|\tilde{\Psi}(t)\right\rangle = \Theta \left|\Psi(0)\right\rangle \tag{4.61}$$

which can alternately be written

$$\Theta^{-1}\left|\tilde{\Psi}(t)\right\rangle = \left|\Psi(-t)\right\rangle = e^{i\hat{H}t/\hbar}\left|\Psi(0)\right\rangle \tag{4.62}$$

The left hand side can be expanded as the evolution of the state as found at time $-t$

$$\begin{aligned} \Theta^{-1}\left|\tilde{\Psi}(t)\right\rangle &= \Theta^{-1}e^{-i\hat{H}t/\hbar}\left|\tilde{\Psi}(-t)\right\rangle \\ &= \Theta^{-1}e^{-i\hat{H}t/\hbar}\Theta\left|\Psi(0)\right\rangle. \end{aligned} \tag{4.63}$$

To first order for a small time increment δt, we have

$$\left(1 + i\frac{\hat{H}}{\hbar}\delta t\right)\left|\Psi(0)\right\rangle = \Theta^{-1}\left(1 - i\frac{\hat{H}}{\hbar}\delta t\right)\Theta\left|\Psi(0)\right\rangle, \tag{4.64}$$

or

$$i\frac{\hat{H}}{\hbar}\delta t\left|\Psi(0)\right\rangle = \Theta^{-1}(-i)\frac{\hat{H}}{\hbar}\delta t\Theta\left|\Psi(0)\right\rangle. \tag{4.65}$$

Since this holds for any state $\left|\Psi(0)\right\rangle$, the time reversal operator satisfies

$$i\hat{H} = \Theta^{-1}(-i)\hat{H}\Theta. \tag{4.66}$$

Note that the factors of i have not been canceled on purpose, since we are allowing for the time reversal operator to not necessarily commute with imaginary numbers.

There are two possible solutions

- If Θ is unitary where $\Theta i = i\Theta$, then

  $$\hat{H} = -\Theta^{-1}\hat{H}\Theta, \tag{4.67}$$

  or

  $$\Theta\hat{H} = -\hat{H}\Theta. \tag{4.68}$$

  Consider the implications of this on energy eigenstates

  $$\hat{H}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle, \tag{4.69}$$

$$\Theta\hat{H}\left|\Psi_n\right\rangle = E_n\Theta\left|\Psi_n\right\rangle, \tag{4.70}$$

but

$$-\hat{H}\Theta\left|\Psi_n\right\rangle = E_n\Theta\left|\Psi_n\right\rangle, \tag{4.71}$$

or

$$\hat{H}\left(\Theta\left|\Psi_n\right\rangle\right) = -E_n\left(\Theta\left|\Psi_n\right\rangle\right). \tag{4.72}$$

This would mean that $\left(\Theta\left|\Psi_n\right\rangle\right)$ is an eigenket of $\hat{H}$, but with a negative energy eigenvalue.

- Θ is antiunitary, where $\Theta i = -i\Theta$.

  This time

$$i\hat{H} = i\Theta^{-1}\hat{H}\Theta, \tag{4.73}$$

so

$$\Theta\hat{H} = \hat{H}\Theta. \tag{4.74}$$

Acting on an energy eigenket, we've got

$$\Theta\hat{H}\left|\Psi_n\right\rangle = E_n\left(\Theta\left|\Psi_n\right\rangle\right), \tag{4.75}$$

and

$$\left(\hat{H}\Theta\right)\left|\Psi_n\right\rangle = \hat{H}\left(\Theta\left|\Psi_n\right\rangle\right), \tag{4.76}$$

so $\Theta\left|\Psi_n\right\rangle$ is an eigenstate with energy E_n.

What properties do we expect from Θ? We expect

$$\begin{aligned}\hat{x} &\rightarrow \hat{x}\\ \hat{p} &\rightarrow -\hat{p}\\ \hat{\mathbf{L}} &\rightarrow -\hat{\mathbf{L}}\end{aligned} \tag{4.77}$$

where we have a sign flip in the time dependent momentum operator (and therefore angular momentum), but not for position. If we have

$$\Theta^{-1}\hat{x}\Theta = \hat{x}, \tag{4.78}$$

if that's true, then how about the momentum operator in the position basis

$$\begin{aligned}
\Theta^{-1}\hat{p}\Theta &= \Theta^{-1}\left(-i\hbar\frac{\partial}{\partial x}\right)\Theta \\
&= \Theta^{-1}(-i\hbar)\Theta\frac{\partial}{\partial x} \\
&= i\hbar\Theta^{-1}\Theta\frac{\partial}{\partial x} \\
&= -\hat{p}.
\end{aligned} \tag{4.79}$$

How about the x, p commutator? For that we have

$$\begin{aligned}
\Theta^{-1}[\hat{x},\hat{p}]\Theta &= \Theta^{-1}(i\hbar)\Theta \\
&= -i\hbar\Theta^{-1}\Theta \\
&= -[\hat{x},\hat{p}].
\end{aligned} \tag{4.80}$$

For the the angular momentum operators

$$\hat{L}_i = \epsilon_{ijk}\hat{r}_j\hat{p}_k, \tag{4.81}$$

the time reversal operator should flip the sign due to its action on $\hat{p}_k$.

Time reversal acting on spin 1/2 (Fermions). Attempt I. Consider two spin states $|\uparrow\rangle, |\downarrow\rangle$. What should the action of the time reversal operator on such a state be? Let's (incorrectly) start by supposing that the time reversal operator effects are

$$\begin{aligned}
\Theta|\uparrow\rangle &\stackrel{?}{=} |\downarrow\rangle \\
\Theta|\downarrow\rangle &\stackrel{?}{=} |\uparrow\rangle.
\end{aligned} \tag{4.82}$$

Given a general state so that if

$$|\Psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle, \tag{4.83}$$

the action of the time reversal operator would be

$$\Theta|\Psi\rangle = a^*|\downarrow\rangle + b^*|\uparrow\rangle. \tag{4.84}$$

That action is:

$$
\begin{aligned}
a &\rightarrow b^* \\
b &\rightarrow a^*
\end{aligned}
\tag{4.85}
$$

Let's consider whether or not such an action a spin operator with properties

$$
\left[\hat{S}_i, \hat{S}_j\right] = i\epsilon_{ijk}\hat{S}_k. \tag{4.86}
$$

produce the desired inversion of sign

$$
\Theta^{-1}\hat{S}_i\Theta = -\hat{S}_i. \tag{4.87}
$$

The expectations of the spin operators (without any application of time reversal) are

$$
\begin{aligned}
\langle\Psi|\,\hat{S}_x\,|\Psi\rangle &= \frac{\hbar}{2}\left(a^*\,\langle\uparrow| + b^*\,\langle\downarrow|\right)\sigma_x\left(a\,|\uparrow\rangle + b\,|\downarrow\rangle\right) \\
&= \frac{\hbar}{2}\left(a^*\,\langle\uparrow| + b^*\,\langle\downarrow|\right)\left(a\,|\downarrow\rangle + b\,|\uparrow\rangle\right) \\
&= \frac{\hbar}{2}\left(a^*b + b^*a\right),
\end{aligned}
\tag{4.88}
$$

$$
\begin{aligned}
\langle\Psi|\,\hat{S}_y\,|\Psi\rangle &= \frac{\hbar}{2}\left(a^*\,\langle\uparrow| + b^*\,\langle\downarrow|\right)\sigma_y\left(a\,|\uparrow\rangle + b\,|\downarrow\rangle\right) \\
&= \frac{i\hbar}{2}\left(a^*\,\langle\uparrow| + b^*\,\langle\downarrow|\right)\left(a\,|\downarrow\rangle - b\,|\uparrow\rangle\right) \\
&= \frac{\hbar}{2i}\left(a^*b - b^*a\right),
\end{aligned}
\tag{4.89}
$$

$$
\begin{aligned}
\langle\Psi|\,\hat{S}_z\,|\Psi\rangle &= \frac{\hbar}{2}\left(a^*\,\langle\uparrow| + b^*\,\langle\downarrow|\right)\sigma_z\left(a\,|\uparrow\rangle - b\,|\downarrow\rangle\right) \\
&= \frac{\hbar}{2}\left(|a|^2 - |b|^2\right)
\end{aligned}
\tag{4.90}
$$

The time reversed actions are

$$
\begin{aligned}
\langle\Psi|\,\Theta^{-1}\hat{S}_x\Theta\,|\Psi\rangle &= \frac{\hbar}{2}\left(a^*\,\langle\downarrow| + b^*\,\langle\uparrow|\right)\sigma_x\left(a\,|\downarrow\rangle + b\,|\uparrow\rangle\right) \\
&= \frac{\hbar}{2}\left(a^*\,\langle\downarrow| + b^*\,\langle\uparrow|\right)\left(a\,|\uparrow\rangle + b\,|\downarrow\rangle\right) \\
&= \frac{\hbar}{2}\left(a^*b + b^*a\right),
\end{aligned}
\tag{4.91}
$$

$$\begin{aligned}\langle\Psi|\,\Theta^{-1}\hat{S}_y\Theta\,|\Psi\rangle &= \frac{\hbar}{2}\left(a^*\langle\downarrow| + b^*\langle\uparrow|\right)\sigma_y\left(a\,|\downarrow\rangle + b\,|\uparrow\rangle\right)\\ &= \frac{i\hbar}{2}\left(a^*\langle\downarrow| + b^*\langle\uparrow|\right)\left(-a\,|\uparrow\rangle + b\,|\downarrow\rangle\right)\\ &= \frac{\hbar}{2i}\left(-a^*b + b^*a\right),\end{aligned} \tag{4.92}$$

$$\begin{aligned}\langle\Psi|\,\Theta^{-1}\hat{S}_z\Theta\,|\Psi\rangle &= \frac{\hbar}{2}\left(a^*\langle\downarrow| + b^*\langle\uparrow|\right)\sigma_z\left(a\,|\downarrow\rangle + b\,|\uparrow\rangle\right)\\ &= \frac{\hbar}{2}\left(a^*\langle\downarrow| + b^*\langle\uparrow|\right)\left(-a\,|\downarrow\rangle + b\,|\uparrow\rangle\right)\\ &= \frac{\hbar}{2}\left(-|a|^2 + |b|^2\right)\end{aligned} \tag{4.93}$$

We see that this is not right, because the sign for the x component has not been flipped.

Spin 1/2 (Fermions). Attempt II. Again assuming

$$|\Psi\rangle = a\,|\uparrow\rangle + b\,|\downarrow\rangle\,, \tag{4.94}$$

now try the action

$$\Theta\,|\Psi\rangle = a^*\,|\downarrow\rangle - b^*\,|\uparrow\rangle\,. \tag{4.95}$$

This is the action:

$$\begin{aligned} a &\to -b^*\\ b &\to a^*\end{aligned} \tag{4.96}$$

The correct action of time reversal on the basis states (up to a phase choice) is

$$\boxed{\begin{aligned}\Theta\,|\uparrow\rangle &= |\downarrow\rangle\\ \Theta\,|\downarrow\rangle &= -\,|\uparrow\rangle\end{aligned}} \tag{4.97}$$

Note that acting the time reversal operator twice has the effects

$$\begin{aligned}\Theta^2\,|\uparrow\rangle &= \Theta\,|\downarrow\rangle\\ &= -\,|\uparrow\rangle\end{aligned} \tag{4.98}$$

$$
\begin{aligned}
\Theta^2 \left|\downarrow\right\rangle &= \Theta(-\left|\uparrow\right\rangle) \\
&= -\left|\uparrow\right\rangle .
\end{aligned}
\tag{4.99}
$$

We end up with the same state we started with, but with the opposite sign. This means that as an operator

$$
\boxed{\Theta^2 = -1.}
\tag{4.100}
$$

This is try for half integer particles (Fermions) $S = 1/2, 3/2, 5/2, \cdots$, but for Bosons with integer spin S.

$$
\boxed{\Theta^2 = 1.}
\tag{4.101}
$$

Kramer's degeneracy for Spin 1/2 (Fermions) Suppose we imagine there is state for which the action of the time reversal operator produces the same state, just different in phase. Let

$$
\left|\psi\right\rangle' = \Theta\left|\psi\right\rangle = e^{i\delta}\left|\psi\right\rangle .
\tag{4.102}
$$

For a Fermion we have

$$
\Theta^2\left|\psi\right\rangle = -\left|\psi\right\rangle ,
\tag{4.103}
$$

but if such the time reversal action posited above is possible we also have

$$
\begin{aligned}
\Theta^2\left|\psi\right\rangle &= \Theta e^{i\delta}\left|\psi\right\rangle \\
&= e^{-i\delta}\Theta\left|\psi\right\rangle \\
&= e^{-i\delta}e^{i\delta}\left|\psi\right\rangle \\
&= \left|\psi\right\rangle \neq -\left|\psi\right\rangle .
\end{aligned}
\tag{4.104}
$$

This is a contradiction, so we must have at least a two-fold degeneracy. This is called Kramer's degeneracy. In the homework we will show that this is not the case for integer spin particles.

Time reversal implications for wave functions For spin and angular momentum states, the implications of time reversal on the states is worked out above. If a spinless Hamiltonian has time reversal symmetry then the implication is really just the fact that the wave functions can be real valued.

4.6 PROBLEMS

Exercise 4.1 No Kramers theorem for spin-1. (*2015 ps5 p1*)

Consider a spin-1 particle. Even with time-reversal invariance, there is no Kramers theorem, so each eigenvalue of a generic spin-1 Hamiltonian will be non-degenerate. Systematically construct a Hamiltonian which is time-reversal invariant and obviously also Hermitian to illustrate this point, making clear the logic of your construction (i.e., why you are including terms which you are including).

Answer for Exercise 4.1

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Exercise 4.2 Boosts. (*2015 ps5 p2*)

The momentum operator $\hat{p}$ was shown, in class, to act as the generator of space translations. Show by following the exact same steps that the position operator $\hat{x}$ acts as the generator of momentum boosts (i.e., $\hat{x}$ is a generator of 'momentum translation').

Answer for Exercise 4.2

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Exercise 4.3 Simultaneous eigenstates. (*2015 ps5 p3*)

A quantum state $|\Psi\rangle$ is a simultaneous eigenstate of two anticommuting Hermitian operators A, B, with $AB + BA = 0$. What can you say about the eigenvalues of A, B for the state $|\Psi\rangle$? Illustrate your point using the parity operator and the momentum operator.

Answer for Exercise 4.3

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Exercise 4.4 Angular momentum. (*2015 ps5 p4*)

a. What is the time-reversed version of $\mathcal{D}(R)\,|j, m\rangle$?

b. Prove that time-reversal implies $\Theta\,|j, m\rangle = (-1)^m\,|j, -m\rangle$.

Answer for Exercise 4.4

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Exercise 4.5 Non-interacting particles in a box. (*[11] pr. 4.1*)

Calculate the three lowest energy levels and their degeneracies for equal mass distinguishable spin half particles in a box of length L.

Consider

a. Two particles.
b. Three particles.
c. Four particles.

Answer for Exercise 4.5

Part a. The problem statement doesn't include the dimensionality of the box. The simplest case is the one dimensional box, for which the wave function of one particle is

$$\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \tag{4.105}$$

and the energy of that particle is

$$E = \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2 n^2. \tag{4.106}$$

If the box is two dimensional the energy is

$$E = \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2 \left(n_1^2 + n_2^2\right), \tag{4.107}$$

and if it's a 3D box, we have

$$E = \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2 \left(n_1^2 + n_2^2 + n_3^2\right). \tag{4.108}$$

Suppose we are considering the 3D box. In statistical mechanics when we are considering particles Fermions, they are indistinguishable, and thus not allowed to share the same spin state at a given energy level. However, for distinguishable particles, that restriction doesn't exist, and we can have two (or more) such particles in the lowest order energy state. The lowest such energy is

$$\begin{aligned} E_{1,1,1;1,1,1} &= \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2 \left(6 \times 1^2\right) \\ &= \frac{6}{2m}\left(\frac{\hbar\pi}{L}\right)^2. \end{aligned} \tag{4.109}$$

The particle spin states can be any of $\lvert ++ \rangle, \lvert +- \rangle, \lvert -+ \rangle, \lvert -- \rangle$, so there is a four way degeneracy in the ground state.

the next lowest energy level is

$$\begin{aligned} E_{1,1,2;1,1,1} &= \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2 \left(5\times 1^2 + 2^2\right) \\ &= \frac{9}{2m}\left(\frac{\hbar\pi}{L}\right)^2, \end{aligned} \tag{4.110}$$

where there are $\binom{6}{1} = 6$ ways to pick such a state for each variation of spin, for a total $6\times 4 = 24$ way degeneracy. Finally, since $2^2 + 2^2 < 3^2 + 1^2$, the next lowest energy level is

$$\begin{aligned} E_{1,2,2;1,1,1} &= \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2 \left(4\times 1^2 + 2\times 2^2\right) \\ &= \frac{12}{2m}\left(\frac{\hbar\pi}{L}\right)^2, \end{aligned} \tag{4.111}$$

with a $\binom{6}{2}\times 4 = 15\times 4 = 60$ way degeneracy for this energy level.

Part b. For three particles (the two particle case wasn't actually in the problem statement, but seemed an easier starting place), the lowest energy state for a 3D box is

$$\begin{aligned} E &= \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2 \left(9\times 1^2\right) \\ &= \frac{9}{2m}\left(\frac{\hbar\pi}{L}\right)^2. \end{aligned} \tag{4.112}$$

There are now $2^3 = 8$ variations of spin $\left|+++\right\rangle, \left|++-\right\rangle, \cdots$, so the ground state is 8-way degenerate. Next up is

$$\begin{aligned} E &= \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2 \left(8\times 1^2 + 2^2\right) \\ &= \frac{12}{2m}\left(\frac{\hbar\pi}{L}\right)^2, \end{aligned} \tag{4.113}$$

where there is a $\binom{9}{1}\times 8 = 9\times 8 = 72$ way degeneracy in this energy level. Finally, the next lowest energy level is

$$\begin{aligned} E &= \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2 \left(7\times 1^2 + 2\times 2^2\right) \\ &= \frac{15}{2m}\left(\frac{\hbar\pi}{L}\right)^2, \end{aligned} \tag{4.114}$$

with a $\binom{9}{2}\times 8 = 36\times 8 = 288$ way degeneracy for this energy level.

Part c. For four particles the lowest energy state for a 3D box is

$$\begin{aligned} E &= \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2\left(12\times 1^2\right) \\ &= \frac{12}{2m}\left(\frac{\hbar\pi}{L}\right)^2. \end{aligned} \tag{4.115}$$

There are now $2^4 = 16$ variations of spin $|+++ +\rangle, |+++-\rangle, \cdots$, so the ground state is 16-way degenerate. For the second level

$$\begin{aligned} E &= \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2\left(11\times 1^2 + 2^2\right) \\ &= \frac{15}{2m}\left(\frac{\hbar\pi}{L}\right)^2, \end{aligned} \tag{4.116}$$

where there is a $\binom{12}{1}\times 16 = 12\times 16 = 192$ way degeneracy in this energy level. Finally, the next lowest energy level is

$$\begin{aligned} E &= \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2\left(7\times 1^2 + 2\times 2^2\right) \\ &= \frac{15}{2m}\left(\frac{\hbar\pi}{L}\right)^2, \end{aligned} \tag{4.117}$$

with a $\binom{12}{2}\times 16 = 66\times 16 = 1056$ way degeneracy for this energy level.

Exercise 4.6 Commutators for some symmetry operators. (*[11] pr. 4.2*)

If $\mathcal{T}_{\mathbf{d}}$, $\mathcal{D}(\hat{\mathbf{n}}, \phi)$, and π denote the translation, rotation, and parity operators respectively. Which of the following commute and why

a. $\mathcal{T}_{\mathbf{d}}$ and $\mathcal{T}_{\mathbf{d}'}$, translations in different directions.

b. $\mathcal{D}(\hat{\mathbf{n}}, \phi)$ and $\mathcal{D}(\hat{\mathbf{n}}', \phi')$, rotations in different directions.

c. $\mathcal{T}_{\mathbf{d}}$ and π.

d. $\mathcal{D}(\hat{\mathbf{n}}, \phi)$ and π.

Answer for Exercise 4.6

Part a. Consider

$$\begin{aligned}\mathcal{T}_{\mathbf{d}}\mathcal{T}_{\mathbf{d}'}\left|\mathbf{x}\right\rangle &= \mathcal{T}_{\mathbf{d}}\left|\mathbf{x}+\mathbf{d}'\right\rangle \\ &= \left|\mathbf{x}+\mathbf{d}'+\mathbf{d}\right\rangle,\end{aligned} \tag{4.118}$$

and the reverse application of the translation operators

$$\begin{aligned}\mathcal{T}_{\mathbf{d}'}\mathcal{T}_{\mathbf{d}}\left|\mathbf{x}\right\rangle &= \mathcal{T}_{\mathbf{d}'}\left|\mathbf{x}+\mathbf{d}\right\rangle \\ &= \left|\mathbf{x}+\mathbf{d}+\mathbf{d}'\right\rangle \\ &= \left|\mathbf{x}+\mathbf{d}'+\mathbf{d}\right\rangle.\end{aligned} \tag{4.119}$$

so we see that

$$[\mathcal{T}_{\mathbf{d}}, \mathcal{T}_{\mathbf{d}'}]\left|\mathbf{x}\right\rangle = 0, \tag{4.120}$$

for any position state $\left|\mathbf{x}\right\rangle$, and therefore in general they commute.

Part b. That rotations do not commute when they are in different directions (like any two orthogonal directions) need not be belaboured.

Part c. We have

$$\begin{aligned}\mathcal{T}_{\mathbf{d}}\pi\left|\mathbf{x}\right\rangle &= \mathcal{T}_{\mathbf{d}}\left|-\mathbf{x}\right\rangle \\ &= \left|-\mathbf{x}+\mathbf{d}\right\rangle,\end{aligned} \tag{4.121}$$

yet

$$\begin{aligned}\pi\mathcal{T}_{\mathbf{d}}\left|\mathbf{x}\right\rangle &= \pi\left|\mathbf{x}+\mathbf{d}\right\rangle \\ &= \left|-\mathbf{x}-\mathbf{d}\right\rangle \ne \left|-\mathbf{x}+\mathbf{d}\right\rangle.\end{aligned} \tag{4.122}$$

so, in general $[\mathcal{T}_{\mathbf{d}}, \pi] \ne 0$.

Part d. We have

$$\begin{aligned}\pi\mathcal{D}(\hat{\mathbf{n}},\phi)\left|\mathbf{x}\right\rangle &= \pi\mathcal{D}(\hat{\mathbf{n}},\phi)\pi^\dagger\pi\left|\mathbf{x}\right\rangle \\ &= \pi\mathcal{D}(\hat{\mathbf{n}},\phi)\pi^\dagger\pi\left|\mathbf{x}\right\rangle \\ &= \pi\left(\sum_{k=0}^\infty \frac{(-i\mathbf{J}\cdot\hat{\mathbf{n}})^k}{k!}\right)\pi^\dagger\pi\left|\mathbf{x}\right\rangle \\ &= \sum_{k=0}^\infty \frac{(-i(\pi\mathbf{J}\pi^\dagger)\cdot(\pi\hat{\mathbf{n}}\pi^\dagger))^k}{k!}\pi\left|\mathbf{x}\right\rangle \\ &= \sum_{k=0}^\infty \frac{(-i\mathbf{J}\cdot\hat{\mathbf{n}})^k}{k!}\pi\left|\mathbf{x}\right\rangle \\ &= \mathcal{D}(\hat{\mathbf{n}},\phi)\pi\left|\mathbf{x}\right\rangle,\end{aligned} \tag{4.123}$$

so $\left[\mathcal{D}(\hat{\mathbf{n}}, \phi), \pi\right] |\mathbf{x}\rangle = 0$, for any position state $|\mathbf{x}\rangle$, and therefore these operators commute in general.

Exercise 4.7 Plane wave and spinor under time reversal. ([11] pr. 4.7)

a. Find the time reversed form of a spinless plane wave state in three dimensions.
b. For the eigenspinor of $\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}$ expressed in terms of polar and azimuthal angles β and γ, show that $-i\sigma_y \chi^*(\hat{\mathbf{n}})$ has the reversed spin direction.

Answer for Exercise 4.7

Part a. The Hamiltonian for a plane wave is

$$H = \frac{\mathbf{p}^2}{2m} = i\frac{\partial.}{\partial t} \tag{4.124}$$

Under time reversal the momentum side transforms as

$$\begin{aligned}\Theta\frac{\mathbf{p}^2}{2m}\Theta^{-1} &= \frac{\left(\Theta\mathbf{p}\Theta^{-1}\right) \cdot \left(\Theta\mathbf{p}\Theta^{-1}\right)}{2m} \\ &= \frac{(-\mathbf{p}) \cdot (-\mathbf{p})}{2m} \\ &= \frac{\mathbf{p}^2}{2m}.\end{aligned} \tag{4.125}$$

The time derivative side of the equation is also time reversal invariant

$$\begin{aligned}\Theta i\frac{\partial}{\partial t}\Theta^{-1} &= \Theta i\Theta^{-1}\Theta\frac{\partial}{\partial t}\Theta^{-1} \\ &= -i\frac{\partial}{\partial(-t)} \\ &= i\frac{\partial}{\partial t}.\end{aligned} \tag{4.126}$$

Solutions to this equation are linear combinations of

$$\psi(\mathbf{x}, t) = e^{i\mathbf{k}\cdot\mathbf{x} - iEt/\hbar}, \tag{4.127}$$

where $\hbar^2\mathbf{k}^2/2m = E$, the energy of the particle. Under time reversal we have

$$\begin{aligned}\psi(\mathbf{x}, t) &\rightarrow e^{-i\mathbf{k}\cdot\mathbf{x} + iE(-t)/\hbar} \\ &= \left(e^{i\mathbf{k}\cdot\mathbf{x} - iE(-t)/\hbar}\right)^* \\ &= \psi^*(\mathbf{x}, -t)\end{aligned} \tag{4.128}$$

Part b. The text uses a requirement for time reversal of spin states to show that the Pauli matrix form of the time reversal operator is

$$\Theta = -i\sigma_y \eta K, \tag{4.129}$$

where K is a complex conjugating operator, and η is a phase factor with $|\eta|^2 = 1$. The form of the spin up state used in that demonstration was

$$\begin{aligned}
|\hat{\mathbf{n}}; +\rangle &= e^{-iS_z\beta/\hbar} e^{-iS_y\gamma/\hbar} |+\rangle \\
&= e^{-i\sigma_z\beta/2} e^{-i\sigma_y\gamma/2} |+\rangle \\
&= (\cos(\beta/2) - i\sigma_z \sin(\beta/2)) \left(\cos(\gamma/2) - i\sigma_y \sin(\gamma/2)\right) |+\rangle \\
&= \left(\cos(\beta/2) - i \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \sin(\beta/2)\right) \left(\cos(\gamma/2) - i \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \sin(\gamma/2)\right) |+\rangle \\
&= \begin{bmatrix} e^{-i\beta/2} & 0 \\ 0 & e^{i\beta/2} \end{bmatrix} \begin{bmatrix} \cos(\gamma/2) & -\sin(\gamma/2) \\ \sin(\gamma/2) & \cos(\gamma/2) \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\
&= \begin{bmatrix} e^{-i\beta/2} & 0 \\ 0 & e^{i\beta/2} \end{bmatrix} \begin{bmatrix} \cos(\gamma/2) \\ \sin(\gamma/2) \end{bmatrix} \\
&= \begin{bmatrix} \cos(\gamma/2) e^{-i\beta/2} \\ \sin(\gamma/2) e^{i\beta/2} \end{bmatrix}.
\end{aligned} \tag{4.130}$$

The state orthogonal to this one is claimed to be

$$\begin{aligned}
|\hat{\mathbf{n}}; -\rangle &= e^{-iS_z\beta/\hbar} e^{-iS_y(\gamma+\pi)/\hbar} |+\rangle \\
&= e^{-i\sigma_z\beta/2} e^{-i\sigma_y(\gamma+\pi)/2} |+\rangle .
\end{aligned} \tag{4.131}$$

We have

$$\cos((\gamma + \pi)/2) = \operatorname{Re} e^{i(\gamma+\pi)/2} = \operatorname{Re} i e^{i\gamma/2} = -\sin(\gamma/2), \tag{4.132}$$

and

$$\sin((\gamma + \pi)/2) = \operatorname{Im} e^{i(\gamma+\pi)/2} = \operatorname{Im} i e^{i\gamma/2} = \cos(\gamma/2), \tag{4.133}$$

so we should have

$$|\hat{\mathbf{n}}; -\rangle = \begin{bmatrix} -\sin(\gamma/2) e^{-i\beta/2} \\ \cos(\gamma/2) e^{i\beta/2} \end{bmatrix}. \tag{4.134}$$

This looks right, but we can sanity check orthogonality

$$\langle \hat{\mathbf{n}}; - | \hat{\mathbf{n}}; + \rangle = \begin{bmatrix} -\sin(\gamma/2)e^{i\beta/2} & \cos(\gamma/2)e^{-i\beta/2} \end{bmatrix} \begin{bmatrix} \cos(\gamma/2)e^{-i\beta/2} \\ \sin(\gamma/2)e^{i\beta/2} \end{bmatrix} = 0, \tag{4.135}$$

as expected.

The task at hand appears to be the operation on the column representation of $|\hat{\mathbf{n}}; +\rangle$ using the Pauli representation of the time reversal operator. With the phase factor $\eta = 1$ the time reversal action on the spin up state is

$$\begin{aligned} \Theta \,|\hat{\mathbf{n}}; +\rangle &= -i\sigma_y K \begin{bmatrix} e^{-i\beta/2}\cos(\gamma/2) \\ e^{i\beta/2}\sin(\gamma/2) \end{bmatrix} \\ &= -i \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} e^{i\beta/2}\cos(\gamma/2) \\ e^{-i\beta/2}\sin(\gamma/2) \end{bmatrix} \\ &= \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} e^{i\beta/2}\cos(\gamma/2) \\ e^{-i\beta/2}\sin(\gamma/2) \end{bmatrix} \\ &= \begin{bmatrix} -e^{-i\beta/2}\sin(\gamma/2) \\ e^{i\beta/2}\cos(\gamma/2) \end{bmatrix} \\ &= |\hat{\mathbf{n}}; -\rangle . \qquad \square \end{aligned} \tag{4.136}$$

Observe that we need $\eta = i$ to have this match eq. (4.79) in the text where $\Theta = i^{2m} \,|j, -m\rangle$.

Exercise 4.8 Totally asymmetric potential. (*[11] pr. 4.11*)

a. Given a time reversal invariant Hamiltonian, show that for any energy eigenket

$$\langle \mathbf{L} \rangle = 0. \tag{4.137}$$

b. If the wave function of such a state is expanded as

$$\sum_{l,m} F_{lm} Y_{lm}(\theta, \phi), \tag{4.138}$$

what are the phase restrictions on F_{lm}?

Answer for Exercise 4.8

Part a. For a time reversal invariant Hamiltonian H we have

$$H\Theta = \Theta H. \tag{4.139}$$

If $|\psi\rangle$ is an energy eigenstate with eigenvalue E, we have

$$
\begin{aligned}
H\Theta |\psi\rangle &= \Theta H |\psi\rangle \\
&= \lambda \Theta |\psi\rangle ,
\end{aligned}
\tag{4.140}
$$

so $\Theta |\psi\rangle$ is also an eigenvalue of H, so can only differ from $|\psi\rangle$ by a phase factor. That is

$$
\begin{aligned}
\left|\psi'\right\rangle &= \Theta |\psi\rangle \\
&= e^{i\delta} |\psi\rangle .
\end{aligned}
\tag{4.141}
$$

Now consider the expectation of $\mathbf{L}$ with respect to a time reversed state

$$
\begin{aligned}
\left\langle\psi'\right| \mathbf{L} \left|\psi'\right\rangle &= \langle\psi| \Theta^{-1} \mathbf{L} \Theta |\psi\rangle \\
&= \langle\psi| (-\mathbf{L}) |\psi\rangle ,
\end{aligned}
\tag{4.142}
$$

however, we also have

$$
\begin{aligned}
\left\langle\psi'\right| \mathbf{L} \left|\psi'\right\rangle &= \left(\langle\psi| e^{-i\delta}\right) \mathbf{L} \left(e^{i\delta} |\psi\rangle\right) \\
&= \langle\psi| \mathbf{L} |\psi\rangle ,
\end{aligned}
\tag{4.143}
$$

so we have $\langle\psi| \mathbf{L} |\psi\rangle = -\langle\psi| \mathbf{L} |\psi\rangle$ which is only possible if $\langle\mathbf{L}\rangle = \langle\psi| \mathbf{L} |\psi\rangle = 0$.

Part b. Consider the expansion of the wave function of a time reversed energy eigenstate

$$
\begin{aligned}
\langle\mathbf{x}| \Theta |\psi\rangle &= \langle\mathbf{x}| e^{i\delta} |\psi\rangle \\
&= e^{i\delta} \langle\mathbf{x}|\psi\rangle ,
\end{aligned}
\tag{4.144}
$$

and then consider the same state expanded in the position basis

$$
\begin{aligned}
\langle\mathbf{x}| \Theta |\psi\rangle &= \langle\mathbf{x}| \Theta \int d^3\mathbf{x}' \left(\left|\mathbf{x}'\right\rangle \left\langle\mathbf{x}'\right|\right) |\psi\rangle \\
&= \langle\mathbf{x}| \Theta \int d^3\mathbf{x}' \left(\left\langle\mathbf{x}'\middle|\psi\right\rangle\right) \left|\mathbf{x}'\right\rangle \\
&= \langle\mathbf{x}| \int d^3\mathbf{x}' \left(\left\langle\mathbf{x}'\middle|\psi\right\rangle\right)^* \Theta \left|\mathbf{x}'\right\rangle \\
&= \langle\mathbf{x}| \int d^3\mathbf{x}' \left(\left\langle\mathbf{x}'\middle|\psi\right\rangle\right)^* \left|\mathbf{x}'\right\rangle \\
&= \int d^3\mathbf{x}' \left(\left\langle\mathbf{x}'\middle|\psi\right\rangle\right)^* \left\langle\mathbf{x}\middle|\mathbf{x}'\right\rangle \\
&= \int d^3\mathbf{x}' \left\langle\psi\middle|\mathbf{x}'\right\rangle \delta(\mathbf{x} - \mathbf{x}') \\
&= \langle\psi|\mathbf{x}\rangle .
\end{aligned}
\tag{4.145}
$$

This demonstrates a relationship between the wave function and its complex conjugate

$$\langle \mathbf{x}|\psi\rangle = e^{-i\delta} \langle \psi|\mathbf{x}\rangle . \tag{4.146}$$

Now expand the wave function in the spherical harmonic basis

$$\begin{aligned}
\langle \mathbf{x}|\psi\rangle &= \int d\Omega \, \langle \mathbf{x}|\hat{\mathbf{n}}\rangle \langle \hat{\mathbf{n}}|\psi\rangle \\
&= \sum_{lm} F_{lm}(r) Y_{lm}(\theta, \phi) \\
&= e^{-i\delta} \left(\sum_{lm} F_{lm}(r) Y_{lm}(\theta, \phi) \right)^* \\
&= e^{-i\delta} \sum_{lm} \left(F_{lm}(r)\right)^* Y^*_{lm}(\theta, \phi) \\
&= e^{-i\delta} \sum_{lm} \left(F_{lm}(r)\right)^* (-1)^m Y_{l,-m}(\theta, \phi) \\
&= e^{-i\delta} \sum_{lm} \left(F_{l,-m}(r)\right)^* (-1)^m Y_{l,m}(\theta, \phi),
\end{aligned} \tag{4.147}$$

so the F_{lm} functions are constrained by

$$F_{lm}(r) = e^{-i\delta} \left(F_{l,-m}(r)\right)^* (-1)^m. \tag{4.148}$$

Exercise 4.9 Time reversal behavior of solutions to crystal spin Hamiltonian. ([11] *pr. 4.12*)

Solve the spin 1 Hamiltonian

$$H = A S_z^2 + B(S_x^2 - S_y^2). \tag{4.149}$$

Is this Hamiltonian invariant under time reversal?
How do the eigenkets change under time reversal?

Answer for Exercise 4.9

In spinMatrices.nb the matrix representation of the Hamiltonian is found to be

$$H = \hbar^2 \begin{bmatrix} A + \frac{B}{2} & 0 & \frac{B}{2} \\ -\frac{iB}{\sqrt{2}} & B & -\frac{iB}{\sqrt{2}} \\ \frac{B}{2} & 0 & A + \frac{B}{2} \end{bmatrix}. \tag{4.150}$$

The eigenvalues are

$$\left\{ \hbar^2 A, \hbar^2 B, \hbar^2 (A + B) \right\}, \tag{4.151}$$

and the respective eigenvalues (unnormalized) are

$$\left\{ \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ -\frac{i\sqrt{2}B}{A} \\ 1 \end{bmatrix} \right\}. \tag{4.152}$$

Under time reversal, the Hamiltonian is

$$H \rightarrow A(-S_z)^2 + B((-S_x)^2 - (-S_y)^2) = H, \tag{4.153}$$

so we expect the eigenkets for this Hamiltonian to vary by at most a phase factor. To check this, first recall that the time reversal action on a spin one state is

$$\Theta \left|1, m\right\rangle = (-1)^m \left|1, -m\right\rangle, \tag{4.154}$$

or

$$\begin{aligned} \Theta \left|1\right\rangle &= -\left|-1\right\rangle \\ \Theta \left|0\right\rangle &= \left|0\right\rangle \\ \Theta \left|-1\right\rangle &= -\left|1\right\rangle. \end{aligned} \tag{4.155}$$

Let's write the eigenkets respectively as

$$\begin{aligned} \left|A\right\rangle &= -\left|1\right\rangle + \left|-1\right\rangle \\ \left|B\right\rangle &= \left|0\right\rangle \\ \left|A+B\right\rangle &= \left|1\right\rangle + \left|-1\right\rangle - \frac{i\sqrt{2}B}{A}\left|0\right\rangle. \end{aligned} \tag{4.156}$$

Noting that the time reversal operator maps complex numbers onto their conjugates, the time reversed eigenkets are

$$\begin{aligned} \left|A\right\rangle &\rightarrow \left|-1\right\rangle - \left|-1\right\rangle = -\left|A\right\rangle \\ \left|B\right\rangle &\rightarrow \left|0\right\rangle = \left|B\right\rangle \\ \left|A+B\right\rangle &\rightarrow -\left|1\right\rangle - \left|-1\right\rangle + \frac{i\sqrt{2}B}{A}\left|0\right\rangle = -\left|A+B\right\rangle. \end{aligned} \tag{4.157}$$

Up to a sign, the time reversed states match the unreversed states.

5 THEORY OF ANGULAR MOMENTUM

5.1 ANGULAR MOMENTUM

In classical mechanics the (orbital) angular momentum is

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}. \tag{5.1}$$

Here "orbital" is to distinguish from spin angular momentum.
In quantum mechanics, the mapping to operators, in component form, is

$$\hat{L}_i = \epsilon_{ijk} \hat{r}_j \hat{p}_k. \tag{5.2}$$

These operators do not commute

$$\left[\hat{L}_i, \hat{L}_j\right] = i\hbar \epsilon_{ijk} \hat{L}_k. \tag{5.3}$$

which means that we can't simultaneously determine $\hat{L}_i$ for all i.
Aside: In quantum mechanics, we define an operator $\hat{\mathbf{V}}$ to be a vector operator if

$$\left[\hat{L}_i, \hat{V}_j\right] = i\hbar \epsilon_{ijk} \hat{V}_k. \tag{5.4}$$

The commutator of the squared angular momentum operator with any $\hat{L}_i$, say $\hat{L}_x$ is zero

$$\begin{aligned}
\left[\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x\right] &= \hat{L}_y \hat{L}_y \hat{L}_x - \hat{L}_x \hat{L}_y \hat{L}_y + \hat{L}_z \hat{L}_z \hat{L}_x - \hat{L}_x \hat{L}_z \hat{L}_z \\
&= \hat{L}_y \left(\left[\hat{L}_y, \hat{L}_x\right] + \cancel{\hat{L}_x \hat{L}_y}\right) - \left(\left[\hat{L}_x, \hat{L}_y\right] + \cancel{\hat{L}_y \hat{L}_x}\right) \hat{L}_y \\
&\quad + \hat{L}_z \left(\left[\hat{L}_z, \hat{L}_x\right] + \cancel{\hat{L}_x \hat{L}_z}\right) - \left(\left[\hat{L}_x, \hat{L}_z\right] + \cancel{\hat{L}_z \hat{L}_x}\right) \hat{L}_z \\
&= \hat{L}_y \left[\hat{L}_y, \hat{L}_x\right] - \left[\hat{L}_x, \hat{L}_y\right] \hat{L}_y + \hat{L}_z \left[\hat{L}_z, \hat{L}_x\right] - \left[\hat{L}_x, \hat{L}_z\right] \hat{L}_z \\
&= i\hbar \left(-\hat{L}_y \hat{L}_z - \hat{L}_z \hat{L}_y + \hat{L}_z \hat{L}_y + \hat{L}_y \hat{L}_z\right) \\
&= 0.
\end{aligned} \tag{5.5}$$

Suppose we have a state $|\Psi\rangle$ with a well defined $\hat{L}_z$ eigenvalue and well defined $\hat{\mathbf{L}}^2$ eigenvalue, written as

$$|\Psi\rangle = |a, b\rangle, \tag{5.6}$$

where the label a is used for the eigenvalue of $\hat{\mathbf{L}}^2$ and b labels the eigenvalue of $\hat{L}_z$. Then

$$\begin{aligned}\hat{\mathbf{L}}^2 |a,b\rangle &= \hbar^2 a\,|a,b\rangle \\ \hat{L}_z\,|a,b\rangle &= \hbar b\,|a,b\rangle\,.\end{aligned} \tag{5.7}$$

Things aren't so nice when we act with other angular momentum operators, producing a scrambled mess

$$\begin{aligned}\hat{L}_x\,|a,b\rangle &= \sum_{a',b'} \mathcal{A}^x_{a,b,a',b'}\,\left|a',b'\right\rangle \\ \hat{L}_y\,|a,b\rangle &= \sum_{a',b'} \mathcal{A}^y_{a,b,a',b'}\,\left|a',b'\right\rangle\end{aligned} \tag{5.8}$$

With this representation, we have

$$\hat{L}_x\hat{\mathbf{L}}^2\,|a,b\rangle = \hat{L}_x\,\hbar^2 a \sum_{a',b'} \mathcal{A}^x_{a,b,a',b'}\,\left|a',b'\right\rangle. \tag{5.9}$$

$$\hat{\mathbf{L}}^2\hat{L}_x\,|a,b\rangle = \hbar^2 \sum_{a',b'} a'\,\mathcal{A}^x_{a,b,a',b'}\,\left|a',b'\right\rangle. \tag{5.10}$$

Since $\hat{\mathbf{L}}^2, \hat{L}_x$ commute, we must have

$$\mathcal{A}^x_{a,b,a',b'} = \delta_{a,a'}\mathcal{A}^x_{a';b,b'}, \tag{5.11}$$

and similarly

$$\mathcal{A}^y_{a,b,a',b'} = \delta_{a,a'}\mathcal{A}^y_{a';b,b'}. \tag{5.12}$$

Simplifying things we can write the action of $\hat{L}_x, \hat{L}_y$ on the state as

$$\begin{aligned}\hat{L}_x\,|a,b\rangle &= \sum_{b'} \mathcal{A}^x_{a;b,b'}\,\left|a,b'\right\rangle \\ \hat{L}_y\,|a,b\rangle &= \sum_{b'} \mathcal{A}^y_{a;b,b'}\,\left|a,b'\right\rangle\end{aligned} \tag{5.13}$$

Let's define

$$\begin{aligned}\hat{L}_+ &\equiv \hat{L}_x + i\hat{L}_y \\ \hat{L}_- &\equiv \hat{L}_x - i\hat{L}_y\end{aligned} \tag{5.14}$$

Because these are sums of $\hat{L}_x, \hat{L}_y$ they must also commute with $\hat{\mathbf{L}}^2$

$$\left[\hat{\mathbf{L}}^2, \hat{L}_\pm\right] = 0. \tag{5.15}$$

The commutators with $\hat{L}_z$ are non-zero

$$\begin{aligned}
\left[\hat{L}_z, \hat{L}_\pm\right] &= \hat{L}_z\left(\hat{L}_x \pm i\hat{L}_y\right) - \left(\hat{L}_x \pm i\hat{L}_y\right)\hat{L}_z \\
&= \left[\hat{L}_z, \hat{L}_x\right] \pm i\left[\hat{L}_z, \hat{L}_y\right] \\
&= i\hbar\left(\hat{L}_y \mp i\hat{L}_x\right) \\
&= \hbar\left(i\hat{L}_y \pm \hat{L}_x\right) \\
&= \pm\hbar\left(\hat{L}_x \pm i\hat{L}_y\right) \\
&= \pm\hbar\hat{L}_\pm.
\end{aligned} \tag{5.16}$$

Explicitly, that is

$$\begin{aligned}
\hat{L}_z\hat{L}_+ - \hat{L}_+\hat{L}_z &= \hbar\hat{L}_+ \\
\hat{L}_z\hat{L}_- - \hat{L}_-\hat{L}_z &= -\hbar\hat{L}_-
\end{aligned} \tag{5.17}$$

Now we are set to compute actions of these (assumed) raising and lowering operators on the eigenstate of $\hat{L}_z, \hat{\mathbf{L}}^2$

$$\begin{aligned}
\hat{L}_z\hat{L}_\pm |a, b\rangle &= \hbar\hat{L}_\pm |a, b\rangle \pm \hat{L}_\pm\hat{L}_z |a, b\rangle \\
&= \hbar\hat{L}_\pm |a, b\rangle \pm \hbar b\hat{L}_\pm |a, b\rangle \\
&= \hbar(b \pm 1)\hat{L}_\pm |a, b\rangle .
\end{aligned} \tag{5.18}$$

There must be a proportionality of the form

$$\left|\hat{L}_\pm\right\rangle \propto |a, b \pm 1\rangle , \tag{5.19}$$

The products of the raising and lowering operators are

$$\begin{aligned}
\hat{L}_-\hat{L}_+ &= \left(\hat{L}_x - i\hat{L}_y\right)\left(\hat{L}_x + i\hat{L}_y\right) \\
&= \hat{L}_x^2 + \hat{L}_y^2 + i\hat{L}_x\hat{L}_y - i\hat{L}_y\hat{L}_x \\
&= \left(\hat{\mathbf{L}}^2 - \hat{L}_z^2\right) + i\left[\hat{L}_x, \hat{L}_y\right] \\
&= \hat{\mathbf{L}}^2 - \hat{L}_z^2 - \hbar\hat{L}_z,
\end{aligned} \tag{5.20}$$

and

$$\begin{aligned}
\hat{L}_+\hat{L}_- &= \left(\hat{L}_x + i\hat{L}_y\right)\left(\hat{L}_x - i\hat{L}_y\right) \\
&= \hat{L}_x^2 + \hat{L}_y^2 - i\hat{L}_x\hat{L}_y + i\hat{L}_y\hat{L}_x \\
&= \left(\hat{\mathbf{L}}^2 - \hat{L}_z^2\right) - i\left[\hat{L}_x, \hat{L}_y\right] \\
&= \hat{\mathbf{L}}^2 - \hat{L}_z^2 + \hbar\hat{L}_z,
\end{aligned} \tag{5.21}$$

So we must have

$$0 \leq \langle a, b| \hat{L}_- \hat{L}_+ |a, b\rangle = \langle a, b| \left(\hat{\mathbf{L}}^2 - \hat{L}_z^2 - \hbar \hat{L}_z\right) |a, b\rangle = \hbar^2 a - \hbar^2 b^2 - \hbar^2 b, \tag{5.22}$$

and

$$0 \leq \langle a, b| \hat{L}_+ \hat{L}_- |a, b\rangle = \langle a, b| \left(\hat{\mathbf{L}}^2 - \hat{L}_z^2 + \hbar \hat{L}_z\right) |a, b\rangle = \hbar^2 a - \hbar^2 b^2 + \hbar^2 b. \tag{5.23}$$

This puts constraints on a, b, roughly of the form

1. $$a - b(b+1) \geq 0 \tag{5.24}$$

   With $b_{\max} > 0$, $b_{\max} \approx \sqrt{a}$.

2. $$a - b(b-1) \geq 0 \tag{5.25}$$

   With $b_{\min} < 0$, $b_{\min} \approx -\sqrt{a}$.

Assuming that the $b_{\max}$ and $b_{\min}$ values are satisfied at the equality extremes we have

$$\begin{aligned} b_{\max}\left(b_{\max} + 1\right) &= a \\ b_{\min}\left(b_{\min} - 1\right) &= a. \end{aligned} \tag{5.26}$$

Equating these pair of equations and rearranging, we have

$$\left(b_{\max} + \frac{1}{2}\right)^2 - \frac{1}{4} = \left(b_{\min} - \frac{1}{2}\right)^2 - \frac{1}{4}, \tag{5.27}$$

which has solutions at

$$b_{\max} + \frac{1}{2} = \pm\left(b_{\min} - \frac{1}{2}\right). \tag{5.28}$$

One of the solutions is

$$-b_{\min} = b_{\max}, \tag{5.29}$$

as desired. The other solution is $b_{\max} = b_{\min} - 1$, which we discard.

The final constraint is therefore

$$\boxed{-b_{\max} \leq b \leq b_{\max},} \tag{5.30}$$

and

$$\begin{aligned} \hat{L}_+ \left| a, b_{\max} \right\rangle &= 0 \\ \hat{L}_- \left| a, b_{\min} \right\rangle &= 0 \end{aligned} \tag{5.31}$$

If we had the sequence, which must terminate at $b_{\min}$ or else it will go on forever

$$\begin{aligned} \left| a, b_{\max} \right\rangle &\xrightarrow{\hat{L}_-} \left| a, b_{\max} - 1 \right\rangle \\ &\xrightarrow{\hat{L}_-} \left| a, b_{\max} - 2 \right\rangle \cdots \\ &\xrightarrow{\hat{L}_-} \left| a, b_{\min} \right\rangle, \end{aligned} \tag{5.32}$$

then we know that $b_{\max} - b_{\min} \in \mathbb{Z}$, or

$$b_{\max} - n = b_{\min} = -b_{\max} \tag{5.33}$$

or

$$b_{\max} = \frac{n}{2}, \tag{5.34}$$

this is either an integer or a $1/2$ odd integer, depending on whether n is even or odd. These are called “orbital” or “spin” respectively.

The convention is to write m for the $\hat{L}_z$ eigenvalue (the magnetic quantum number), and j, the azimthual quantum number, to describe the $j(j+1)$ eigenvalue of the $\hat{\mathbf{L}}^2$ operator.

$$\begin{aligned} b_{\max} &= j \\ a &= j(j+1). \end{aligned} \tag{5.35}$$

so for $m \in -j, -j+1, \cdots, +j$

$$\boxed{\begin{aligned} \hat{\mathbf{L}}^2 \left| j, m \right\rangle &= \hbar^2 j(j+1) \left| j, m \right\rangle \\ L_z \left| j, m \right\rangle &= \hbar m \left| j, m \right\rangle. \end{aligned}} \tag{5.36}$$

5.2 SCHWINGER'S HARMONIC OSCILLATOR REPRESENTATION OF ANGULAR MOMENTUM OPERATORS.

In [13] a powerful method for describing angular momentum with harmonic oscillators was introduced, which will be outlined here. The question is whether we can construct a set of harmonic oscillators that allows a mapping from

$$\hat{L}_+ \leftrightarrow a^+? \tag{5.37}$$

Picture two harmonic oscillators, one with states counted from one zero towards ∞ and another with states counted from a different zero towards $-\infty$, as pictured in fig. 5.1.

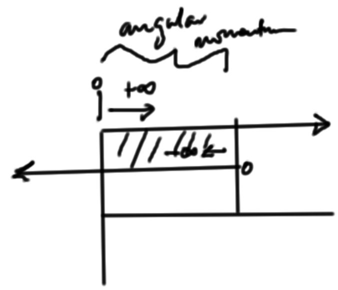

Figure 5.1: Overlapping SHO domains.

Is it possible that such an overlapping set of harmonic oscillators can provide the properties of the angular momentum operators? Let's relabel the counting so that we have two sets of positive counted SHO systems, each counted in a positive direction as sketched in fig. 5.2.

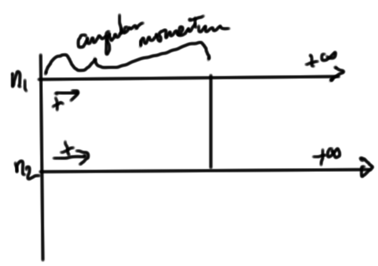

Figure 5.2: Relabeling the counting for overlapping SHO systems.

It turns out that given a constraint there the number of ways to distribute particles between a pair of SHO systems, the process that can be viewed as reproducing the angular momentum action is a transfer of particles from one harmonic oscillator to the other. For $\hat{L}_z = +j$

$$\begin{aligned} n_1 &= n_{\text{max}} \\ n_2 &= 0, \end{aligned} \tag{5.38}$$

and for $\hat{L}_z = -j$

$$\begin{aligned} n_1 &= 0 \\ n_2 &= n_{\text{max}}. \end{aligned} \tag{5.39}$$

We can make the identifications

$$\hat{L}_z = (n_1 - n_2)\frac{\hbar}{2}, \tag{5.40}$$

and

$$j = \frac{1}{2} n_{\text{max}}, \tag{5.41}$$

or

$$n_1 + n_2 = \text{fixed} = n_{\text{max}} \tag{5.42}$$

Changes that keep $n_1 + n_2$ fixed are those that change n_1, n_2 by $+1$ or -1 respectively, as sketched in fig. 5.3.

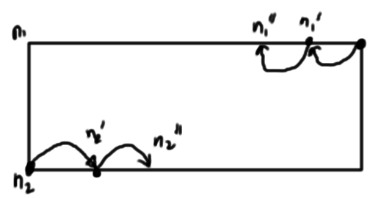

Figure 5.3: Number conservation constraint.

Can we make an identification that takes

$$|n_1, n_2\rangle \xrightarrow{\hat{L}_-} |n_1 - 1, n_2 + 1\rangle\,? \tag{5.43}$$

What operator in the SHO problem has this effect? Let's try

$$\boxed{\begin{aligned}\hat{L}_- &= \hbar a_2^\dagger a_1\\ \hat{L}_+ &= \hbar a_1^\dagger a_2\\ \hat{L}_z &= \frac{\hbar}{2}\left(n_1 - n_2\right)\end{aligned}} \tag{5.44}$$

Is this correct? Do we need to make any scalar adjustments? We want

$$\left[\hat{L}_z, \hat{L}_\pm\right] = \pm\hbar\hat{L}_\pm. \tag{5.45}$$

First check this with the $\hat{L}_+$ commutator

$$\begin{aligned}\left[\hat{L}_z, \hat{L}_+\right] &= \frac{1}{2}\hbar^2\left[n_1 - n_2, a_1^\dagger a_2\right]\\ &= \frac{1}{2}\hbar^2\left[a_1^\dagger a_1 - a_2^\dagger a_2, a_1^\dagger a_2\right]\\ &= \frac{1}{2}\hbar^2\left(\left[a_1^\dagger a_1, a_1^\dagger a_2\right] - \left[a_2^\dagger a_2, a_1^\dagger a_2\right]\right)\\ &= \frac{1}{2}\hbar^2\left(a_2\left[a_1^\dagger a_1, a_1^\dagger\right] - a_1^\dagger\left[a_2^\dagger a_2, a_2\right]\right).\end{aligned} \tag{5.46}$$

But

$$\begin{aligned}\left[a^\dagger a, a^\dagger\right] &= a^\dagger a a^\dagger - a^\dagger a^\dagger a\\ &= a^\dagger\left(1 + a^\dagger a\right) - a^\dagger a^\dagger a\\ &= a^\dagger,\end{aligned} \tag{5.47}$$

and

$$\begin{aligned}\left[a^\dagger a, a\right] &= a^\dagger a a - a a^\dagger a\\ &= a^\dagger a a - \left(1 + a^\dagger a\right) a\\ &= -a,\end{aligned} \tag{5.48}$$

so

$$\left[\hat{L}_z, \hat{L}_+\right] = \hbar^2 a_2 a_1^\dagger = \hbar\hat{L}_+, \tag{5.49}$$

as desired. Similarly

$$
\begin{aligned}
\left[\hat{L}_z, \hat{L}_-\right] &= \frac{1}{2}\hbar^2 \left[n_1 - n_2, a_2^\dagger a_1\right] \\
&= \frac{1}{2}\hbar^2 \left[a_1^\dagger a_1 - a_2^\dagger a_2, a_2^\dagger a_1\right] \\
&= \frac{1}{2}\hbar^2 \left(a_2^\dagger \left[a_1^\dagger a_1, a_1\right] - a_1 \left[a_2^\dagger a_2, a_2^\dagger\right]\right) \\
&= \frac{1}{2}\hbar^2 \left(a_2^\dagger(-a_1) - a_1 a_2^\dagger\right) \\
&= -\hbar^2 a_2^\dagger a_1 \\
&= -\hbar \hat{L}_-.
\end{aligned}
\tag{5.50}
$$

With

$$
\begin{aligned}
j &= \frac{n_1 + n_2}{2} \\
m &= \frac{n_1 - n_2}{2}
\end{aligned}
\tag{5.51}
$$

We can make the identification

$$
|n_1, n_2\rangle = |j + m, j - m\rangle . \tag{5.52}
$$

Another way With

$$
\hat{L}_+ |j, m\rangle = d^+_{j,m} |j, m+1\rangle \tag{5.53}
$$

or

$$
\hbar a_1^\dagger a_2 |j + m, j - m\rangle = d^+_{j,m} |j + m + 1, j - m - 1\rangle , \tag{5.54}
$$

we can seek this factor $d^+_{j,m}$ by operating with $\hat{L}_+$

$$
\begin{aligned}
\hat{L}_+ |j, m\rangle &= \hbar a_1^\dagger a_2 |n_1, n_2\rangle \\
&= \hbar a_1^\dagger a_2 |j + m, j - m\rangle \\
&= \hbar \sqrt{n + 1} \sqrt{n_2} |j + m + 1, j - m - 1\rangle \\
&= \hbar \sqrt{(j + m + 1)(j - m)} |j + m + 1, j - m - 1\rangle
\end{aligned}
\tag{5.55}
$$

That gives

$$\begin{aligned} d^{+}_{j,m} &= \hbar\sqrt{(j-m)\,(j+m+1)} \\ d^{-}_{j,m} &= \hbar\sqrt{(j+m)\,(j-m+1)}. \end{aligned} \tag{5.56}$$

This equivalence can be used to model spin interaction in crystals as harmonic oscillators. This equivalence of lattice vibrations and spin oscillations is called "spin waves".

5.3 REPRESENTATIONS

It's possible to compute matrix representations of the rotation operators

$$\hat{R}_{\hat{\mathbf{n}}}(\phi) = e^{i\hat{\mathbf{L}}\cdot\hat{\mathbf{n}}\phi/\hbar}. \tag{5.57}$$

With respect to a ket it's possible to find

$$e^{i\hat{\mathbf{L}}\cdot\hat{\mathbf{n}}\phi/\hbar}\,|j,m\rangle = \sum_{m'} d^{j}_{mm'}(\hat{\mathbf{n}},\phi)\,\left|j,m'\right\rangle. \tag{5.58}$$

This has a block diagonal form that's sketched in fig. 5.4.

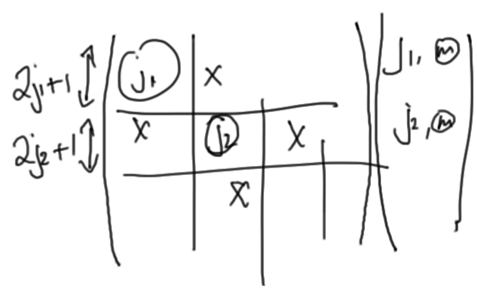

Figure 5.4: Block diagonal form for angular momentum matrix representation.

We can view $d^{j}_{mm'}(\hat{\mathbf{n}},\phi)$ as a matrix, representing the rotation. The problem of determining these matrices can be reduced to that of determining the matrix for $\hat{\mathbf{L}}$, because once we have that we can exponentiate that.

Example 5.1: Spin half

From the eigenvalue relationships, with basis states

$$
\begin{aligned}
|\uparrow\rangle &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\
|\downarrow\rangle &= \begin{bmatrix} 0 \\ 1 \end{bmatrix}
\end{aligned}
\tag{5.59}
$$

we find

$$
\begin{aligned}
\hat{L}_z &= \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\
\hat{L}_+ &= \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \\
\hat{L}_- &= \frac{\hbar}{2} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.
\end{aligned}
\tag{5.60}
$$

Rearranging we find the Pauli matrices

$$
\hat{L}_k = \frac{1}{2} \hbar \sigma_i. \tag{5.61}
$$

Noting that $(\boldsymbol{\sigma} \cdot \hat{\mathbf{n}})^2 = 1$, and $(\boldsymbol{\sigma} \cdot \hat{\mathbf{n}})^3 = \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}$, the rotation matrix is

$$
e^{i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\phi/2} \left| \frac{1}{2}, m \right\rangle = (\cos(\phi/2) + i\boldsymbol{\sigma} \cdot \hat{\mathbf{n}} \sin(\phi/2)) \left| \frac{1}{2}, m \right\rangle. \tag{5.62}
$$

The steps taken in the example above, which apply to all values of j were

1. Enumerate the states.

$$
j_1 = \frac{1}{2} \leftrightarrow \text{ 2 states (dimension of irreducible representation = 2)} \tag{5.63}
$$

2. Construct the $\hat{\mathbf{L}}$ matrices.
3. Construct $d^j_{mm'}(\hat{\mathbf{n}}, \phi)$.

5.4 SPHERICAL HARMONICS

For $L = 1$ it turns out that the rotation matrices turn out to be the 3D rotation matrices. In the space representation

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}, \tag{5.64}$$

the coordinates of the operator are

$$\hat{L}_k = i\epsilon_{kmn} r_m \left(-i\hbar \frac{\partial}{\partial r_n}\right) \tag{5.65}$$

We see that scaling $\mathbf{r} \to \alpha\mathbf{r}$ does not change this operator, allowing for an angular representation $\hat{L}_k(\theta, \phi)$ that have the form

$$\begin{aligned} \hat{L}_z &= -i\hbar \frac{\partial}{\partial \phi} \\ \hat{L}_\pm &= \hbar \left(\pm \frac{\partial}{\partial \theta} + i \cot\theta \frac{\partial}{\partial \phi}\right). \end{aligned} \tag{5.66}$$

Here θ and ϕ are the polar and azimuthal angles respectively as illustrated in fig. 5.5.

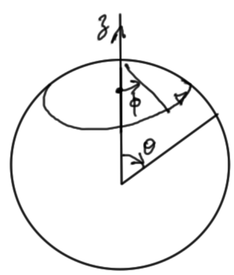

Figure 5.5: Spherical coordinate convention.

Introducing the spherical harmonics Y_{lm}, the equivalent wave function representation of the problem is

$$\begin{aligned} \hat{\mathbf{L}} Y_{lm}(\theta, \phi) &= \hbar^2 l(l+1) Y_{lm}(\theta, \phi) \\ \hat{L}_z Y_{lm}(\theta, \phi) &= \hbar m Y_{lm}(\theta, \phi) \end{aligned} \tag{5.67}$$

One can find these functions

$$Y_{lm}(\theta, \phi) = P_{l,m}(\cos\theta) e^{im\phi}, \tag{5.68}$$

where $P_{l,m}(\cos\theta)$ are called the associated Legendre polynomials. This can be applied whenever we have

$$\left[H, \hat{L}_k\right] = 0. \tag{5.69}$$

where all the eigenfunctions will have the form

$$\Psi(r,\theta,\phi) = R(r)Y_{lm}(\theta,\phi). \tag{5.70}$$

5.5 ADDITION OF ANGULAR MOMENTUM

Since $\hat{\mathbf{L}}$ is a vector we expect to be able to add angular momentum in some way similar to the addition of classical vectors as illustrated in fig. 5.6.

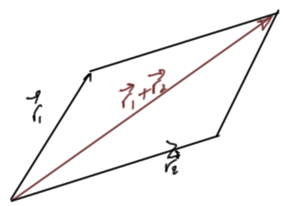

Figure 5.6: Classical vector addition.

When we have a potential that depends only on the difference in position $V(\mathbf{r}_1 - \mathbf{r}_2)$ then we know from classical problems it is effective to work in center of mass coordinates

$$\begin{aligned}\hat{\mathbf{R}}_{\mathrm{cm}} &= \frac{\hat{\mathbf{r}}_1 + \hat{\mathbf{r}}_2}{2} \\ \hat{\mathbf{P}}_{\mathrm{cm}} &= \hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2\end{aligned} \tag{5.71}$$

where

$$\left[\hat{R}_i, \hat{P}_j\right] = i\hbar\delta_{ij}. \tag{5.72}$$

Given

$$\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2 = \hat{\mathbf{L}}_{\mathrm{tot}}, \tag{5.73}$$

do we have

$$\left[\hat{L}_{\mathrm{tot},i}, \hat{L}_{\mathrm{tot},j}\right] = i\hbar\epsilon_{ijk}\hat{L}_{\mathrm{tot},k}? \tag{5.74}$$

That is

$$\left[\hat{L}_{1,i} + \hat{L}_{1,j}, \hat{L}_{2,i} + \hat{L}_{2,j}\right] = i\hbar\epsilon_{ijk}\left(\hat{L}_{1,k} + \hat{L}_{1,k}\right) \tag{5.75}$$

FIXME: Right at the end of the lecture, there was a mention of something about whether or not $\hat{\mathbf{L}}_1^2$ and $\hat{L}_{1,z}$ were sharply defined, but I missed it. Ask about this if not covered in the next lecture.

5.6 ADDITION OF ANGULAR MOMENTA (CONT.)

- For orbital angular momentum

$$\begin{aligned}\hat{\mathbf{L}}_1 &= \hat{\mathbf{r}}_1 \times \hat{\mathbf{p}}_1 \\ \hat{\mathbf{L}}_1 &= \hat{\mathbf{r}}_1 \times \hat{\mathbf{p}}_1,\end{aligned} \tag{5.76}$$

We can show that it is true that

$$\left[L_{1i} + L_{2i}, L_{1j} + L_{2j}\right] = i\hbar\epsilon_{ijk}\left(L_{1k} + L_{2k}\right), \tag{5.77}$$

because the angular momentum of the independent particles commute. Given this is it fair to consider that the sum

$$\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2 \tag{5.78}$$

is also angular momentum.

- Given $|l_1, m_1\rangle$ and $|l_2, m_2\rangle$, if a measurement is made of $\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2$, what do we get? Specifically, what do we get for

$$\left(\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2\right)^2, \tag{5.79}$$

and for

$$\left(\hat{L}_{1z} + \hat{L}_{2z}\right). \tag{5.80}$$

For the latter, we get

$$\left(\hat{L}_{1z} + \hat{L}_{2z}\right)|l_1, m_1; l_2, m_2\rangle = (\hbar m_1 + \hbar m_2)\,|l_1, m_1; l_2, m_2\rangle \tag{5.81}$$

Given

$$\hat{L}_{1z} + \hat{L}_{2z} = \hat{L}_z^{\text{tot}}, \tag{5.82}$$

we find

$$\begin{aligned}\left[\hat{L}_z^{\text{tot}}, \hat{\mathbf{L}}_1^2\right] &= 0 \\ \left[\hat{L}_z^{\text{tot}}, \hat{\mathbf{L}}_2^2\right] &= 0 \\ \left[\hat{L}_z^{\text{tot}}, \hat{\mathbf{L}}_{1z}\right] &= 0 \\ \left[\hat{L}_z^{\text{tot}}, \hat{\mathbf{L}}_{1z}\right] &= 0.\end{aligned} \tag{5.83}$$

We also find

$$\begin{aligned}\left[(\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2)^2, \hat{\mathbf{L}}_1^2\right] &= \left[\hat{\mathbf{L}}_1^2 + \hat{\mathbf{L}}_2^2 + 2\hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_2, \hat{\mathbf{L}}_1^2\right] \\ &= 0,\end{aligned} \tag{5.84}$$

but for

$$\begin{aligned}\left[(\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2)^2, \hat{L}_{1z}\right] &= \left[\hat{\mathbf{L}}_1^2 + \hat{\mathbf{L}}_2^2 + 2\hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_2, \hat{L}_{1z}\right] \\ &= 2\left[\hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_2, \hat{L}_{1z}\right] \neq 0.\end{aligned} \tag{5.85}$$

Classically if we have measured $\hat{\mathbf{L}}_1$ and $\hat{\mathbf{L}}_2$ then we know the total angular momentum as sketched in fig. 5.7.

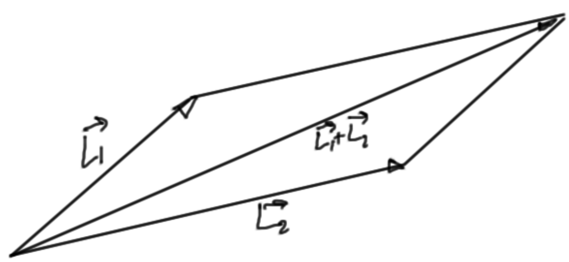

Figure 5.7: Classical addition of angular momenta.

In QM where we don't know all the components of the angular momentum simultaneously, things get fuzzier. For example, if the $\hat{L}_{1z}$ and $\hat{L}_{2z}$ components have been measured, we have the angular momentum defined within a conical region as sketched in fig. 5.8.

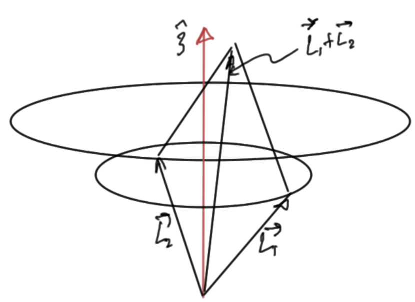

Figure 5.8: Addition of angular momenta given measured $\hat{L}_z$.

Suppose we know $\hat{L}_z^{\text{tot}}$ precisely, but have imprecise information about $\left(\hat{\mathbf{L}}^{\text{tot}}\right)^2$. Can we determine bounds for this? Let $|\psi\rangle = |l_1, m_2; l_2, m_2\rangle$, so

$$\begin{aligned}\langle\psi| \left(\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2\right)^2 |\psi\rangle &= \langle\psi| \hat{\mathbf{L}}_1^2 |\psi\rangle + \langle\psi| \hat{\mathbf{L}}_2^2 |\psi\rangle + 2 \langle\psi| \hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_2 |\psi\rangle \\ &= l_1 (l_1 + 1) \hbar^2 + l_2 (l_2 + 1) \hbar^2 + 2 \langle\psi| \hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_2 |\psi\rangle .\end{aligned} \tag{5.86}$$

Using the Cauchy-Schwartz inequality

$$|\langle\phi|\psi\rangle|^2 \le |\langle\phi|\phi\rangle||\langle\psi|\psi\rangle|, \tag{5.87}$$

which is the equivalent of the classical relationship

$$(\mathbf{A} \cdot \mathbf{B})^2 \le \mathbf{A}^2\mathbf{B}^2. \tag{5.88}$$

Applying this to the last term, we have

$$\begin{aligned}\left(\langle\psi| \hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_2 |\psi\rangle\right)^2 &\le \langle\psi| \hat{\mathbf{L}}_1 \cdot \hat{\mathbf{L}}_1 |\psi\rangle \langle\psi| \hat{\mathbf{L}}_2 \cdot \hat{\mathbf{L}}_2 |\psi\rangle \\ &= \hbar^4 l_1 (l_1 + 1) l_2 (l_2 + 2) .\end{aligned} \tag{5.89}$$

Thus for the max we have

$$\langle\psi| \left(\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2\right)^2 |\psi\rangle \le \hbar^2 l_1 (l_1 + 1) + \hbar^2 l_2 (l_2 + 1) + 2 \hbar^2 \sqrt{l_1 (l_1 + 1) l_2 (l_2 + 2)} \tag{5.90}$$

and for the min

$$\langle\psi| \left(\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2\right)^2 |\psi\rangle \ge \hbar^2 l_1 (l_1 + 1) + \hbar^2 l_2 (l_2 + 1) - 2 \hbar^2 \sqrt{l_1 (l_1 + 1) l_2 (l_2 + 2)}. \tag{5.91}$$

To try to pretty up these estimate, starting with the max, note that if we replace a portion of the RHS with something bigger, we are left with a strict less than relationship.

That is

$$\begin{aligned}l_1 (l_1 + 1) &< \left(l_1 + \frac{1}{2}\right)^2 \\ l_2 (l_2 + 1) &< \left(l_2 + \frac{1}{2}\right)^2\end{aligned} \tag{5.92}$$

That is

$$\begin{aligned}\langle\psi| \left(\hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2\right)^2 |\psi\rangle &< \hbar^2 \left(l_1 (l_1 + 1) + l_2 (l_2 + 1) + 2 \left(l_1 + \frac{1}{2}\right)\left(l_2 + \frac{1}{2}\right)\right) \\ &= \hbar^2 \left(l_1^2 + l_2^2 + l_1 + l_2 + 2 l_1 l_2 + l_1 + l_2 + \frac{1}{2}\right) \\ &= \hbar^2 \left(\left(l_1 + l_2 + \frac{1}{2}\right)\left(l_1 + l_2 + \frac{3}{2}\right) - \frac{1}{4}\right)\end{aligned} \tag{5.93}$$

or

$$l_{\text{tot}}\left(l_{\text{tot}}+1\right)<\left(l_1+l_2+\frac{1}{2}\right)\left(l_1+l_2+\frac{3}{2}\right), \tag{5.94}$$

which, gives

$$l_{\text{tot}}<l_1+l_2+\frac{1}{2}. \tag{5.95}$$

Finally, given a quantization requirement, that is

$$\boxed{l_{\text{tot}}\leq l_1+l_2.} \tag{5.96}$$

Similarly, for the min, we find

$$\begin{aligned}\langle\psi|\left(\hat{\mathbf{L}}_1+\hat{\mathbf{L}}_2\right)^2|\psi\rangle &> \hbar^2\left(l_1\left(l_1+1\right)+l_2\left(l_2+1\right)-2\left(l_1+\frac{1}{2}\right)\left(l_2+\frac{1}{2}\right)\right)\\ &= \hbar^2\left(l_1^2+l_2^2-2l_1l_2-\frac{1}{2}\right)\\ &= \hbar^2\left(\left(l_1-l_2-\frac{1}{2}\right)\left(l_1-l_2+\frac{1}{2}\right)-\frac{1}{4}\right).\end{aligned} \tag{5.97}$$

The total angular momentum quantum number must then satisfy

$$l_{\text{tot}}(l_{\text{tot}}+1)>\left(l_1-l_2-\frac{1}{2}\right)\left(l_1-l_2+\frac{1}{2}\right)-\frac{1}{4} \tag{5.98}$$

Is it true that

$$l_{\text{tot}}(l_{\text{tot}}+1)>\left(l_1-l_2-\frac{1}{2}\right)\left(l_1-l_2+\frac{1}{2}\right)? \tag{5.99}$$

This is true when $l_{\text{tot}}>l_1-l_2-\frac{1}{2}$, assuming that $l_1>l_2$. Suppose $l_{\text{tot}}=l_1-l_2-\frac{1}{2}$, then

$$\begin{aligned}l_{\text{tot}}(l_{\text{tot}}+1) &= \left(l_1-l_2-\frac{1}{2}\right)\left(l_1-l_2+\frac{1}{2}\right)\\ &= (l_1-l_2)^2-\frac{1}{4}.\end{aligned} \tag{5.100}$$

So, is it true that

$$(l_1-l_2)^2-\frac{1}{4}\geq l_1^2+l_1+l_2^2+l_2-2\sqrt{l_1(l_1+1)l_2(l_2+1)}? \tag{5.101}$$

If that is the case we have

$$-2l_1l_2 - \frac{1}{4} \geq l_1 + l_2 - 2\sqrt{l_1(l_1+1)l_2(l_2+1)}, \tag{5.102}$$

$$\begin{aligned} 2\sqrt{l_2(l_1+1)l_1(l_2+1)} &\geq l_1 + l_2 + 2l_1l_2 + \frac{1}{4} \\ &= l_1(l_2+1) + l_2(l_1+1) + \frac{1}{4}. \end{aligned} \tag{5.103}$$

This has the structure

$$2\sqrt{xy} \geq x + y + \frac{1}{4}, \tag{5.104}$$

or

$$4xy \geq (x+y)^2 + \frac{1}{16} + \frac{1}{2}(x+y), \tag{5.105}$$

or

$$0 \geq (x-y)^2 + \frac{1}{16} + \frac{1}{2}(x+y), \tag{5.106}$$

But since $x + y \geq 0$ this inequality is not satisfied when $l_{\text{tot}} = l_1 - l_2 - \frac{1}{2}$. We can conclude

$$l_1 - l_2 - \frac{1}{2} < l_{\text{tot}} < l_1 + l_2 + \frac{1}{2}. \tag{5.107}$$

Is it true that

$$l_1 - l_2 \geq l_{\text{tot}} \geq l_1 + l_2? \tag{5.108}$$

Note that we have two separate Hilbert spaces $l_1 \otimes l_2$ of dimension $2l_1 + 1$ and $2l_2 + 1$ respectively. The total number of states is

$$\begin{aligned} \sum_{l_{\text{tot}}=l_1-l_2}^{l_1+l_2} (2l_{\text{tot}}+1) &= 2\sum_{n=l_1-l_2}^{l_1+l_2} n + \cancel{l_1} + l_2 - (\cancel{l_1} - l_2) + 1 \\ &= 2\frac{1}{2}\left(l_1 + l_2 + (l_1 - l_2)\right)\left(l_1 + l_2 - (l_1 - l_2) + 1\right) + 2l_2 + 1 \\ &= 2l_1\left(2l_2 + 1\right) + 2l_2 + 1 \\ &= (2l_1 + 1)(2l_2 + 1). \end{aligned} \tag{5.109}$$

So the end result is that given $|l_1, m_1\rangle, |l_2, m_2\rangle$, with $l_1 \geq l_2$, where, in steps of 1,

$$\boxed{l_1 - l_2 \leq l_{\text{tot}} \leq l_1 + l_2.} \tag{5.110}$$

5.7 CLEBSCH-GORDAN

How can we related total momentum states to individual momentum states in the $1 \otimes 2$ space?

$$|l_1, l_2, l, m\rangle = \sum_{m_1, m_2} C^{l_1 l_2 l m}_{l_1 l_2 m_1 m_2} |l_1 m_1; l_2 m_2\rangle \tag{5.111}$$

The values $C^{l_1 l_2 l m}_{l_1 l_2 m_1 m_2}$ are called the Clebsch-Gordan coefficients.

Example 5.2: Example: spin one and spin one half

With individual momentum states $|l_1 m_1; l_2 m_2\rangle$

$$\begin{aligned} l_1 &= 1 \\ m_1 &= \pm 1, 0 \\ l_2 &= \frac{1}{2} \\ m_2 &= \pm\frac{1}{2} \end{aligned} \tag{5.112}$$

The total angular momentum numbers are

$$l_{\text{tot}} \in [l_1 - l_2, l_1 + l_2] = [1/2, 3/2] \tag{5.113}$$

The possible states $|l_{\text{tot}}, m_{\text{tot}}\rangle$ are

$$\left|\frac{1}{2}, \frac{1}{2}\right\rangle, \left|\frac{1}{2}, -\frac{1}{2}\right\rangle, \tag{5.114}$$

and

$$\left|\frac{3}{2}, \frac{3}{2}\right\rangle, \left|\frac{3}{2}, \frac{1}{2}\right\rangle, \left|\frac{3}{2}, -\frac{1}{2}\right\rangle \left|\frac{3}{2}, -\frac{3}{2}\right\rangle. \tag{5.115}$$

The Clebsch-Gordan procedure is the search for an orthogonal angular momentum basis, built up from the individual momentum bases. For the total momentum basis we want the basis states to satisfy the ladder operators, but also have them satisfy the consistent ladder operators for the individual particle angular momenta. This procedure is sketched in fig. 5.9.

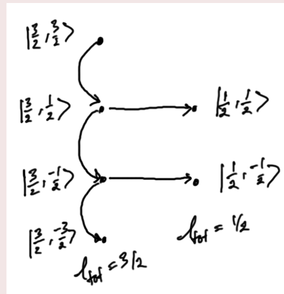

Figure 5.9: Spin one,one-half Clebsch-Gordan procedure.

Demonstrating by example, let the highest total momentum state be proportional to the highest product of individual momentum states

$$\left|\frac{3}{2}\frac{3}{2}\right\rangle = |11\rangle \otimes \left|\frac{1}{2}\frac{1}{2}\right\rangle. \tag{5.116}$$

A lowered state can be constructed in two different ways, one using the total angular momentum lowering operator

$$\begin{aligned}
\left|\frac{3}{2}\frac{1}{2}\right\rangle &= \hat{L}_-^{\text{tot}} \left|\frac{3}{2}\frac{3}{2}\right\rangle \\
&= \hbar \sqrt{\left(\frac{3}{2}+\frac{3}{2}\right)\left(\frac{3}{2}-\frac{3}{2}+1\right)} \left|\frac{3}{2}\frac{1}{2}\right\rangle \\
&= \hbar \sqrt{3} \left|\frac{3}{2}\frac{1}{2}\right\rangle.
\end{aligned} \tag{5.117}$$

On the other hand, the lowering operator can also be expressed as $\hat{L}_-^{\text{tot}} = \hat{L}_-^{(1)} \otimes 1 + 1 \otimes \hat{L}_-^{(2)}$. Operating with that gives

$$
\begin{aligned}
\left|\frac{3}{2}\frac{1}{2}\right\rangle &= \hat{L}_-^{\text{tot}}\,|11\rangle \otimes \left|\frac{1}{2}\frac{1}{2}\right\rangle \\
&= \hat{L}_-^{(1)}\,|11\rangle \otimes \left|\frac{1}{2}\frac{1}{2}\right\rangle + |11\rangle \otimes \hat{L}_-^{2}\left|\frac{1}{2}\frac{1}{2}\right\rangle \\
&= \hbar\sqrt{(1+1)\,(1-1+1)}\,|10\rangle \otimes \left|\frac{1}{2}\frac{1}{2}\right\rangle + \hbar\sqrt{\left(\frac{1}{2}+\frac{1}{2}\right)\left(\frac{1}{2}-\frac{1}{2}+1\right)}\,|11\rangle \otimes \left|\frac{1}{2}-\frac{1}{2}\right\rangle \\
&= \hbar\sqrt{2}\,|10\rangle \otimes \left|\frac{1}{2}\frac{1}{2}\right\rangle + \hbar\,|11\rangle \otimes \left|\frac{1}{2}-\frac{1}{2}\right\rangle.
\end{aligned}
\tag{5.118}
$$

Equating both sides and dispensing with the direct product notation, this is

$$
\sqrt{3}\left|\frac{3}{2}\frac{1}{2}\right\rangle = \sqrt{2}\left|10;\frac{1}{2}\frac{1}{2}\right\rangle + \left|11;\frac{1}{2}-\frac{1}{2}\right\rangle,
\tag{5.119}
$$

or

$$
\boxed{\left|\frac{3}{2}\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|10;\frac{1}{2}\frac{1}{2}\right\rangle + \frac{1}{\sqrt{3}}\left|11;\frac{1}{2}-\frac{1}{2}\right\rangle.}
\tag{5.120}
$$

This is clearly both a unit ket, and normal to $\left|\frac{3}{2}\frac{3}{2}\right\rangle$. We can continue operating with the lowering operator for the total angular momentum to construct all the states down to $\left|\frac{3}{2}\frac{-3}{2}\right\rangle$. Working with $\hbar = 1$ since we see it cancel out, the next lower state follows from

$$
\begin{aligned}
\hat{L}_-^{\text{tot}}\left|\frac{3}{2}\frac{1}{2}\right\rangle &= \sqrt{2\times 2}\left|\frac{3}{2}\frac{-1}{2}\right\rangle \\
&= 2\left|\frac{3}{2}\frac{-1}{2}\right\rangle.
\end{aligned}
\tag{5.121}
$$

and from the individual lowering operators on the components of $\left|\frac{3}{2}\frac{1}{2}\right\rangle$.

$$
\hat{L}_-^{(1)}\left|10;\frac{1}{2}\frac{1}{2}\right\rangle = \sqrt{1\times 2}\left|1-1;\frac{1}{2}\frac{1}{2}\right\rangle,
\tag{5.122}
$$

and

$$
\hat{L}_-^{(2)}\left|10;\frac{1}{2}\frac{1}{2}\right\rangle = \sqrt{1\times 1}\left|10;\frac{1}{2}\frac{-1}{2}\right\rangle,
\tag{5.123}
$$

and

$$\hat{L}_-^1 \left|11; \frac{1}{2} - \frac{1}{2}\right\rangle = \sqrt{2\times 1}\left|10; \frac{1}{2} - \frac{1}{2}\right\rangle. \tag{5.124}$$

This gives

$$2\left|\frac{3}{2}\frac{-1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left(\sqrt{2}\left|1-1; \frac{1}{2}\frac{1}{2}\right\rangle + \left|10; \frac{1}{2}\frac{-1}{2}\right\rangle\right) + \frac{1}{\sqrt{3}}\sqrt{2}\left|10; \frac{1}{2} - \frac{1}{2}\right\rangle, \tag{5.125}$$

or

$$\boxed{\left|\frac{3}{2}\frac{-1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left|1-1; \frac{1}{2}\frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\left|10; \frac{1}{2}\frac{-1}{2}\right\rangle.} \tag{5.126}$$

There's one more possible state with total angular momentum $\frac{3}{2}$. This time

$$\begin{aligned}
\hat{L}_-^{\text{tot}}\left|\frac{3}{2}\frac{-1}{2}\right\rangle &= \sqrt{1\times 3}\left|\frac{3}{2}\frac{-3}{2}\right\rangle \\
&= \frac{1}{\sqrt{3}}\hat{L}_-^{(2)}\left|1-1; \frac{1}{2}\frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\hat{L}_-^{(1)}\left|10; \frac{1}{2}\frac{-1}{2}\right\rangle \\
&= \frac{1}{\sqrt{3}}\sqrt{1\times 1}\left|1-1; \frac{1}{2}\frac{-1}{2}\right\rangle + \sqrt{\frac{2}{3}}\sqrt{1\times 2}\left|1-1; \frac{1}{2}\frac{-1}{2}\right\rangle,
\end{aligned} \tag{5.127}$$

or

$$\boxed{\left|\frac{3}{2}\frac{-3}{2}\right\rangle = \left|1-1; \frac{1}{2}\frac{-1}{2}\right\rangle.} \tag{5.128}$$

The $\left|\frac{1}{2}\frac{1}{2}\right\rangle$ state is constructed as normal to $\left|\frac{3}{2}\frac{1}{2}\right\rangle$, or

$$\boxed{\left|\frac{1}{2}\frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left|10; \frac{1}{2}\frac{1}{2}\right\rangle - \sqrt{\frac{2}{3}}\left|11; \frac{1}{2} - \frac{1}{2}\right\rangle,} \tag{5.129}$$

and $\left|\frac{1}{2} - \frac{1}{2}\right\rangle$ by lowering that. With

$$\hat{L}_-^{\text{tot}}\left|\frac{1}{2}\frac{1}{2}\right\rangle = \sqrt{1\times 1}\left|\frac{1}{2} - \frac{1}{2}\right\rangle, \tag{5.130}$$

we have

$$\left|\frac{1}{2}\,-\frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left(\sqrt{1\times 2}\left|1\,-1;\frac{1}{2}\,\frac{1}{2}\right\rangle + \left|10;\frac{1}{2}\,-\frac{1}{2}\right\rangle\right) - \sqrt{\frac{2}{3}}\sqrt{2\times 1}\left|10;\frac{1}{2}\,-\frac{1}{2}\right\rangle, \tag{5.131}$$

or

$$\boxed{\left|\frac{1}{2}\,-\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|1\,-1;\frac{1}{2}\,\frac{1}{2}\right\rangle - \frac{1}{\sqrt{3}}\left|10;\frac{1}{2}\,-\frac{1}{2}\right\rangle.} \tag{5.132}$$

Observe that further lowering this produces zero

$$\begin{aligned}\hat{L}_-^{\text{tot}}\left|\frac{1}{2}\,-\frac{1}{2}\right\rangle &= \sqrt{\frac{2}{3}}\sqrt{1\times 1}\left|1\,-1;\frac{1}{2}\,-\frac{1}{2}\right\rangle - \frac{1}{\sqrt{3}}\sqrt{1\times 2}\left|1\,-1;\frac{1}{2}\,-\frac{1}{2}\right\rangle.\\ &= 0.\end{aligned} \tag{5.133}$$

All the basis elements have been determined, and are summarized in table 5.1.

Table 5.1: Spin one,half total angular momentum basis.

$\left\lvert\frac{3}{2}\,\frac{3}{2}\right\rangle = \left\lvert 11;\frac{1}{2}\,\frac{1}{2}\right\rangle$	
$\left\lvert\frac{3}{2}\,\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left\lvert 10;\frac{1}{2}\,\frac{1}{2}\right\rangle + \frac{1}{\sqrt{3}}\left\lvert 11;\frac{1}{2}\,-\frac{1}{2}\right\rangle$	$\left\lvert\frac{1}{2}\,\frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left\lvert 10;\frac{1}{2}\,\frac{1}{2}\right\rangle - \sqrt{\frac{2}{3}}\left\lvert 11;\frac{1}{2}\,-\frac{1}{2}\right\rangle$
$\left\lvert\frac{3}{2}\,\frac{-1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left\lvert 1\,-1;\frac{1}{2}\,\frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\left\lvert 10;\frac{1}{2}\,\frac{-1}{2}\right\rangle$	$\left\lvert\frac{1}{2}\,-\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left\lvert 1\,-1;\frac{1}{2}\,\frac{1}{2}\right\rangle - \frac{1}{\sqrt{3}}\left\lvert 10;\frac{1}{2}\,-\frac{1}{2}\right\rangle$
$\left\lvert\frac{3}{2}\,\frac{-3}{2}\right\rangle = \left\lvert 1\,-1;\frac{1}{2}\,\frac{-1}{2}\right\rangle$	

Example 5.3: Spin two, spin one.

With $j_1 = 2$ and $j_2 = 1$, we have $j \in 1, 2, 3$, and can proceed the same way as sketched in fig. 5.10.

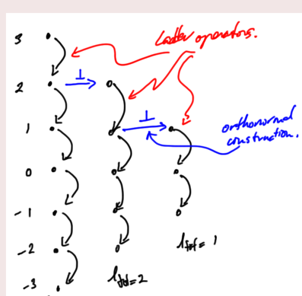

Figure 5.10: Spin two,one Clebsch-Gordan procedure.

Working through the details for this example is left to the problem set.

5.8 PROBLEMS

Exercise 5.1 Angular momentum commutators.

Using $\hat{L}_i = \epsilon_{ijk}\hat{r}_j\hat{p}_k$, show that

$$\left[\hat{L}_i, \hat{L}_j\right] = i\hbar\epsilon_{ijk}\hat{L}_k \tag{5.134}$$

Answer for Exercise 5.1

Let's start without using abstract index expressions, computing the commutator for $\hat{L}_1, \hat{L}_2$, which should show the basic steps required

$$\begin{aligned}\left[\hat{L}_1, \hat{L}_2\right] &= \left[\hat{r}_2\hat{p}_3 - \hat{r}_3\hat{p}_2, \hat{r}_3\hat{p}_1 - \hat{r}_1\hat{p}_3\right] \\ &= \left[\hat{r}_2\hat{p}_3, \hat{r}_3\hat{p}_1\right] - \left[\hat{r}_2\hat{p}_3, \hat{r}_1\hat{p}_3\right] - \left[\hat{r}_3\hat{p}_2, \hat{r}_3\hat{p}_1\right] + \left[\hat{r}_3\hat{p}_2, \hat{r}_1\hat{p}_3\right].\end{aligned} \tag{5.135}$$

The first of these commutators is

$$\begin{aligned}\left[\hat{r}_2\hat{p}_3, \hat{r}_3\hat{p}_1\right] &= \hat{r}_2\hat{p}_3\hat{r}_3\hat{p}_1 - \hat{r}_3\hat{p}_1\hat{r}_2\hat{p}_3 \\ &= \hat{r}_2\hat{p}_1\left[\hat{p}_3, \hat{r}_3\right] \\ &= -i\hbar\hat{r}_2\hat{p}_1.\end{aligned} \tag{5.136}$$

We see that any factors in the commutator don't have like indexes (i.e. $\hat{r}_k, \hat{p}_k$) on both position and momentum terms, can be pulled out of the commutator. This leaves

$$\begin{aligned}\left[\hat{L}_1, \hat{L}_2\right] &= \hat{r}_2\hat{p}_1\left[\hat{p}_3, \hat{r}_3\right] - \cancel{\left[\hat{r}_2\hat{p}_3, \hat{r}_1\hat{p}_3\right]} - \cancel{\left[\hat{r}_3\hat{p}_2, \hat{r}_3\hat{p}_1\right]} + \hat{r}_1\hat{p}_2\left[\hat{r}_3, \hat{p}_3\right] \\ &= i\hbar\left(\hat{r}_1\hat{p}_2 - \hat{r}_2\hat{p}_1\right) \\ &= i\hbar\hat{L}_3.\end{aligned} \tag{5.137}$$

With cyclic permutation this is really enough to consider eq. (5.134) proven. However, can we do this in the general case with the abstract index expression? The quantity to simplify looks forbidding

$$\left[\hat{L}_i, \hat{L}_j\right] = \epsilon_{iab}\epsilon_{jst}\left[\hat{r}_a\hat{p}_b, \hat{r}_s\hat{p}_t\right] \tag{5.138}$$

Because there are no repeated indexes, this doesn't submit to any of the normal reduction identities. Note however, since we only care about the $i \neq j$ case, that one of the indexes a, b must be j for this quantity to be non-zero. Therefore (for $i \neq j$)

$$\begin{aligned}
\left[\hat{L}_i, \hat{L}_j\right] &= \epsilon_{ijb}\epsilon_{jst}\left[\hat{r}_j\hat{p}_b, \hat{r}_s\hat{p}_t\right] + \epsilon_{iaj}\epsilon_{jst}\left[\hat{r}_a\hat{p}_j, \hat{r}_s\hat{p}_t\right] \\
&= \epsilon_{ijb}\epsilon_{jst}\left(\left[\hat{r}_j\hat{p}_b, \hat{r}_s\hat{p}_t\right] - \left[\hat{r}_b\hat{p}_j, \hat{r}_s\hat{p}_t\right]\right) \\
&= -\delta^{st}_{[ib]}\left[\hat{r}_j\hat{p}_b - \hat{r}_b\hat{p}_j, \hat{r}_s\hat{p}_t\right] \\
&= \left[\hat{r}_j\hat{p}_b - \hat{r}_b\hat{p}_j, \hat{r}_b\hat{p}_i - \hat{r}_i\hat{p}_b\right] \\
&= \left[\hat{r}_j\hat{p}_b, \hat{r}_b\hat{p}_i\right] - \cancel{\left[\hat{r}_j\hat{p}_b, \hat{r}_i\hat{p}_b\right]} - \cancel{\left[\hat{r}_b\hat{p}_j, \hat{r}_b\hat{p}_i\right]} + \left[\hat{r}_b\hat{p}_j, \hat{r}_i\hat{p}_b\right] \\
&= \hat{r}_j\hat{p}_i\left[\hat{p}_b, \hat{r}_b\right] + \hat{r}_i\hat{p}_j\left[\hat{r}_b, \hat{p}_b\right] \\
&= i\hbar\left(\hat{r}_i\hat{p}_j - \hat{r}_j\hat{p}_i\right) \\
&= i\hbar\epsilon_{ijk}\hat{r}_i\hat{p}_j.
\end{aligned} \tag{5.139}$$

Exercise 5.2 S_y eigenvectors. ([11] pr. 4.1)

Find the eigenvectors of σ_y, and then find the probability that a measurement of S_y will be $\hbar/2$ when the state is initially

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} \tag{5.140}$$

Answer for Exercise 5.2

The eigenvalues should be ± 1, which is easily checked

$$\begin{aligned}
0 &= \left|\sigma_y - \lambda\right| \\
&= \begin{vmatrix} -\lambda & -i \\ i & -\lambda \end{vmatrix} \\
&= \lambda^2 - 1.
\end{aligned} \tag{5.141}$$

For $|+\rangle = (a, b)^{\mathrm{T}}$ we must have

$$-1a - ib = 0, \tag{5.142}$$

so

$$|+\rangle \propto \begin{bmatrix} -i \\ 1 \end{bmatrix}, \tag{5.143}$$

or

$$|+\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}. \tag{5.144}$$

For $|-\rangle$ we must have

$$a - ib = 0, \tag{5.145}$$

so

$$|+\rangle \propto \begin{bmatrix} i \\ 1 \end{bmatrix}, \tag{5.146}$$

or

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix}. \tag{5.147}$$

The normalized eigenvectors are

$$\boxed{|\pm\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm i \end{bmatrix}.} \tag{5.148}$$

For the probability question we are interested in

$$\begin{aligned}
\left| \left\langle S_y; + \right| \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \right|^2 &= \frac{1}{2} \left| \begin{bmatrix} 1 & -i \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \right|^2 \\
&= \frac{1}{2} \left(|\alpha|^2 + |\beta|^2 \right) \\
&= \frac{1}{2}.
\end{aligned} \tag{5.149}$$

There is a 50% chance of finding the particle in the $|S_x; +\rangle$ state, independent of the initial state.

Exercise 5.3 **Magnetic Hamiltonian eigenvectors. (*[11] pr. 3.2*)**

Using Pauli matrices, find the eigenvectors for the magnetic spin interaction Hamiltonian

$$H = -\frac{1}{\hbar} 2\mu \mathbf{S} \cdot \mathbf{B}. \tag{5.150}$$

Answer for Exercise 5.3

$$\begin{aligned} H &= -\mu \boldsymbol{\sigma} \cdot \mathbf{B} \\ &= -\mu \left(B_x \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + B_y \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + B_z \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right) \\ &= -\mu \begin{bmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{bmatrix}. \end{aligned} \tag{5.151}$$

The characteristic equation is

$$\begin{aligned} 0 &= \begin{vmatrix} -\mu B_z - \lambda & -\mu(B_x - iB_y) \\ -\mu(B_x + iB_y) & \mu B_z - \lambda \end{vmatrix} \\ &= -\left((\mu B_z)^2 - \lambda^2 \right) - \mu^2 \left(B_x^2 - (iB_y)^2 \right) \\ &= \lambda^2 - \mu^2 \mathbf{B}^2. \end{aligned} \tag{5.152}$$

That is

$$\boxed{\lambda = \pm \mu B.} \tag{5.153}$$

Now for the eigenvectors. We are looking for $|\pm\rangle = (a, b)^{\mathrm{T}}$ such that

$$0 = (-\mu B_z \mp \mu B) a - \mu (B_x - iB_y) b \tag{5.154}$$

or

$$|\pm\rangle \propto \begin{bmatrix} B_x - iB_y \\ B_z \pm B \end{bmatrix}. \tag{5.155}$$

This squares to

$$B_x^2 + B_y^2 + B_z^2 + B^2 \pm 2BB_z = 2B(B \pm B_z), \tag{5.156}$$

so the normalized eigenkets are

$$\boxed{|\pm\rangle = \frac{1}{\sqrt{2B(B \pm B_z)}} \begin{bmatrix} B_x - iB_y \\ B_z \pm B \end{bmatrix}.} \tag{5.157}$$

Exercise 5.4 Unimodular transformation. ([11] pr. 3.3)

Given the matrix

$$U = \frac{a_0 + i\sigma \cdot \mathbf{a}}{a_0 - i\sigma \cdot \mathbf{a}}, \tag{5.158}$$

where $a_0, \mathbf{a}$ are real valued constant and vector respectively.

a. Show that this is a unimodular and unitary transformation.
b. A unitary transformation can represent an arbitrary rotation. Determine the rotation angle and direction in terms of $a_0, \mathbf{a}$.

Answer for Exercise 5.4

Part a. Let's call these factors $A_\pm$, which expand to

$$\begin{aligned} A_\pm &= a_0 \pm i\sigma \cdot \mathbf{a} \\ &= \begin{bmatrix} a_0 \pm ia_z & \pm\left(a_y + ia_x\right) \\ \mp(a_y - ia_x) & a_0 \mp ia_z \end{bmatrix}, \end{aligned} \tag{5.159}$$

or with $z = a_0 + ia_z$, and $w = a_y + ia_x$, these are

$$A_+ = \begin{bmatrix} z & w \\ -w^* & z^* \end{bmatrix} \tag{5.160}$$

$$A_- = \begin{bmatrix} z^* & -w \\ w^* & z \end{bmatrix}. \tag{5.161}$$

These both have a determinant of

$$\begin{aligned} |z|^2 + |w|^2 &= |a_0 + ia_z|^2 + \left|a_y + ia_x\right|^2 \\ &= a_0^2 + \mathbf{a}^2. \end{aligned} \tag{5.162}$$

The inverse of the latter is

$$A_-^{-1} = \frac{1}{a_0^2 + \mathbf{a}^2} \begin{bmatrix} z & w \\ -w^* & z^* \end{bmatrix} \tag{5.163}$$

Noting that the numerator and denominator commute the inverse can be applied in either order. Picking one, the transformation of interest, after writing $A = a_0^2 + \mathbf{a}^2$, is

$$\begin{aligned} U &= \frac{1}{A} \begin{bmatrix} z & w \\ -w^* & z^* \end{bmatrix} \begin{bmatrix} z & w \\ -w^* & z^* \end{bmatrix} \\ &= \frac{1}{A} \begin{bmatrix} z^2 - |w|^2 & w(z + z^*) \\ -w^*(z^* + z) & (z^*)^2 - |w|^2 \end{bmatrix}. \end{aligned} \tag{5.164}$$

Recall that a unimodular transformation is one that has the form

$$
\begin{bmatrix}
z & w \\
-w^* & z^*
\end{bmatrix},
\tag{5.165}
$$

provided $|z|^2 + |w|^2 = 1$, so eq. (5.164) is unimodular if the following sum is unity, which is the case

$$
\begin{aligned}
\frac{\left|z^2 - |w|^2\right|^2}{\left(|z|^2 + |w|^2\right)^2} + |w|^2 \frac{|z + z^*|^2}{\left(|z|^2 + |w|^2\right)^2}
&= \frac{\left(z^2 - |w|^2\right)\left((z^*)^2 - |w|^2\right) + |w|^2 (z + z^*)^2}{\left(|z|^2 + |w|^2\right)^2} \\
&= \frac{|z|^4 + |w|^4 - |w|^2 \left(\cancel{z^2 + (z^*)^2}\right) + |w|^2 \left(\cancel{z^2 + (z^*)^2} + 2|z|^2\right)}{\left(|z|^2 + |w|^2\right)^2} \\
&= 1.
\end{aligned}
\tag{5.166}
$$

Part b. The most general rotation of a vector $\mathbf{a}$, described by Pauli matrices is

$$
e^{i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\theta/2}\boldsymbol{\sigma}\cdot\mathbf{a}e^{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\theta/2} = \boldsymbol{\sigma}\cdot\hat{\mathbf{n}} + (\boldsymbol{\sigma}\cdot\mathbf{a} - (\mathbf{a}\cdot\hat{\mathbf{n}})\boldsymbol{\sigma}\cdot\hat{\mathbf{n}})\cos\theta + \boldsymbol{\sigma}\cdot(\mathbf{a}\times\hat{\mathbf{n}})\sin\theta.
\tag{5.167}
$$

If the unimodular matrix above, applied as $\boldsymbol{\sigma}\cdot\mathbf{a}' = U^\dagger\boldsymbol{\sigma}\cdot\mathbf{a}U$ is to also describe this rotation, we want the equivalence

$$
U = e^{-i\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}\theta/2},
\tag{5.168}
$$

or

$$
\begin{aligned}
&\frac{1}{a_0^2 + \mathbf{a}^2}
\begin{bmatrix}
a_0^2 - \mathbf{a}^2 + 2ia_0a_z & 2a_0(a_y + ia_x) \\
-2a_0(a_y - ia_x) & a_0^2 - \mathbf{a}^2 - 2ia_0a_z
\end{bmatrix} \\
&= \begin{bmatrix}
\cos(\theta/2) - in_z\sin(\theta/2) & (-n_y - in_x)\sin(\theta/2) \\
-(-n_y + in_x)\sin(\theta/2) & \cos(\theta/2) + in_z\sin(\theta/2)
\end{bmatrix}.
\end{aligned}
\tag{5.169}
$$

Equating components, that is

$$
\begin{aligned}
\cos(\theta/2) &= \frac{a_0^2 - \mathbf{a}^2}{a_0^2 + \mathbf{a}^2} \\
-n_x\sin(\theta/2) &= \frac{2a_0a_x}{a_0^2 + \mathbf{a}^2} \\
-n_y\sin(\theta/2) &= \frac{2a_0a_y}{a_0^2 + \mathbf{a}^2} \\
-n_z\sin(\theta/2) &= \frac{2a_0a_y}{a_0^2 + \mathbf{a}^2}
\end{aligned}
\tag{5.170}
$$

Noting that

$$
\begin{aligned}
\sin(\theta/2) &= \sqrt{1 - \frac{(a_0^2 - \mathbf{a}^2)^2}{(a_0^2 + \mathbf{a}^2)^2}} \\
&= \frac{\sqrt{(a_0^2 + \mathbf{a}^2)^2 - (a_0^2 - \mathbf{a}^2)^2}}{a_0^2 + \mathbf{a}^2} \\
&= \frac{\sqrt{4a_0^2\mathbf{a}^2}}{a_0^2 + \mathbf{a}^2} \\
&= \frac{2a_0|\mathbf{a}|}{a_0^2 + \mathbf{a}^2}
\end{aligned}
\tag{5.171}
$$

The vector normal direction can be written

$$
\mathbf{n} = -\frac{2a_0}{(a_0^2 + \mathbf{a}^2)\sin(\theta/2)}\mathbf{a},
\tag{5.172}
$$

or

$$
\boxed{\mathbf{n} = -\frac{\mathbf{a}}{|\mathbf{a}|}.}
\tag{5.173}
$$

The angle of rotation is

$$
\boxed{\theta = 2\,\mathrm{atan}\,\frac{2a_0|\mathbf{a}|}{a_0^2 - \mathbf{a}^2}.}
\tag{5.174}
$$

Exercise 5.5 **Rotation angle and normal for a rotation through Euler angles.** (*[11] pr. 3.9*)

Consider a sequence of Euler rotations represented by

$$
\mathcal{D}^{1/2}(\alpha, \beta, \gamma) = e^{-i\sigma_z\alpha/2} e^{-i\sigma_y\beta/2} e^{-i\sigma_z\gamma_2}.
\tag{5.175}
$$

Because rotations form a group, this sequence of rotations corresponds to a single rotation by an angle θ about a new axis $\hat{\mathbf{n}}$. What is θ? What is $\hat{\mathbf{n}}$?

Answer for Exercise 5.5

PROBLEM SET RELATED MATERIAL REDACTED IN THIS DOCUMENT.PLEASE FEEL FREE TO EMAIL ME FOR THE FULL VERSION IF YOU AREN'T TAKING PHY1520.[redacted]

[redacted]. END-REDACTION

Exercise 5.6 **Angular momentum addition.** (*2015 ps6 p2*)

You have to add angular momenta $j_1 = 1$ and $j_2 = 2$ to form total angular momentum states with $j = 1, 2, 3$. There are a total of 15 $|j, m\rangle$ states in the total angular momentum basis. Express each of them in terms of the old basis $|j_1, j_2; m_1, m_2\rangle$ set.

Answer for Exercise 5.6

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Exercise 5.7 **Spin-1 rotations.** (*2015 ps6 p3*)

Consider angular momentum $j = 1$.

a. Express $\langle j = 1, m' | \hat{J}_y | j = 1, m\rangle$ as a 3×3 matrix.

b. Show that for $j = 1$

$$e^{-i\hat{J}_y\beta/\hbar} = 1 - i\frac{\hat{J}_y}{\hbar}\sin\beta - \frac{\hat{J}_y^2}{\hbar^2}(1 - \cos\beta)\,. \tag{5.176}$$

Answer for Exercise 5.7

PROBLEM SET RELATED MATERIAL REDACTED IN THIS DOCUMENT.PLEASE FEEL FREE TO EMAIL ME FOR THE FULL VERSION IF YOU AREN'T TAKING PHY1520.[redacted]

[redacted]. END-REDACTION

Exercise 5.8 **L_z and $\mathbf{L}^2$ eigenvalues and probabilities for a wave function.** ([11] *pr. 3.17*)

Given a wave function

$$\psi(r, \theta, \phi) = f(r)\,(x + y + 3z)\,, \tag{5.177}$$

a. Determine if this wave function is an eigenfunction of $\mathbf{L}^2$, and the value of l if it is an eigenfunction.
b. Determine the probabilities for the particle to be found in any given $|l, m\rangle$ state,
c. If it is known that ψ is an energy eigenfunction with energy E indicate how we can find $V(r)$.

Answer for Exercise 5.8

Part a. Using

$$\mathbf{L}^2 = -\hbar^2 \left(\frac{1}{\sin^2\theta} \partial_{\phi\phi} + \frac{1}{\sin\theta} \partial_\theta \left(\sin\theta \partial_\theta \right) \right), \tag{5.178}$$

and

$$\begin{aligned} x &= r \sin\theta \cos\phi \\ y &= r \sin\theta \sin\phi \\ z &= r \cos\theta \end{aligned} \tag{5.179}$$

it's a quick computation to show that

$$\mathbf{L}^2 \psi = 2\hbar^2 \psi = 1(1+1)\hbar^2 \psi, \tag{5.180}$$

so this function is an eigenket of $\mathbf{L}^2$ with an eigenvalue of $2\hbar^2$, which corresponds to $l = 1$, a p-orbital state.

Part b. Recall that the angular representation of L_z is

$$L_z = -i\hbar\frac{\partial,}{\partial\phi} \tag{5.181}$$

so we have

$$\begin{aligned} L_z x &= i\hbar y \\ L_z y &= -i\hbar x \\ L_z z &= 0, \end{aligned} \tag{5.182}$$

The L_z action on ψ is

$$L_z\psi = -i\hbar r f(r)\left(-y + x\right). \tag{5.183}$$

This wave function is not an eigenket of L_z. Expressed in terms of the L_z basis states $e^{im\phi}$, this wave function is

$$\begin{aligned} \psi &= r f(r)\left(\sin\theta\left(\cos\phi + \sin\phi\right) + \cos\theta\right) \\ &= r f(r)\left(\frac{\sin\theta}{2}\left(e^{i\phi}\left(1 + \frac{1}{i}\right) + e^{-i\phi}\left(1 - \frac{1}{i}\right)\right) + \cos\theta\right) \\ &= r f(r)\left(\frac{(1-i)\sin\theta}{2}e^{1i\phi} + \frac{(1+i)\sin\theta}{2}e^{-1i\phi} + \cos\theta e^{0i\phi}\right) \end{aligned} \tag{5.184}$$

Assuming that ψ is normalized, the probabilities for measuring $m = 1, -1, 0$ respectively are

$$\begin{aligned} P_{\pm 1} &= 2\pi\rho\left|\frac{1 \mp i}{2}\right|^2 \int_0^\pi \sin\theta d\theta \sin^2\theta \\ &= -2\pi\rho\int_1^{-1} du(1 - u^2) \\ &= 2\pi\rho\left(u - \frac{u^3}{3}\right)\Big|_{-1}^{1} \\ &= 2\pi\rho\left(2 - \frac{2}{3}\right) \\ &= \frac{8\pi\rho}{3}, \end{aligned} \tag{5.185}$$

and

$$\begin{aligned} P_0 &= 2\pi\rho \int_0^{\pi} \sin\theta \cos\theta \\ &= 0, \end{aligned} \tag{5.186}$$

where

$$\rho = \int_0^{\infty} r^4 |f(r)|^2 dr. \tag{5.187}$$

Because the probabilities must sum to 1, this means the $m = \pm 1$ states are equiprobable with $P_\pm = 1/2$, fixing $\rho = 3/16\pi$, even without knowing $f(r)$.

Part c. The operator $r^2\mathbf{p}^2$ can be decomposed into a $\mathbf{L}^2$ component and some other portions, from which we can write

$$\begin{aligned} H\psi &= \left(\frac{\mathbf{p}^2}{2m} + V(r) \right) \psi \\ &= \left(-\frac{\hbar^2}{2m} \left(\partial_{rr} + \frac{2}{r}\partial_r - \frac{1}{\hbar^2 r^2}\mathbf{L}^2 \right) + V(r) \right) \psi. \end{aligned} \tag{5.188}$$

(See: [11] eq. 6.21)
In this case where $\mathbf{L}^2\psi = 2\hbar^2\psi$ we can rearrange for $V(r)$

$$\begin{aligned} V(r) &= E + \frac{1}{\psi}\frac{\hbar^2}{2m} \left(\partial_{rr} + \frac{2}{r}\partial_r - \frac{2}{r^2} \right) \psi \\ &= E + \frac{1}{f(r)}\frac{\hbar^2}{2m} \left(\partial_{rr} + \frac{2}{r}\partial_r - \frac{2}{r^2} \right) f(r). \end{aligned} \tag{5.189}$$

See sakuraiProblem3.17.nb for some verifications of some of the algebra for this problem.

Exercise 5.9 Angular momentum expectation values. (*[11] pr. 3.18*)

Compute the expectation values for the first and second powers of the angular momentum operators with respect to states $|lm\rangle$.

Answer for Exercise 5.9

We can write the expectation values for the L_z powers immediately

$$\langle L_z \rangle = m\hbar, \tag{5.190}$$

and

$$\left\langle L_z^2 \right\rangle = (m\hbar)^2. \tag{5.191}$$

For the x and y components first express the operators in terms of the ladder operators.

$$
\begin{aligned}
L_+ &= L_x + iL_y \\
L_- &= L_x - iL_y.
\end{aligned}
\tag{5.192}
$$

Rearranging gives

$$
\begin{aligned}
L_x &= \frac{1}{2}\left(L_+ + L_-\right) \\
L_y &= \frac{1}{2i}\left(L_+ - L_-\right).
\end{aligned}
\tag{5.193}
$$

The first order expectations $\langle L_x \rangle, \left\langle L_y \right\rangle$ are both zero since $\langle L_+ \rangle = \langle L_- \rangle$. For the second order expectation values we have

$$
\begin{aligned}
L_x^2 &= \frac{1}{4}\left(L_+ + L_-\right)\left(L_+ + L_-\right) \\
&= \frac{1}{4}\left(L_+L_+ + L_-L_- + L_+L_- + L_-L_+\right) \\
&= \frac{1}{4}\left(L_+L_+ + L_-L_- + 2(L_x^2 + L_y^2)\right) \\
&= \frac{1}{4}\left(L_+L_+ + L_-L_- + 2(\mathbf{L}^2 - L_z^2)\right),
\end{aligned}
\tag{5.194}
$$

and

$$
\begin{aligned}
L_y^2 &= -\frac{1}{4}\left(L_+ - L_-\right)\left(L_+ - L_-\right) \\
&= -\frac{1}{4}\left(L_+L_+ + L_-L_- - L_+L_- - L_-L_+\right) \\
&= -\frac{1}{4}\left(L_+L_+ + L_-L_- - 2(L_x^2 + L_y^2)\right) \\
&= -\frac{1}{4}\left(L_+L_+ + L_-L_- - 2(\mathbf{L}^2 - L_z^2)\right).
\end{aligned}
\tag{5.195}
$$

Any expectation value $\langle lm| L_+L_+ |lm\rangle$ or $\langle lm| L_-L_- |lm\rangle$ will be zero, leaving

$$
\begin{aligned}
\left\langle L_x^2 \right\rangle &= \left\langle L_y^2 \right\rangle \\
&= \frac{1}{4}\left\langle 2(\mathbf{L}^2 - L_z^2) \right\rangle \\
&= \frac{1}{2}\left(\hbar^2 l(l+1) - (\hbar m)^2\right).
\end{aligned}
\tag{5.196}
$$

Observe that we have

$$\left\langle L_x^2 \right\rangle + \left\langle L_y^2 \right\rangle + \left\langle L_z^2 \right\rangle = \hbar^2 l(l+1) = \left\langle \mathbf{L}^2 \right\rangle, \tag{5.197}$$

which is the quantum mechanical analogue of the classical scalar equation $\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$.

Exercise 5.10 Spin three halves spin interaction. ([11] pr. 3.33)

A spin 3/2 nucleus subjected to an external electric field has an interaction Hamiltonian of the form

$$H = \frac{eQ}{2s(s-1)\hbar^2} \left(\left(\frac{\partial^2 \phi}{\partial x^2} \right)_0 S_x^2 + \left(\frac{\partial^2 \phi}{\partial y^2} \right)_0 S_y^2 + \left(\frac{\partial^2 \phi}{\partial z^2} \right)_0 S_z^2 \right). \tag{5.198}$$

a. Show that the interaction energy can be written as

$$A(3S_z^2 - \mathbf{S}^2) + B(S_+^2 + S_-^2). \tag{5.199}$$

b. Find the energy eigenvalues for such a Hamiltonian.

Answer for Exercise 5.10

Part a. Reordering

$$\begin{aligned} S_+ &= S_x + iS_y \\ S_- &= S_x - iS_y, \end{aligned} \tag{5.200}$$

gives

$$\begin{aligned} S_x &= \frac{1}{2} \left(S_+ + S_- \right) \\ S_y &= \frac{1}{2i} \left(S_+ - S_- \right). \end{aligned} \tag{5.201}$$

The squared spin operators are

$$\begin{aligned} S_x^2 &= \frac{1}{4} \left(S_+^2 + S_-^2 + S_+ S_- + S_- S_+ \right) \\ &= \frac{1}{4} \left(S_+^2 + S_-^2 + 2(S_x^2 + S_y^2) \right) \\ &= \frac{1}{4} \left(S_+^2 + S_-^2 + 2(\mathbf{S}^2 - S_z^2) \right), \end{aligned} \tag{5.202}$$

$$
\begin{aligned}
S_y^2 &= -\frac{1}{4}\left(S_+^2 + S_-^2 - S_+S_- - S_-S_+\right) \\
&= -\frac{1}{4}\left(S_+^2 + S_-^2 - 2(S_x^2 + S_y^2)\right) \\
&= -\frac{1}{4}\left(S_+^2 + S_-^2 - 2(\mathbf{S}^2 - S_z^2)\right).
\end{aligned}
\tag{5.203}
$$

This gives

$$
\begin{aligned}
H = \frac{eQ}{2s(s-1)\hbar^2}(&\frac{1}{4}\left(\frac{\partial^2\phi}{\partial x^2}\right)_0 \left(S_+^2 + S_-^2 + 2(\mathbf{S}^2 - S_z^2)\right) \\
&- \left(\frac{\partial^2\phi}{\partial y^2}\right)_0 \left(S_+^2 + S_-^2 - 2(\mathbf{S}^2 - S_z^2)\right) \\
&+ \left(\frac{\partial^2\phi}{\partial z^2}\right)_0 S_z^2) \\
= \frac{eQ}{2s(s-1)\hbar^2}(&\frac{1}{4}\left(\left(\frac{\partial^2\phi}{\partial x^2}\right)_0 - \left(\frac{\partial^2\phi}{\partial y^2}\right)_0\right)\left(S_+^2 + S_-^2\right) \\
&+ \frac{1}{2}\left(\left(\frac{\partial^2\phi}{\partial x^2}\right)_0 + \left(\frac{\partial^2\phi}{\partial y^2}\right)_0\right)\mathbf{S}^2 \\
&+ \left(\left(\frac{\partial^2\phi}{\partial z^2}\right)_0 - \frac{1}{2}\left(\frac{\partial^2\phi}{\partial x^2}\right)_0 - \frac{1}{2}\left(\frac{\partial^2\phi}{\partial y^2}\right)_0\right) S_z^2).
\end{aligned}
\tag{5.204}
$$

For a static electric field we have

$$
\boldsymbol{\nabla}^2\phi = -\frac{\rho}{\epsilon_0},
\tag{5.205}
$$

but are evaluating it at a point away from the generating charge distribution, so $\boldsymbol{\nabla}^2\phi = 0$ at that point. This gives

$$
\begin{aligned}
H = \frac{eQ}{4s(s-1)\hbar^2}(&\frac{1}{2}\left(\left(\frac{\partial^2\phi}{\partial x^2}\right)_0 - \left(\frac{\partial^2\phi}{\partial y^2}\right)_0\right)\left(S_+^2 + S_-^2\right) \\
&+ \left(\left(\frac{\partial^2\phi}{\partial x^2}\right)_0 + \left(\frac{\partial^2\phi}{\partial y^2}\right)_0\right)(\mathbf{S}^2 - 3S_z^2)),
\end{aligned}
\tag{5.206}
$$

so

$$
A = -\frac{eQ}{4s(s-1)\hbar^2}\left(\left(\frac{\partial^2\phi}{\partial x^2}\right)_0 + \left(\frac{\partial^2\phi}{\partial y^2}\right)_0\right)
\tag{5.207}
$$

$$
B = \frac{eQ}{8s(s-1)\hbar^2}\left(\left(\frac{\partial^2\phi}{\partial x^2}\right)_0 - \left(\frac{\partial^2\phi}{\partial y^2}\right)_0\right).
\tag{5.208}
$$

Part b. Using sakuraiProblem3.33.nb, matrix representations for the spin three halves operators and the Hamiltonian were constructed with respect to the basis $\{|3/2\rangle, |1/2\rangle, |-1/2\rangle, |-3/2\rangle\}$

$$
\begin{aligned}
S_+ &= \hbar \begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{bmatrix} \\
S_- &= \hbar \begin{bmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{bmatrix} \\
S_x &= \hbar \begin{bmatrix} 0 & \sqrt{3}/2 & 0 & 0 \\ \sqrt{3}/2 & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{3}/2 \\ 0 & 0 & \sqrt{3}/2 & 0 \end{bmatrix} \\
S_y &= i\hbar \begin{bmatrix} 0 & -\sqrt{3}/2 & 0 & 0 \\ \sqrt{3}/2 & 0 & -1 & 0 \\ 0 & 1 & 0 & -\sqrt{3}/2 \\ 0 & 0 & \sqrt{3}/2 & 0 \end{bmatrix} \\
S_z &= \frac{\hbar}{2} \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix} \\
H &= \begin{bmatrix} 3A & 0 & 2\sqrt{3}B & 0 \\ 0 & -3A & 0 & 2\sqrt{3}B \\ 2\sqrt{3}B & 0 & -3A & 0 \\ 0 & 2\sqrt{3}B & 0 & 3A \end{bmatrix}.
\end{aligned}
\tag{5.209}
$$

The energy eigenvalues are found to be

$$
E = \pm \hbar^2 \sqrt{9A^2 + 12B^2}, \tag{5.210}
$$

with two fold degeneracies for each eigenvalue.

6 APPROXIMATION METHODS

6.1 APPROXIMATION METHODS

Suppose we have a perturbed Hamiltonian

$$H = H_0 + \lambda V, \tag{6.1}$$

where $\lambda = 0$ represents a solvable (perhaps known) system, and $\lambda = 1$ is the case of interest. There are two approaches of interest

1. Direct solution of H with $\lambda = 1$.
2. Take λ small, and do a series expansion. This is perturbation theory.

6.2 VARIATIONAL METHODS

Given

$$H \left|\phi_n\right\rangle = E_n \left|\phi_n\right\rangle, \tag{6.2}$$

where we don't know $\left|\phi_n\right\rangle$, we can compute the expectation with respect to an arbitrary state $\left|\psi\right\rangle$

$$\begin{aligned}
\left\langle\psi\right| H \left|\psi\right\rangle &= \left\langle\psi\right| H \left(\sum_n \left|\phi_n\right\rangle \left\langle\phi_n\right|\right) \left|\psi\right\rangle \\
&= \sum_n E_n \left\langle\psi|\phi_n\right\rangle \left\langle\phi_n|\psi\right\rangle \\
&= \sum_n E_n \left|\left\langle\psi|\phi_n\right\rangle\right|^2.
\end{aligned} \tag{6.3}$$

Define

$$\overline{E} = \frac{\left\langle\psi\right| H \left|\psi\right\rangle}{\left\langle\psi|\psi\right\rangle}. \tag{6.4}$$

Assuming that it is possible to express the state in the Hamiltonian energy basis

$$|\psi\rangle = \sum_n a_n |\phi_n\rangle, \tag{6.5}$$

this average energy is

$$\begin{aligned}\overline{E} &= \frac{\sum_{m,n} \langle\phi_m| a_m^* H a_n |\phi_n\rangle}{\sum_n |a_n|^2} \\ &= \frac{\sum_n |a_n|^2 E_n}{\sum_n |a_n|^2}. \\ &= \sum_n \frac{|a_n|^2}{\sum_n |a_n|^2} E_n \\ &= \sum_n \frac{P_n}{\sum_m P_m} E_n,\end{aligned} \tag{6.6}$$

where $P_m = |a_m|^2$, which has the structure of a probability coefficient once divided by $\sum_m P_m$, as sketched in fig. 6.1.

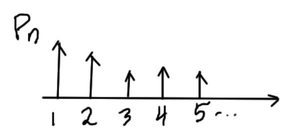

Figure 6.1: A decreasing probability distribution.

This average energy is a probability weighted average of the individual energy basis states. One of those energies is the ground state energy E_1, so we necessarily have

$$\boxed{\overline{E} \ge E_1.} \tag{6.7}$$

Example 6.1: Particle in an offset box.

For the infinite potential box sketched in fig. 6.2.

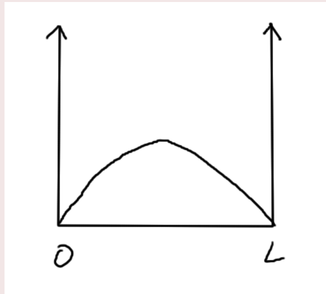

Figure 6.2: Infinite potential $[0, L]$ box.

The exact solutions for such a system are found to be

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right), \tag{6.8}$$

where the energies are

$$E = \frac{\hbar^2}{2m} \frac{n^2\pi^2}{L^2}. \tag{6.9}$$

The function $\psi' = x(L - x)$ also satisfies the boundary value constraints? How close in energy is that function to the ground state?

$$\begin{aligned}
\overline{E} &= -\frac{\hbar^2}{2m} \frac{\int_0^L dx x(L-x) \frac{d^2}{dx^2} (x(L-x))}{\int_0^L dx x^2 (L-x)^2} \\
&= \frac{\hbar^2}{2m} \frac{\frac{2L^3}{6}}{\frac{L^5}{30}} \\
&= \frac{\hbar^2}{2m} \frac{10}{L^2}.
\end{aligned} \tag{6.10}$$

This average energy is quite close to the ground state energy

$$\begin{aligned}
\frac{\overline{E}}{E_1} &= \frac{10}{\pi^2} \\
&= 1.014.
\end{aligned} \tag{6.11}$$

Example 6.2: Particle in a symmetric box.

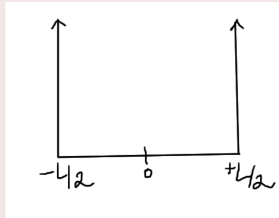

Figure 6.3: Infinite potential $[-L/2, L/2]$ box.

Shifting the boundaries, as sketched in fig. 6.3 doesn't change the energy levels. For this potential let's try a shifted trial function

$$\begin{aligned} \psi(x) &= \left(x - \frac{L}{2}\right)\left(x + \frac{L}{2}\right) \\ &= x^2 - \frac{L^2}{4}, \end{aligned} \tag{6.12}$$

without worrying about the form of the exact solution. This produces the same result as above

$$\begin{aligned} \overline{E} &= -\frac{\hbar^2}{2m} \frac{\int_0^L dx \left(x^2 - \frac{L^2}{4}\right) \frac{d^2}{dx^2} \left(x^2 - \frac{L^2}{4}\right)}{\int_0^L dx \left(x^2 - \frac{L^2}{4}\right)^2} \\ &= -\frac{\hbar^2}{2m} \frac{-2L^3/6}{\frac{L^5}{30}} \\ &= \frac{\hbar^2}{2m} \frac{10}{L^2}. \end{aligned} \tag{6.13}$$

Summary (Nishant) The above example is that of a particle in a box. The actual wave function is a sin as shown. But we can come up with a guess wave function that meets the boundary conditions and ask how accurate it is compared to the actual one.

Basically we are assuming a wave function form and then seeing how it differs from the exact form. We cannot do this if we have nothing to compare it against. But, we note that the variance of the number operator in the systems eigenstate is zero. So we can still calculate the variance and try to minimize it. This is one way of coming up with an approximate wave function. This does not necessarily give the ground state wave function though. For this we need to minimize the energy itself.

6.3 VARIATIONAL METHOD

Today we want to use the variational degree of freedom to try to solve some problems that we don't have analytic solutions for.

Anharmonic oscillator

$$V(x) = \frac{1}{2}m\omega^2 x^2 + \lambda x^4, \qquad \lambda \ge 0. \tag{6.14}$$

With the potential growing faster than the harmonic oscillator, which had a ground state solution

$$\psi(x) = \frac{1}{\pi^{1/4}} \frac{1}{a_0^{1/2}} e^{-x^2/2a_0^2}, \tag{6.15}$$

where

$$a_0 = \sqrt{\frac{\hbar}{m\omega}}. \tag{6.16}$$

Let's try allowing $a_0 \rightarrow a$, to be a variational degree of freedom

$$\psi_a(x) = \frac{1}{\pi^{1/4}} \frac{1}{a^{1/2}} e^{-x^2/2a^2}, \tag{6.17}$$

$$\langle \psi_a | H | \psi_a \rangle = \langle \psi_a | \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \lambda x^4 | \psi_a \rangle \tag{6.18}$$

We can find

$$\left\langle x^2 \right\rangle = \frac{1}{2}a^2 \tag{6.19}$$

$$\left\langle x^4 \right\rangle = \frac{3}{4}a^4 \tag{6.20}$$

Define

$$\tilde{\omega} = \frac{\hbar}{ma^2}, \tag{6.21}$$

so that

$$\begin{aligned}
\overline{E}_a &= \langle \psi_a | \left(\frac{p^2}{2m} + \frac{1}{2}m\tilde{\omega}^2 x^2 \right) + \left(\frac{1}{2}m\left(\omega^2 - \tilde{\omega}^2\right) x^2 + \lambda x^4 \right) | \psi_a \rangle \\
&= \frac{1}{2}\hbar\tilde{\omega} + \frac{1}{2}m\left(\omega^2 - \tilde{\omega}^2\right)\frac{1}{2}a^2 + \frac{3}{4}\lambda a^4.
\end{aligned} \tag{6.22}$$

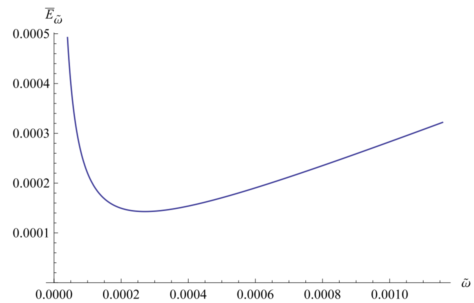

Figure 6.4: Energy after perturbation.

Write this as

$$\overline{E}_{\tilde{\omega}} = \frac{1}{2}\hbar\tilde{\omega} + \frac{1}{4}\frac{\hbar}{\tilde{\omega}}\left(\omega^2 - \tilde{\omega}^2\right) + \frac{3}{4}\lambda\frac{\hbar^2}{m^2\tilde{\omega}^2}. \tag{6.23}$$

This might look something like fig. 6.4.

Demand that

$$\begin{aligned} 0 &= \frac{\partial \overline{E}_{\tilde{\omega}}}{\partial \tilde{\omega}} \\ &= \frac{\hbar}{2} - \frac{\hbar}{4}\frac{\omega^2}{\tilde{\omega}^2} - \frac{\hbar}{4} + \frac{3}{4}(-2)\frac{\lambda\hbar^2}{m^2\tilde{\omega}^3} \\ &= \frac{\hbar}{4}\left(1 - \frac{\omega^2}{\tilde{\omega}^2} - 6\frac{\lambda\hbar}{m^2\tilde{\omega}^3}\right) \end{aligned} \tag{6.24}$$

or

$$\tilde{\omega}^3 - \omega^2\tilde{\omega} - \frac{6\lambda\hbar}{m^2} = 0. \tag{6.25}$$

for $\lambda a_0^4 \ll \hbar\omega$, we have something like $\tilde{\omega} = \omega + \epsilon$. Expanding eq. (6.25) to first order in ϵ, this gives

$$\omega^3 + 3\omega^2\epsilon - \omega^2\left(\omega + \epsilon\right) - \frac{6\lambda\hbar}{m^2} = 0, \tag{6.26}$$

so that

$$2\omega^2\epsilon = \frac{6\lambda\hbar}{m^2}, \tag{6.27}$$

and

$$\hbar\epsilon = \frac{3\lambda\hbar^2}{m^2\omega^2} = 3\lambda a_0^4. \tag{6.28}$$

Plugging into

$$\begin{aligned}
\overline{E}_{\omega+\epsilon} &= \frac{1}{2}\hbar(\omega+\epsilon) + \frac{1}{4}\frac{\hbar}{\omega}\left(-2\omega\epsilon+\epsilon^2\right) + \frac{3}{4}\lambda\frac{\hbar^2}{m^2\omega^2} \\
&\approx \frac{1}{2}\hbar(\omega+\epsilon) - \frac{1}{2}\hbar\epsilon + \frac{3}{4}\lambda\frac{\hbar^2}{m^2\omega^2} \\
&= \frac{1}{2}\hbar\omega + \frac{3}{4}\lambda a_0^4.
\end{aligned} \tag{6.29}$$

With eq. (6.28), that is

$$\overline{E}_{\tilde{\omega}=\omega+\epsilon} \approx \frac{1}{2}\hbar\left(\omega+\frac{\epsilon}{2}\right). \tag{6.30}$$

The energy levels are shifted slightly for each shift in the Hamiltonian frequency.
What do we have in the extreme anharmonic limit, where $\lambda a_0^4 \gg \hbar\omega$. Now we get

$$\tilde{\omega}^* = \left(\frac{6\hbar\lambda}{m^2}\right)^{1/3}, \tag{6.31}$$

and

$$\overline{E}_{\tilde{\omega}^*} = \frac{\hbar^{4/3}\lambda^{1/3}}{m^{2/3}}\frac{3}{8}6^{1/3}. \tag{6.32}$$

(this last result is pulled from a web treatment somewhere of the anharmonic oscillator). Note that the first factor in this energy, with $\hbar^4\lambda/m^2$ traveling together could have been worked out on dimensional grounds.

This variational method tends to work quite well in these limits. For a system where $m = \omega = \hbar = 1$, for this problem, we have

Example: (sketch) double well potential

$$V(x) = \frac{m\omega^2}{8a^2}(x-a)^2(x+a)^2. \tag{6.33}$$

Note that this potential, and the Hamiltonian, both commute with parity.

Table 6.1: Comparing numeric and variational solutions

$\hbar/\omega$	numeric	variational
100	3.13	3.16
1000	6.69	6.81

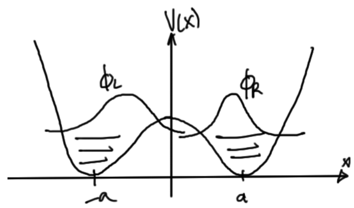

Figure 6.5: Double well potential.

We are interested in the regime where $a_0^2 = \frac{\hbar}{m\omega} \ll a^2$.
Near $x = \pm a$, this will be approximately

$$V(x) = \frac{1}{2} m\omega^2 \left(x \pm a\right)^2 . \tag{6.34}$$

Guessing a wave function that is an eigenstate of parity

$$\Psi_\pm = g_\pm \left(\phi_{\mathrm{R}}(x) \pm \phi_{\mathrm{L}}(x)\right) . \tag{6.35}$$

perhaps looking like the even and odd functions sketched in fig. 6.6, and fig. 6.7.

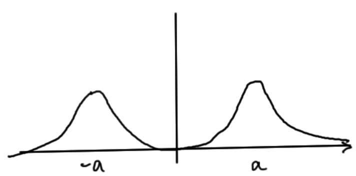

Figure 6.6: Even double well function.

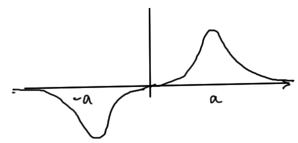

Figure 6.7: Odd double well function.

Using harmonic oscillator functions

$$\begin{aligned} \phi_{\mathrm{L}}(x) &= \Psi_{\mathrm{H.O.}}(x+a) \\ \phi_{\mathrm{R}}(x) &= \Psi_{\mathrm{H.O.}}(x-a) \end{aligned} \tag{6.36}$$

After doing a lot of integral (i.e. in the problem set), we will see a splitting of the variational energy levels as sketched in fig. 6.8.

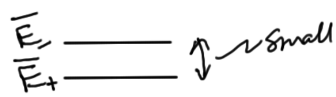

Figure 6.8: Splitting for double well potential.

This sort of level splitting was what was used in the very first mazers.

6.4 PERTURBATION THEORY (OUTLINE)

Given

$$H = H_0 + \lambda V, \tag{6.37}$$

where λV is "small". We want to figure out the eigenvalues and eigenstates of this Hamiltonian

$$H |n\rangle = E_n |n\rangle . \tag{6.38}$$

We don't know what these are, but do know that

$$H_0 \left| n^{(0)} \right\rangle = E_n^{(0)} \left| n^{(0)} \right\rangle . \tag{6.39}$$

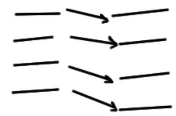

Figure 6.9: Adiabatic transitions.

We are hoping that the level transitions have adiabatic transitions between the original and perturbed levels as sketched in fig. 6.9.

and not crossed level transitions as sketched in fig. 6.10.

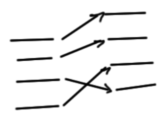

Figure 6.10: Crossed level transitions.

If we have level crossings (which can in general occur), as opposed to adiabatic transitions, then we have no hope of using perturbation theory.

6.5 SIMPLEST PERTURBATION EXAMPLE.

Given a 2×2 Hamiltonian $H = H_0 + V$, where

$$H = \begin{bmatrix} a & c \\ c^* & b \end{bmatrix}, \tag{6.40}$$

note that if $c = 0$ is

$$H = H_0 = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}. \tag{6.41}$$

The off diagonal terms can be considered to be a perturbation

$$V = \begin{bmatrix} 0 & c \\ c^* & 0 \end{bmatrix}, \tag{6.42}$$

with $H = H_0 + V$.

Energy levels after perturbation We can solve for the eigenvalues of H easily, finding

$$\lambda_\pm = \frac{a+b}{2} \pm \sqrt{\left(\frac{a-b}{2}\right)^2 + |c|^2}. \tag{6.43}$$

Plots of a few a, b variations of $\lambda_\pm$ are shown in fig. 6.11. The quadratic (non-degenerate) domain is found near the $c = 0$ points of all but the first ($a = b$) plot, and the degenerate (linear in $|c|^2$) regions are visible for larger values of c.

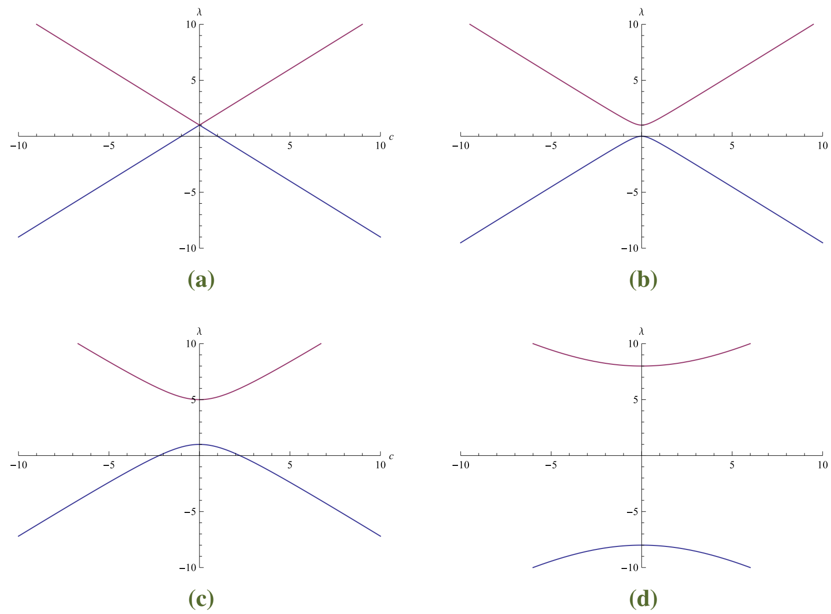

Figure 6.11: Plots of $\lambda_\pm$ for $(a, b) \in \{(1, 1), (1, 0), (1, 5), (-8, 8)\}$

Some approximations Suppose that $|c| \ll |a - b|$, then

$$\lambda_\pm \approx \frac{a+b}{2} \pm \left|\frac{a-b}{2}\right| \left(1 + 2\frac{|c|^2}{|a-b|^2}\right). \tag{6.44}$$

If $a > b$, then

$$\lambda_\pm \approx \frac{a+b}{2} \pm \frac{a-b}{2} \left(1 + 2\frac{|c|^2}{(a-b)^2}\right). \tag{6.45}$$

$$
\begin{aligned}
\lambda_+ &= \frac{a+b}{2} + \frac{a-b}{2}\left(1 + 2\frac{|c|^2}{(a-b)^2}\right) \\
&= a + (a-b)\,\frac{|c|^2}{(a-b)^2} \\
&= a + \frac{|c|^2}{a-b},
\end{aligned}
\tag{6.46}
$$

and

$$
\begin{aligned}
\lambda_- &= \frac{a+b}{2} - \frac{a-b}{2}\left(1 + 2\frac{|c|^2}{(a-b)^2}\right) \\
&= b + (a-b)\,\frac{|c|^2}{(a-b)^2} \\
&= b + \frac{|c|^2}{a-b}.
\end{aligned}
\tag{6.47}
$$

This adiabatic evolution displays a “level repulsion”, quadratic in $|c|$, and is described as a non-degenerate permutation.

If $|c| \gg |a-b|$, then

$$
\begin{aligned}
\lambda_\pm &= \frac{a+b}{2} \pm |c|\sqrt{1 + \frac{1}{|c|^2}\left(\frac{a-b}{2}\right)^2} \\
&\approx \frac{a+b}{2} \pm |c|\left(1 + \frac{1}{2|c|^2}\left(\frac{a-b}{2}\right)^2\right) \\
&= \frac{a+b}{2} \pm |c| \pm \frac{(a-b)^2}{8|c|}.
\end{aligned}
\tag{6.48}
$$

Here we loose the adiabaticity, and have “level repulsion” that is linear in $|c|$. We no longer have the sign of $a-b$ in the expansion. This is described as a degenerate permutation.

6.6 GENERAL NON-DEGENERATE PERTURBATION

Given an unperturbed system with solutions of the form

$$
H_0 \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(0)}\right\rangle,
\tag{6.49}
$$

we want to solve the perturbed Hamiltonian equation

$$
\left(H_0 + \lambda V\right)|n\rangle = \left(E_n^{(0)} + \Delta n\right)|n\rangle.
\tag{6.50}
$$

Here Δn is an energy shift as that goes to zero as $\lambda \rightarrow 0$. We can write this as

$$\left(E_n^{(0)} - H_0\right)|n\rangle = (\lambda V - \Delta_n)|n\rangle . \tag{6.51}$$

We are hoping to iterate with application of the inverse to an initial estimate of $|n\rangle$

$$|n\rangle = \left(E_n^{(0)} - H_0\right)^{-1} (\lambda V - \Delta_n)|n\rangle . \tag{6.52}$$

This gets us into trouble if $\lambda \rightarrow 0$, which can be fixed by using

$$|n\rangle = \left(E_n^{(0)} - H_0\right)^{-1} (\lambda V - \Delta_n)|n\rangle + \left|n^{(0)}\right\rangle , \tag{6.53}$$

which can be seen to be a solution to eq. (6.51). We want to ask if

$$(\lambda V - \Delta_n)|n\rangle , \tag{6.54}$$

contains a bit of $\left|n^{(0)}\right\rangle$? To determine this act with $\left\langle n^{(0)}\right|$ on the left

$$\begin{aligned} \left\langle n^{(0)}\right|(\lambda V - \Delta_n)|n\rangle &= \left\langle n^{(0)}\right|\left(E_n^{(0)} - H_0\right)|n\rangle \\ &= \left(E_n^{(0)} - E_n^{(0)}\right)\left\langle n^{(0)}\middle|n\right\rangle \\ &= 0. \end{aligned} \tag{6.55}$$

This shows that $|n\rangle$ is entirely orthogonal to $\left|n^{(0)}\right\rangle$.
Define a projection operator

$$P_n = \left|n^{(0)}\right\rangle\left\langle n^{(0)}\right| , \tag{6.56}$$

which has the idempotent property $P_n^2 = P_n$ that we expect of a projection operator.
Define a rejection operator

$$\begin{aligned} \overline{P}_n &= 1 - \left|n^{(0)}\right\rangle\left\langle n^{(0)}\right| \\ &= \sum_{m \neq n} \left|m^{(0)}\right\rangle\left\langle m^{(0)}\right| . \end{aligned} \tag{6.57}$$

Because $|n\rangle$ has no component in the direction $\left|n^{(0)}\right\rangle$, the rejection operator can be inserted much like we normally do with the identity operator, yielding

$$|n\rangle' = \left(E_n^{(0)} - H_0\right)^{-1} \overline{P}_n (\lambda V - \Delta_n)|n\rangle + \left|n^{(0)}\right\rangle , \tag{6.58}$$

valid for any initial $|n\rangle$.

Power series perturbation expansion Instead of iterating, suppose that the unknown state and unknown energy difference operator can be expanded in a λ power series, say

$$|n\rangle = |n_0\rangle + \lambda |n_1\rangle + \lambda^2 |n_2\rangle + \lambda^3 |n_3\rangle + \cdots \tag{6.59}$$

and

$$\Delta_n = \Delta_{n_0} + \lambda \Delta_{n_1} + \lambda^2 \Delta_{n_2} + \lambda^3 \Delta_{n_3} + \cdots \tag{6.60}$$

We usually interpret functions of operators in terms of power series expansions. In the case of $\left(E_n^{(0)} - H_0\right)^{-1}$, we have a concrete interpretation when acting on one of the unperturbed eigenstates

$$\frac{1}{E_n^{(0)} - H_0} \left| m^{(0)} \right\rangle = \frac{1}{E_n^{(0)} - E_m^0} \left| m^{(0)} \right\rangle . \tag{6.61}$$

This gives

$$|n\rangle = \frac{1}{E_n^{(0)} - H_0} \sum_{m \neq n} \left| m^{(0)} \right\rangle \left\langle m^{(0)} \right| (\lambda V - \Delta_n) |n\rangle + \left| n^{(0)} \right\rangle , \tag{6.62}$$

or

$$\boxed{|n\rangle = \left| n^{(0)} \right\rangle + \sum_{m \neq n} \frac{\left| m^{(0)} \right\rangle \left\langle m^{(0)} \right|}{E_n^{(0)} - E_m^{(0)}} (\lambda V - \Delta_n) |n\rangle .} \tag{6.63}$$

From eq. (6.51), note that

$$\Delta_n = \frac{\left\langle n^{(0)} \right| \lambda V |n\rangle}{\langle n^0 | n \rangle}, \tag{6.64}$$

however, we will normalize by setting $\left\langle n^0 \middle| n \right\rangle = 1$, so

$$\boxed{\Delta_n = \left\langle n^{(0)} \right| \lambda V |n\rangle .} \tag{6.65}$$

to $O(\lambda^0)$ If all $\lambda^n, n > 0$ are zero, then we have

$$|n_0\rangle = \left| n^{(0)} \right\rangle + \sum_{m \neq n} \frac{\left| m^{(0)} \right\rangle \left\langle m^{(0)} \right|}{E_n^{(0)} - E_m^{(0)}} (-\Delta_{n_0}) |n_0\rangle \tag{6.66a}$$

$$\Delta_{n_0} \left\langle n^{(0)} \middle| n_0 \right\rangle = 0 \tag{6.66b}$$

so

$$\begin{aligned} |n_0\rangle &= \left| n^{(0)} \right\rangle \\ \Delta_{n_0} &= 0. \end{aligned} \tag{6.67}$$

to $O(\lambda^1)$ Requiring identity for all λ^1 terms means

$$\left|n_1\right\rangle \lambda = \sum_{m\neq n} \frac{\left|m^{(0)}\right\rangle\left\langle m^{(0)}\right|}{E_n^{(0)} - E_m^{(0)}} \left(\lambda V - \Delta_{n_1}\lambda\right)\left|n_0\right\rangle, \tag{6.68}$$

so

$$\left|n_1\right\rangle = \sum_{m\neq n} \frac{\left|m^{(0)}\right\rangle\left\langle m^{(0)}\right|}{E_n^{(0)} - E_m^{(0)}} \left(V - \Delta_{n_1}\right)\left|n_0\right\rangle. \tag{6.69}$$

With the assumption that $\left|n^{(0)}\right\rangle$ is normalized, and with the shorthand

$$V_{mn} = \left\langle m^{(0)}\right| V \left|n^{(0)}\right\rangle, \tag{6.70}$$

that is

$$\begin{aligned} \left|n_1\right\rangle &= \sum_{m\neq n} \frac{\left|m^{(0)}\right\rangle}{E_n^{(0)} - E_m^{(0)}} V_{mn} \\ \Delta_{n_1} &= \left\langle n^{(0)}\right| V \left|n^{(0)}\right\rangle = V_{nn}. \end{aligned} \tag{6.71}$$

to $O(\lambda^2)$ The second order perturbation states are found by selecting only the λ^2 contributions to

$$\lambda^2 \left|n_2\right\rangle = \sum_{m\neq n} \frac{\left|m^{(0)}\right\rangle\left\langle m^{(0)}\right|}{E_n^{(0)} - E_m^{(0)}} \left(\lambda V - (\lambda\Delta_{n_1} + \lambda^2\Delta_{n_2})\right)\left(\left|n_0\right\rangle + \lambda\left|n_1\right\rangle\right). \tag{6.72}$$

Because $\left|n_0\right\rangle = \left|n^{(0)}\right\rangle$, the $\lambda^2\Delta_{n_2}$ is killed, leaving

$$\begin{aligned} \left|n_2\right\rangle &= \sum_{m\neq n} \frac{\left|m^{(0)}\right\rangle\left\langle m^{(0)}\right|}{E_n^{(0)} - E_m^{(0)}} \left(V - \Delta_{n_1}\right)\left|n_1\right\rangle \\ &= \sum_{m\neq n} \frac{\left|m^{(0)}\right\rangle\left\langle m^{(0)}\right|}{E_n^{(0)} - E_m^{(0)}} \left(V - \Delta_{n_1}\right) \sum_{l\neq n} \frac{\left|l^{(0)}\right\rangle}{E_n^{(0)} - E_l^{(0)}} V_{ln}, \end{aligned} \tag{6.73}$$

which can be written as

$$\left|n_2\right\rangle = \sum_{l,m\neq n} \left|m^{(0)}\right\rangle \frac{V_{ml}V_{ln}}{\left(E_n^{(0)} - E_m^{(0)}\right)\left(E_n^{(0)} - E_l^{(0)}\right)} - \sum_{m\neq n} \left|m^{(0)}\right\rangle \frac{V_{nn}V_{mn}}{\left(E_n^{(0)} - E_m^{(0)}\right)^2}. \tag{6.74}$$

For the second energy perturbation we have

$$\lambda^2 \Delta_{n_2} = \left\langle n^{(0)} \right| \lambda V \left(\lambda \left| n_1 \right\rangle \right), \tag{6.75}$$

or

$$\begin{aligned} \Delta_{n_2} &= \left\langle n^{(0)} \right| V \left| n_1 \right\rangle \\ &= \left\langle n^{(0)} \right| V \sum_{m \neq n} \frac{\left| m^{(0)} \right\rangle}{E_n^{(0)} - E_m^{(0)}} V_{mn}. \end{aligned} \tag{6.76}$$

That is

$$\Delta_{n_2} = \sum_{m \neq n} \frac{V_{nm} V_{mn}}{E_n^{(0)} - E_m^{(0)}}. \tag{6.77}$$

to $O(\lambda^3)$ Similarly, it can be shown that

$$\Delta_{n_3} = \sum_{l,m \neq n} \frac{V_{nm} V_{ml} V_{ln}}{\left(E_n^{(0)} - E_m^{(0)}\right)\left(E_n^{(0)} - E_l^{(0)}\right)} - \sum_{m \neq n} \frac{V_{nm} V_{nn} V_{mn}}{\left(E_n^{(0)} - E_m^{(0)}\right)^2}. \tag{6.78}$$

In general, the energy perturbation is given by

$$\Delta_n^{(l)} = \left\langle n^{(0)} \right| V \left| n_{l-1} \right\rangle. \tag{6.79}$$

6.7 STARK EFFECT

$$H = H_{\text{atom}} + e\mathcal{E}z, \tag{6.80}$$

where H_{atom} is assumed to be Hydrogen-like with Hamiltonian

$$H_{\text{atom}} = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r}, \tag{6.81}$$

and wave functions

$$\langle \mathbf{r} | \psi_{nlm} \rangle = R_{nl}(r) Y_{lm}(\theta, \phi) \tag{6.82}$$

Referring to eq. (A.117), the first level correction to the energy

$$\begin{aligned} \Delta_1 &= \langle \psi_{100} | \, e\mathcal{E}z \, | \psi_{100} \rangle \\ &= e\mathcal{E} \int \frac{d\Omega}{4\pi} \cos\theta \int dr r^2 R_{100}^2(r) \end{aligned} \tag{6.83}$$

The cosine integral is obliterated, so we have $\Delta_1 = 0$.

How about the second order energy correction? That is

$$\Delta_2 = \sum_{nlm \neq 100} \frac{|\langle \psi_{100}| e\mathcal{E}z |nlm\rangle|^2}{E_{100}^{(0)} - E_{nlm}} \tag{6.84}$$

The matrix element in the numerator is the absolute square of

$$V_{100,nlm} = e\mathcal{E} \int d\Omega \frac{1}{\sqrt{4\pi}} \cos\theta Y_{lm}(\theta,\phi) \int dr r^3 R_{100}(r) R_{nl}(r). \tag{6.85}$$

For all $m \neq 0$, Y_{lm} includes a $e^{im\phi}$ factor, so this cosine integral is zero. For $m = 0$, each of the Y_{lm} functions appears to contain either even or odd powers of cosines (see: eq. (A.115)). This shows that for even $2k = l$, the cosine integral is zero

$$\int_0^\pi \sin\theta \cos\theta \sum_k a_k \cos^{2k}\theta d\theta = 0, \tag{6.86}$$

since $\cos^{2k}(\theta)$ is even and $\sin\theta\cos\theta$ is odd over the same interval. We find zero for $\int_0^\pi \sin\theta\cos\theta Y_{30}(\theta,\phi) d\theta$, and Mathematica appears to show that the rest of these integrals for $l > 1$ are also zero.

FIXME: find the property of the spherical harmonics that can be used to prove that this is true in general for $l > 1$.

This leaves

$$\begin{aligned}\Delta_2 &= \sum_{n \neq 1} \frac{|\langle \psi_{100}| e\mathcal{E}z |n10\rangle|^2}{E_{100}^{(0)} - E_{n10}} \\ &= -e^2\mathcal{E}^2 \sum_{n \neq 1} \frac{|\langle \psi_{100}| z |n10\rangle|^2}{E_{n10} - E_{100}^{(0)}}.\end{aligned} \tag{6.87}$$

This is sometimes written in terms of a polarizability α

$$\Delta_2 = -\frac{\mathcal{E}^2}{2}\alpha, \tag{6.88}$$

where

$$\alpha = 2e^2 \sum_{n \neq 1} \frac{|\langle \psi_{100}| z |n10\rangle|^2}{E_{n10} - E_{100}^{(0)}}. \tag{6.89}$$

With

$$\mathbf{P} = \alpha\mathcal{E}, \tag{6.90}$$

the energy change upon turning on the electric field from $0 \rightarrow \mathcal{E}$ is simply $-\mathbf{P} \cdot d\mathcal{E}$ integrated from $0 \rightarrow \mathcal{E}$. Putting $\mathbf{P} = \alpha\mathcal{E}\hat{\mathbf{z}}$, we have

$$\begin{aligned} -\int_0^{\mathcal{E}} P_z d\mathcal{E} &= -\int_0^{\mathcal{E}} \alpha\mathcal{E} d\mathcal{E} \\ &= -\frac{1}{2}\alpha\mathcal{E}^2 \end{aligned} \tag{6.91}$$

leading to an energy change $-\alpha\mathcal{E}^2/2$, so we can directly compute $\langle \mathbf{P} \rangle$ or we can compute change in energy, and both contain information about the polarization factor α.

There is an exact answer to the sum eq. (6.89), but we aren't going to try to get it here. Instead let's look for bounds

$$\Delta_2^{\min} < \Delta_2 < \Delta_2^{\max} \tag{6.92}$$

$$\alpha^{\min} = 2e^2 \frac{|\langle \psi_{100} | z | \psi_{210} \rangle|^2}{E_{210}^{(0)} - E_{100}^{(0)}} \tag{6.93}$$

For the hydrogen atom we have

$$E_n = -\frac{e^2}{2n^2 a_0}, \tag{6.94}$$

allowing any difference of energy levels to be expressed as a fraction of the ground state energy, such as

$$\begin{aligned} E_{210}^{(0)} &= \frac{1}{4} E_{100}^{(0)} \\ &= \frac{1}{4} \frac{-\hbar^2}{2ma_0^2} \end{aligned} \tag{6.95}$$

So

$$E_{210}^{(0)} - E_{100}^{(0)} = \frac{3}{4} \frac{\hbar^2}{2ma_0^2} \tag{6.96}$$

In the numerator we have

$$
\begin{aligned}
\langle\psi_{100}|\, z\, |\psi_{210}\rangle &= \int r^2 d\Omega \left(\frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0} \right) r\cos\theta \left(\frac{1}{4\sqrt{2\pi} a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \cos\theta \right) \\
&= (2\pi) \frac{1}{\sqrt{\pi}} \frac{1}{4\sqrt{2\pi}} a_0 \int_0^\pi d\theta \sin\theta \cos^2\theta \int_0^\infty \frac{dr}{a_0} \frac{r^4}{a_0^4} e^{-r/a_0 - r/2a_0} \\
&= (2\cancel{\pi}) \frac{1}{\cancel{\sqrt{\pi}}} \frac{1}{4\sqrt{2\cancel{\pi}}} a_0 \left(-\frac{u^3}{3} \Big|_1^{-1} \right) \int_0^\infty s^4 ds e^{-3s/2} \\
&= \frac{1}{2\sqrt{2}} \frac{2}{3} a_0 \frac{256}{81} \\
&= \frac{1}{3\sqrt{2}} \frac{256}{81} a_0 \\
&\approx 0.75 a_0.
\end{aligned}
\tag{6.97}
$$

This gives

$$
\begin{aligned}
\alpha^{\min} &= \frac{2e^2 (0.75)^2 a_0^2}{\frac{3}{4} \frac{\hbar^2}{2ma_0^2}} \\
&= \frac{6}{4} \frac{2me^2 a_0^4}{\hbar^2} \\
&= 3 \frac{me^2 a_0^4}{\hbar^2} \\
&= 3 \frac{4\pi\epsilon_0}{a_0} a_0^4 \\
&\approx 4\pi\epsilon_0 a_0^3 \times 3.
\end{aligned}
\tag{6.98}
$$

The factor $4\pi\epsilon_0 a_0^3$ are the natural units for the polarizability.

There is a neat trick that generalizes to many problems to find the upper bound. Recall that the general polarizability was

$$
\alpha = 2e^2 \sum_{nlm \neq 100} \frac{|\langle 100|\, z\, |nlm\rangle|^2}{E_{nlm} - E_{100}^{(0)}}. \tag{6.99}
$$

If we are looking for the upper bound, and replace the denominator by the smallest energy difference that will be encountered, it can be brought out of the sum, for

$$
\alpha^{\max} = 2e^2 \frac{1}{E_{210} - E_{100}^{(0)}} \sum_{nlm \neq 100} \langle 100|\, z\, |nlm\rangle \langle nlm|\, z\, |100\rangle \tag{6.100}
$$

Because $\langle nlm| z |100\rangle = 0$, the constraint in the sum can be removed, and the identity summation evaluated

$$\begin{aligned}
\alpha^{\max} &= 2e^2 \frac{1}{E_{210} - E_{100}^{(0)}} \sum_{nlm} \langle 100| z |nlm\rangle \langle nlm| z |100\rangle \\
&= \frac{2e^2}{\frac{3}{4}\frac{\hbar^2}{2ma_0^2}} \langle 100| z^2 |100\rangle \\
&= \frac{16e^2 ma_0^2}{3\hbar^2} \times a_0^2 \\
&= 4\pi\epsilon_0 a_0^3 \times \frac{16}{3}.
\end{aligned} \tag{6.101}$$

The bounds are

$$\boxed{3 \ge \frac{\alpha}{\alpha^{\mathrm{at}}} < \frac{16}{3},} \tag{6.102}$$

where

$$\alpha^{\mathrm{at}} = 4\pi\epsilon_0 a_0^3. \tag{6.103}$$

The actual value is

$$\frac{\alpha}{\alpha^{\mathrm{at}}} = \frac{9}{2}. \tag{6.104}$$

See lecture21someSphericalHarmonicsAndTheirIntegrals.nb, for some of the integrals above, and for spherical harmonic tables.

Example: Computing the dipole moment

$$\langle P_z\rangle = \alpha\mathcal{E} = \langle \psi_{100}| ez |\psi_{100}\rangle . \tag{6.105}$$

Without any perturbation this is zero. After perturbation, retaining only the terms that are first order in $\delta\psi_{100}$ we have

$$\langle \psi_{100} + \delta\psi_{100}| ez |\psi_{100} + \delta\psi_{100}\rangle \approx \langle \psi_{100}| ez |\delta\psi_{100}\rangle + \langle \delta\psi_{100}| ez |\psi_{100}\rangle . \tag{6.106}$$

Next time: van der Walls We will look at two hyrdogenic atomic systems interacting where the pair of nuclei are supposed to be infinitely heavy and stationary. The wave functions each set of atoms are individually known, but we can consider the problem of the interactions of atom 1's electrons with atom 2's nucleus and atom 2's electrons, and also the opposite interactions of atom 2's electrons with atom 1's nucleus and its electrons. This leads to a result that is linear in the electric field (unlike the above result, which is called the quadratic Stark effect).

Another approach (for last time?) Imagine we perturb a potential, say a harmonic oscillator with an electric field

$$V_0(x) = \frac{1}{2}kx^2 \tag{6.107}$$

$$V(x) = \mathcal{E}ex \tag{6.108}$$

After minimizing the energy, using $\partial V/\partial x = 0$, we get

$$\begin{aligned}\frac{1}{2}kx^2 + \mathcal{E}ex \rightarrow kx^* \\ = -e\mathcal{E}\end{aligned} \tag{6.109}$$

$$\begin{aligned}p^* &= -ex^* \\ &= -\frac{e^2\mathcal{E}}{k}\end{aligned} \tag{6.110}$$

For such a system the polarizability is

$$\alpha = \frac{e^2}{k} \tag{6.111}$$

$$\begin{aligned}\frac{1}{2}k\left(-\frac{e\mathcal{E}}{k}\right)^2 + \mathcal{E}e\left(-\frac{e\mathcal{E}}{k}\right) &= -\frac{1}{2}\left(\frac{e^2}{k}\right)\mathcal{E}^2 \\ &= -\frac{1}{2}\alpha\mathcal{E}^2\end{aligned} \tag{6.112}$$

6.8 VAN DER WALLS POTENTIAL

$$H_0 = H_{01} + H_{02}, \tag{6.113}$$

where

$$H_{0\alpha} = \frac{p_\alpha^2}{2m} - \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_\alpha - \mathbf{R}_\alpha|}, \qquad \alpha = 1, 2 \tag{6.114}$$

The full interaction potential is

$$V = \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{|\mathbf{R}_1 - \mathbf{R}_2|} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} - \frac{1}{|\mathbf{r}_1 - \mathbf{R}_2|} - \frac{1}{|\mathbf{r}_2 - \mathbf{R}_1|}\right) \tag{6.115}$$

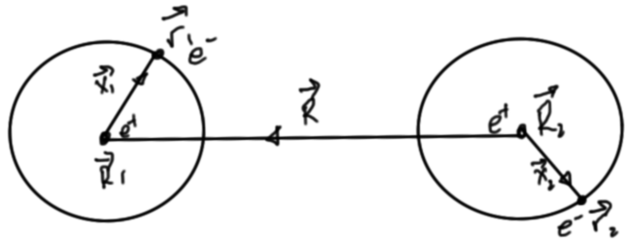

Figure 6.12: Two atom interaction.

Let

$$\mathbf{x}_\alpha = \mathbf{r}_\alpha - \mathbf{R}_\alpha, \tag{6.116}$$

$$\mathbf{R} = \mathbf{R}_1 - \mathbf{R}_2, \tag{6.117}$$

as sketched in fig. 6.12.

$$H_{0\alpha} = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{4\pi\epsilon_0 |\mathbf{x}_\alpha|} \tag{6.118}$$

which allows the total interaction potential to be written

$$V = \frac{e^2}{4\pi\epsilon_0 R}\left(1 + \frac{R}{|\mathbf{x}_1 - \mathbf{x}_2 + \mathbf{R}|} - \frac{R}{|\mathbf{x}_1 + \mathbf{R}|} - \frac{R}{|-\mathbf{x}_2 + \mathbf{R}|}\right) \tag{6.119}$$

For $R \gg x_1, x_2$, this interaction potential, after a multipole expansion, is approximately

$$V = \frac{e^2}{4\pi\epsilon_0}\left(\frac{\mathbf{x}_1 \cdot \mathbf{x}_2}{|\mathbf{R}|^3} - 3\frac{(\mathbf{x}_1 \cdot \mathbf{R})(\mathbf{x}_2 \cdot \mathbf{R})}{|\mathbf{R}|^5}\right) \tag{6.120}$$

Showing this is left as a exercise.

1. *$O(\lambda)$* .

With

$$\psi_0 = |1s, 1s\rangle \tag{6.121}$$

$$\Delta E^{(1)} = \langle \psi_0 | V | \psi_0 \rangle \tag{6.122}$$

The two particle wave functions are of the form

$$\langle \mathbf{x}_1, \mathbf{x}_2 | \psi_0 \rangle = \psi_{1s}(\mathbf{x}_1)\psi_{1s}(\mathbf{x}_2), \tag{6.123}$$

so braket integrals must be evaluated over a six-fold space. Recall that

$$\psi_{1s} = \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0}, \tag{6.124}$$

so

$$\langle \psi_{1s} | x_i | \psi_{1s} \rangle \propto \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi x_i \tag{6.125}$$

where

$$x_i \in \{r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta\}. \tag{6.126}$$

The x, y integrals are zero because of the ϕ integral, and the z integral is proportional to $\int_0^\pi \sin(2\theta) d\theta$, which is also zero. This leads to zero averages

$$\langle \mathbf{x}_1 \rangle = 0 = \langle \mathbf{x}_2 \rangle \tag{6.127}$$

so

$$\Delta E^{(1)} = 0. \tag{6.128}$$

2. $O(\lambda^2)$.

$$\begin{aligned}
\Delta E^{(2)} &= \sum_{n\neq 0} \frac{|\langle \psi_n | V | \psi_0 \rangle|^2}{E_0 - E_n} \\
&= \sum_{n\neq 0} \frac{\langle \psi_0 | V | \psi_n \rangle \langle \psi_n | V | \psi_0 \rangle}{E_0 - E_n}.
\end{aligned} \tag{6.129}$$

This is a sum over all excited states.

We expect that this will be of the form

$$\Delta E^{(2)} = -\left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{C_6}{R^6} \tag{6.130}$$

$\mathbf{x}_1$ and $\mathbf{x}_2$ are dipole operators. The first time this has a non-zero expectation is when we go from the 1s to the 2p states (both 1s and 2s states are spherically symmetric).

Noting that $E_n = -e^2/2n^2 a_0$, we can compute a minimum bound for the energy denominator

$$\begin{aligned}
(E_n - E_0)^{\min} &= 2\left(E_{2p} - E_{1s}\right) \\
&= 2E_{1s}\left(\frac{1}{4} - 1\right) \\
&= 2\frac{3}{4}|E_{1s}| \\
&= \frac{3}{2}|E_{1s}|.
\end{aligned} \tag{6.131}$$

Note that the factor of two above comes from summing over the energies for both electrons. This gives us

$$C_6 = \frac{3}{2}|E_{1s}| \langle\psi_0| \tilde{V} |\psi_0\rangle, \tag{6.132}$$

where

$$\tilde{V} = \left(\mathbf{x}_1 \cdot \mathbf{x}_2 - 3(\mathbf{x}_1 \cdot \hat{\mathbf{R}})(\mathbf{x}_2 \cdot \hat{\mathbf{R}})\right) \tag{6.133}$$

What about degeneracy?

$$\Delta E_n^{(2)} = \sum_{m \neq n} \frac{|\langle\psi_n| V |\psi_0\rangle|^2}{E_0 - E_n} \tag{6.134}$$

If $\langle\psi_n| V |\psi_m\rangle \propto \delta_{nm}$ then it's okay. In general the we can't expect the matrix element will be anything but fully populated, say

$$V = \begin{bmatrix} V_{11} & V_{12} & V_{13} & V_{14} \\ V_{21} & V_{22} & V_{23} & V_{24} \\ V_{31} & V_{32} & V_{33} & V_{34} \\ V_{41} & V_{42} & V_{43} & V_{44} \end{bmatrix}, \tag{6.135}$$

If we choose a basis so that

$$V = \begin{bmatrix} V_{11} & & & \\ & V_{22} & & \\ & & V_{33} & \\ & & & V_{44} \end{bmatrix}. \tag{6.136}$$

When this is the case, we have no mixing of elements in the sum of eq. (6.134)

Degeneracy in the Stark effect

$$H = H_0 + e\mathcal{E}z, \tag{6.137}$$

where

$$H_0 = \frac{\mathbf{p}^2}{2m} - \frac{e}{4\pi\epsilon_0}\frac{1}{|\mathbf{x}|} \tag{6.138}$$

Consider the states $2s, 2p_x, 2p_y, 2p_z$, for which $E_n^{(0)} \equiv E_{2s}$, as sketched in fig. 6.13.

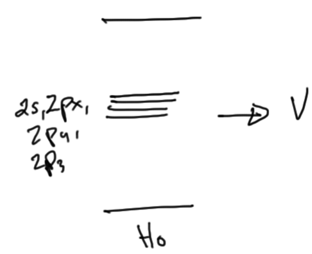

Figure 6.13: 2s 2p degeneracy.

Because of spherical symmetry

$$\begin{aligned}\langle 2s| e\mathcal{E}z |2s\rangle &= 0 \\ \langle 2p_x| e\mathcal{E}z |2p_x\rangle &= 0 \\ \left\langle 2p_y\middle| e\mathcal{E}z \middle|2p_y\right\rangle &= 0 \\ \langle 2p_z| e\mathcal{E}z |2p_z\rangle &= 0\end{aligned} \tag{6.139}$$

Looking at odd and even properties, it turns out that the only off-diagonal matrix element is

$$\langle 2s| e\mathcal{E}z |2p_z\rangle = V_1 = -3e\mathcal{E}a_0. \tag{6.140}$$

With a $\left\{2s, 2p_x, 2p_y, 2p_z\right\}$ basis the potential matrix is

$$\begin{bmatrix} 0 & 0 & 0 & V_1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ V_1^* & 0 & 0 & 0 \end{bmatrix} \tag{6.141}$$

$$\begin{bmatrix} 0 & -|V_1| \\ -|V_1| & 0 \end{bmatrix} \tag{6.142}$$

implies that the energy splitting goes as

$$E_{2s} \rightarrow E_{2s} \pm |V_1|, \tag{6.143}$$

as sketched in fig. 6.14.

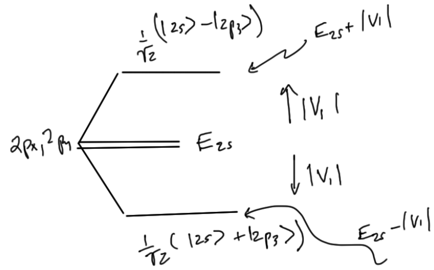

Figure 6.14: Stark effect energy level splitting.

The diagonalizing states corresponding to eigenvalues $\pm 3 a_0 \mathcal{E}$, are $(|2s\rangle \mp |2p_z\rangle)/\sqrt{2}$.

The matrix element above is calculated explicitly in lecture22Integrals.nb.

The degeneracy that is left unsplit here, and has to be accounted for should we attempt higher order perturbation calculations.

6.9 PROBLEMS

Exercise 6.1 van der Walls multipole expansion.

Prove eq. (6.120).

Answer for Exercise 6.1

Noting that

$$(1+\epsilon)^{-1/2} = 1 - \frac{1}{2}\epsilon - \frac{1}{2}\left(\frac{-3}{2}\right)\frac{1}{2!}\epsilon^2 = 1 - \frac{1}{2}\epsilon + \frac{3}{8}\epsilon^2, \tag{6.144}$$

we have

$$\begin{aligned}
\frac{R}{\left|\boldsymbol{\epsilon} + \mathbf{R}\right|} &= \frac{1}{\left|\frac{\boldsymbol{\epsilon}}{R} + \hat{\mathbf{R}}\right|} \\
&= \left(1 + 2\frac{\boldsymbol{\epsilon}}{R}\cdot\hat{\mathbf{R}} + \left(\frac{\boldsymbol{\epsilon}}{R}\right)^2\right)^{-1/2} \\
&= 1 - \frac{\boldsymbol{\epsilon}}{R}\cdot\hat{\mathbf{R}} - \frac{1}{2}\left(\frac{\boldsymbol{\epsilon}}{R}\right)^2 + \frac{3}{8}\left(2\frac{\boldsymbol{\epsilon}}{R}\cdot\hat{\mathbf{R}} + \left(\frac{\boldsymbol{\epsilon}}{R}\right)^2\right)^2 \\
&= 1 - \frac{\boldsymbol{\epsilon}}{R}\cdot\hat{\mathbf{R}} - \frac{1}{2}\left(\frac{\boldsymbol{\epsilon}}{R}\right)^2 + \frac{3}{8}\left(4\left(\frac{\boldsymbol{\epsilon}}{R}\cdot\hat{\mathbf{R}}\right)^2 + \left(\frac{\boldsymbol{\epsilon}}{R}\right)^4 + 4\frac{\boldsymbol{\epsilon}}{R}\cdot\hat{\mathbf{R}}\left(\frac{\boldsymbol{\epsilon}}{R}\right)^2\right) \\
&\approx 1 - \frac{\boldsymbol{\epsilon}}{R}\cdot\hat{\mathbf{R}} - \frac{1}{2}\left(\frac{\boldsymbol{\epsilon}}{R}\right)^2 + \frac{3}{2}\left(\frac{\boldsymbol{\epsilon}}{R}\cdot\hat{\mathbf{R}}\right)^2.
\end{aligned} \tag{6.145}$$

Inserting the values from the brackets of eq. (6.119) we have

$$
\begin{aligned}
1 + \frac{R}{|\mathbf{x}_1 - \mathbf{x}_2 + \mathbf{R}|} - \frac{R}{|\mathbf{x}_1 + \mathbf{R}|} - \frac{R}{|-\mathbf{x}_2 + \mathbf{R}|}
&= -\frac{(\mathbf{x}_1 - \mathbf{x}_2)}{R} \cdot \hat{\mathbf{R}} - \frac{1}{2}\left(\frac{(\mathbf{x}_1 - \mathbf{x}_2)}{R}\right)^2 + \frac{3}{2}\left(\frac{(\mathbf{x}_1 - \mathbf{x}_2)}{R} \cdot \hat{\mathbf{R}}\right)^2 \\
&\quad + \frac{\mathbf{x}_1}{R} \cdot \hat{\mathbf{R}} + \frac{1}{2}\left(\frac{\mathbf{x}_1}{R}\right)^2 - \frac{3}{2}\left(\frac{\mathbf{x}_1}{R} \cdot \hat{\mathbf{R}}\right)^2 \\
&\quad - \frac{\mathbf{x}_2}{R} \cdot \hat{\mathbf{R}} + \frac{1}{2}\left(\frac{\mathbf{x}_2}{R}\right)^2 - \frac{3}{2}\left(\frac{\mathbf{x}_2}{R} \cdot \hat{\mathbf{R}}\right)^2 \\
&= \frac{\mathbf{x}_1}{R} \cdot \frac{\mathbf{x}_2}{R} + \frac{3}{2}\left(\frac{(\mathbf{x}_1 - \mathbf{x}_2)}{R} \cdot \hat{\mathbf{R}}\right)^2 \\
&\quad - \frac{3}{2}\left(\frac{\mathbf{x}_1}{R} \cdot \hat{\mathbf{R}}\right)^2 \\
&\quad - \frac{3}{2}\left(\frac{\mathbf{x}_2}{R} \cdot \hat{\mathbf{R}}\right)^2 \\
&= \frac{\mathbf{x}_1}{R} \cdot \frac{\mathbf{x}_2}{R} - 3\frac{\mathbf{x}_1}{R} \cdot \hat{\mathbf{R}}\frac{\mathbf{x}_2}{R} \cdot \hat{\mathbf{R}}.
\end{aligned}
\tag{6.146}
$$

This proves eq. (6.120).

Exercise 6.2 Harmonic oscillator with energy shift. (*[11] pr. 5.1*)

Given a perturbed 1D SHO Hamiltonian

$$
H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2 + \lambda b x,
\tag{6.147}
$$

calculate the first non-zero perturbation to the ground state energy. Then solve for that energy directly and compare.

Answer for Exercise 6.2

The first order energy shift is seen to be zero

$$
\begin{aligned}
\Delta_0^{(0)} &= V_{00} \\
&= \langle 0| bx |0\rangle \\
&= \frac{x_0}{\sqrt{2}} \langle 0| a + a^\dagger |0\rangle \\
&= \frac{x_0}{\sqrt{2}} \langle 0|1\rangle \\
&= 0.
\end{aligned}
\tag{6.148}
$$

The first order perturbation to the ground state is

$$\begin{aligned}
\left|0^{(1)}\right\rangle &= \sum_{m\neq 0} \frac{|m\rangle\langle m|\, bx\, |0\rangle}{\hbar\omega/2 - \hbar\omega(m-1/2)} \\
&= -b\frac{x_0}{\sqrt{2}\,\hbar\omega} \sum_{m\neq 0} \frac{|m\rangle\langle m|1\rangle}{m} \\
&= -b\frac{x_0}{\sqrt{2}\,\hbar\omega}\,|1\rangle\,.
\end{aligned} \tag{6.149}$$

The second order ground state energy perturbation is

$$\begin{aligned}
\Delta_0^{(2)} &= \langle 0|\, bx \left|0^{(1)}\right\rangle \\
&= \frac{bx_0}{\sqrt{2}}\langle 0|\, a + a^\dagger \left(-b\frac{x_0}{\sqrt{2}\,\hbar\omega}\,|1\rangle\right) \\
&= \frac{bx_0}{\sqrt{2}}\left(-b\frac{x_0}{\sqrt{2}\,\hbar\omega}\right) \\
&= -\frac{b^2x_0^2}{2\,\hbar\omega} \\
&= -\frac{b^2}{2\,\hbar\omega}\frac{\hbar}{m\omega} \\
&= -\frac{b^2}{2m\omega^2},
\end{aligned} \tag{6.150}$$

so the total energy perturbation up to second order is

$$\Delta_0 = -\lambda^2\frac{b^2}{2m\omega^2}. \tag{6.151}$$

To compare to the exact result, rewrite the Hamiltonian as

$$\begin{aligned}
H &= \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2\left(x^2 + \frac{2\lambda bx}{m\omega^2}\right) \\
&= \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2\left(x + \frac{\lambda b}{m\omega^2}\right)^2 - \frac{1}{2}m\omega^2\left(\frac{\lambda b}{m\omega^2}\right)^2 .
\end{aligned} \tag{6.152}$$

The Hamiltonian is subject to a constant energy shift

$$\begin{aligned}
\Delta E &= -\frac{1}{2}m\omega^2\frac{\lambda^2b^2}{m^2\omega^4} \\
&= -\frac{\lambda^2b^2}{2m\omega^2}.
\end{aligned} \tag{6.153}$$

This is an exact match with the second order perturbation result of eq. (6.151).

Exercise 6.3 Double well potential. (*2015 ps7 p1*)

Consider a particle in the double well potential

$$V(x) = \frac{m\omega^2}{8a^2}(x+a)^2(x-a)^2 . \tag{6.154}$$

Expanding $V(x)$ around $x = \pm a$ leads to a harmonic potential with frequency ω. Construct variational states with even/odd parity as $\psi_\pm(x) = g_\pm\left(\phi(x-a) \pm \phi(x+a)\right)$ where $\phi(x)$ is the normalized ground state of the usual harmonic oscillator with frequency ω, i.e.,

$$\phi(x) = \left(\frac{1}{\pi a_0^2}\right)^{1/4} e^{-\frac{x^2}{2a_0^2}}; \qquad a_0 = \sqrt{\frac{\hbar}{m\omega}}. \tag{6.155}$$

a. Determine the normalization constants $g_\pm$. Next using these wavefunctions, determine the variational energies of these two states. Hence determine the 'tunnel splitting' between the two states, induced by the tunneling through the barrier region. In your calculations, you can assume $a \gg a_0$, so retain only the leading terms in any polynomials you might encounter when you do the integrals.

b. If we pay attention to these lowest two states (left well and right well) in the full Hilbert space, we can write a phenomenological 2×2 Hamiltonian

$$H = \begin{bmatrix} \epsilon_0 & -\gamma \\ -\gamma & \epsilon_0 \end{bmatrix}, \tag{6.156}$$

where ϵ_0 is the energy on each side, and γ leads to tunneling, so if we start off in the left well, t leads to a nonzero amplitude to find it in the right well at a later time. Find its eigenvalues and eigenvectors. Comparing with your variational result for the energy splitting, determine the 'tunnel coupling' γ.

Answer for Exercise 6.3

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Exercise 6.4 Helium-4 atom. (*2015 ps7 p2*)

Consider the Helium atom with atomic number $Z = 2$, which leads to the nuclear charge $Z = 2e$, and two electrons with charge $-e$ each.

a. Show that ignoring electron-electron interactions leads to a ground state energy $E_{\mathrm{He}} = 4E_{\mathrm{H}}$ where E_{H} is the ground state energy of the hydrogen atom.

b. Consider the full problem which retains the Coulomb interaction between the electrons, i.e.

$$H = \frac{1}{2m}\left(\mathbf{p}_1^2 + \mathbf{p}_2^2\right) - 2e^2 \frac{1}{4\pi\epsilon_0}\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + e^2 \frac{1}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}. \tag{6.157}$$

and consider the variational wavefunction

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = N e^{-\frac{1}{a}(r_1 + r_2)}. \tag{6.158}$$

where N is the normalization constant, and a is a variational parameter. Determine the variational ground state energy, and minimize with respect to a to find the best estimate for the ground state energy of Helium. Compare with numerical estimates of the energy.

Answer for Exercise 6.4

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Exercise 6.5 Harmonic oscillator variation. (*[2] pr. 24.3*)

Consider a 1D harmonic oscillator with an unnormalized trial wavefunction $\psi_v(x) = e^{-\beta|x|}$. Minimize the ground state energy with respect to β, thus obtaining the optimal β as well as the variational ground state energy. Compare with the exact result. Note that you need to be careful evaluating derivatives since the wavefunction has a 'cusp' at $x = 0$.

Answer for Exercise 6.5

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Exercise 6.6 **Energy estimate for an absolute value potential.** (*[11] pr. 5.21*)

Estimate the lowest eigenvalue λ of the differential equation

$$\frac{d^2}{dx^2}\psi + (\lambda - |x|)\,\psi = 0. \tag{6.159}$$

Using α variation with the trial function

$$\psi = \begin{cases} c(\alpha - |x|) & |x| < \alpha \\ 0 & |x| > \alpha \end{cases} \tag{6.160}$$

Answer for Exercise 6.6

First rewrite the differential equation in a Hamiltonian like fashion

$$H\psi = -\frac{d^2}{dx^2}\psi + |x|\psi = \lambda\psi. \tag{6.161}$$

We need the derivatives of the trial distribution. The first derivative is

$$\begin{aligned}
\frac{d}{dx}\psi &= -c\frac{d}{dx}|x| \\
&= -c\frac{d}{dx}\left(x\theta(x) - x\theta(-x)\right) \\
&= -c\left(\theta(x) - \theta(-x) + x\delta(x) + x\delta(-x)\right) \\
&= -c\left(\theta(x) - \theta(-x) + 2x\delta(x)\right).
\end{aligned} \tag{6.162}$$

The second derivative is

$$\begin{aligned}
\frac{d^2}{dx^2}\psi &= -c\frac{d}{dx}\left(\theta(x) - \theta(-x) + 2x\delta(x)\right) \\
&= -c\left(\delta(x) + \delta(-x) + 2\delta(x) + 2x\delta'(x)\right) \\
&= -c\left(4\delta(x) + 2x\frac{-\delta(x)}{x}\right) \\
&= -2c\delta(x).
\end{aligned} \tag{6.163}$$

This gives

$$H\psi = -2c\delta(x) + |x|c\,(\alpha - |x|)\,. \tag{6.164}$$

We are now set to compute some of the inner products. The normalization is the simplest

$$\begin{aligned}\langle\psi|\psi\rangle &= c^2\int_{-\alpha}^{\alpha}(\alpha - |x|)^2 dx \\ &= 2c^2\int_0^{\alpha}(x-\alpha)^2 dx \\ &= 2c^2\int_{-\alpha}^{0}u^2 du \\ &= 2c^2\left(-\frac{(-\alpha)^3}{3}\right) \\ &= \frac{2}{3}c^2\alpha^3.\end{aligned} \tag{6.165}$$

For the energy

$$\begin{aligned}\langle\psi|H\psi\rangle &= c^2\int dx\,(\alpha - |x|)\left(-2\delta(x) + |x|\,(\alpha - |x|)\right) \\ &= c^2\left(-2\alpha + \int_{-\alpha}^{\alpha}dx\,(\alpha - |x|)^2\,|x|\right) \\ &= c^2\left(-2\alpha + 2\int_{-\alpha}^{0}duu^2\,(u+\alpha)\right) \\ &= c^2\left(-2\alpha + 2\left(\frac{u^4}{4} + \alpha\frac{u^3}{3}\right)\Big|_{-\alpha}^{0}\right) \\ &= c^2\left(-2\alpha - 2\left(\frac{\alpha^4}{4} - \frac{\alpha^4}{3}\right)\right) \\ &= c^2\left(-2\alpha + \frac{1}{6}\alpha^4\right).\end{aligned} \tag{6.166}$$

The energy estimate is

$$\begin{aligned}\overline{E} &= \frac{\langle\psi|H\psi\rangle}{\langle\psi|\psi\rangle} \\ &= \frac{-2\alpha + \frac{1}{6}\alpha^4}{\frac{2}{3}\alpha^3} \\ &= -\frac{3}{\alpha^2} + \frac{1}{4}\alpha.\end{aligned} \tag{6.167}$$

This has its minimum at

$$0 = -\frac{6}{\alpha^3} + \frac{1}{4}, \tag{6.168}$$

or

$$\alpha = 2 \times 3^{1/3}. \tag{6.169}$$

Back substitution into the energy gives

$$\begin{aligned} \overline{E} &= -\frac{3}{4 \times 3^{2/3}} + \frac{1}{2} 3^{1/3} \\ &= \frac{3^{4/3}}{4} \\ &\approx 1.08. \end{aligned} \tag{6.170}$$

The problem says the exact answer is 1.019, so the variation gets within 6 %.

Exercise 6.7 Anharmonic oscillator. (*2015 ps8 p1*)

Consider a quantum particle in the ground state of a 1D anharmonic oscillator potential

$$\begin{aligned} V(x) &= \frac{1}{2} m\omega^2 x^2 + \lambda x^4 \\ &= V_0 + \lambda V'. \end{aligned} \tag{6.171}$$

Compute the first and second order energy shift of this oscillator perturbatively in λ.

Answer for Exercise 6.7

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Exercise 6.8 Quadrupolar potential. (*2015 ps8 p2*)

Consider a p-orbital electron of hydrogen with $|n, l = 1, m\rangle$, with $m = 0, \pm 1$, subject to an external potential

$$V(x, y, z) = \lambda(x^2 - y^2), \tag{6.172}$$

with λ being a constant. For fixed n, obtain the correct eigenstates which diagonalize the perturbation, without worrying about doing radial integrals explicitly. Show that the three-fold degeneracy of the p-orbital is completely broken by the perturbation to linear order in λ.

Answer for Exercise 6.8

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Exercise 6.9 Harmonic oscillator. (*2015 ps8 p3*)

Consider a 2D harmonic oscillator with

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2} m\omega^2 \left(x^2 + y^2\right) \tag{6.173}$$

Turn on an anharmonic perturbation

$$V = \lambda g_1 \frac{m^2\omega^3}{\hbar} \left(x^4 + y^4\right) + \lambda^2 g_2 m\omega^2 xy, \tag{6.174}$$

Note that the potentials have been altered from the original problem statement to have dimensions of energy with dimensionless scale factors g_1, g_2, λ.

a. Derive the equations for the energy shifts and perturbed states for a second order perturbing potential of the form above.
b. Find the perturbed eigenstate and the corresponding energy shifts up to $O(\lambda^2)$ for the ground state. Ignore terms of $O(\lambda^3)$.
c. Do the same for the first two degenerate states.

Answer for Exercise 6.9

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Exercise 6.10 Hyperfine levels. (*2015 ps8 p4*)

We can schematically model the hyperfine interaction between the electron and proton spins as $A\mathbf{S}_\mathrm{e} \cdot \mathbf{S}_\mathrm{p}$ where A is the hyperfine interaction energy.

a. Consider the spin-1/2 proton interacting with a spin-1/2 electron. What are the spin eigenstates and eigenvalues?

b. Now consider applying a magnetic field which leads to an extra term

$$-B\left(g_\mathrm{e}\mu_\mathrm{e}S_\mathrm{e}^z + g_\mathrm{p}\mu_\mathrm{p}S_\mathrm{p}^z\right) \tag{6.175}$$

with gyromagnetic ratios $g_\mathrm{e} \approx -2$ and $g_\mathrm{p} \approx 5.5$, with magnetic moments $\mu_\mathrm{e} = e/2m_\mathrm{e}$ and $\mu_\mathrm{p} = e/2m_\mathrm{p}$. The large nuclear mass ensures $\mu_\mathrm{e}/\mu_\mathrm{p} \sim 2000$, so let us simply set $\mu_\mathrm{p} = 0$. For convenience, set $Bg_\mathrm{e}\mu_\mathrm{e} \rightarrow B_\mathrm{eff}$ so the Hamiltonian becomes

$$H = A\mathbf{S}_\mathrm{e} \cdot \mathbf{S}_\mathrm{p} - B_\mathrm{eff}S_\mathrm{e}^z, \tag{6.176}$$

so the only dimensionless parameter is B_eff/A.
Using perturbation theory (degenerate or non-degenerate as appropriate) find how the coupled hyperfine levels split for weak field $B_\mathrm{eff}/A \ll 1$. Also consider the strong field limit $B_\mathrm{eff}/A \gg 1$.

c. Compute the full field evolution of the levels and compare with the perturbative low field regime result and the high field regime result.

Answer for Exercise 6.10

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Exercise 6.11 **2D SHO xy perturbation.** ([11] *pr. 5.4*)

Given a 2D SHO with Hamiltonian

$$H_0 = \frac{1}{2m}\left(p_x^2 + p_y^2\right) + \frac{m\omega^2}{2}\left(x^2 + y^2\right), \tag{6.177}$$

a. What are the energies and degeneracies of the three lowest states?
b. With perturbation

$$V = m\omega^2 xy, \tag{6.178}$$

calculate the first order energy perturbations and the zeroth order perturbed states.
c. Solve the $H_0 + \delta V$ problem exactly, and compare.

Answer for Exercise 6.11

Part a. Recall that we have

$$H\left|n_1, n_2\right\rangle = \hbar\omega\left(n_1 + n_2 + 1\right)\left|n_1, n_2\right\rangle, \tag{6.179}$$

So the three lowest energy states are $\left|0,0\right\rangle, \left|1,0\right\rangle, \left|0,1\right\rangle$ with energies $\hbar\omega, 2\hbar\omega, 2\hbar\omega$ respectively (with a two fold degeneracy for the second two energy eigenkets).

Part b. Consider the action of xy on the $\beta = \{\left|0,0\right\rangle, \left|1,0\right\rangle, \left|0,1\right\rangle\}$ subspace. Those are

$$\begin{aligned} xy\left|0,0\right\rangle &= \frac{x_0^2}{2}\left(a + a^\dagger\right)\left(b + b^\dagger\right)\left|0,0\right\rangle \\ &= \frac{x_0^2}{2}\left(b + b^\dagger\right)\left|1,0\right\rangle \\ &= \frac{x_0^2}{2}\left|1,1\right\rangle. \end{aligned} \tag{6.180}$$

$$\begin{aligned} xy\,|1,0\rangle &= \frac{x_0^2}{2}\left(a+a^\dagger\right)\left(b+b^\dagger\right)|1,0\rangle \\ &= \frac{x_0^2}{2}\left(a+a^\dagger\right)|1,1\rangle \\ &= \frac{x_0^2}{2}\left(|0,1\rangle+\sqrt{2}\,|2,1\rangle\right). \end{aligned} \tag{6.181}$$

$$\begin{aligned} xy\,|0,1\rangle &= \frac{x_0^2}{2}\left(a+a^\dagger\right)\left(b+b^\dagger\right)|0,1\rangle \\ &= \frac{x_0^2}{2}\left(b+b^\dagger\right)|1,1\rangle \\ &= \frac{x_0^2}{2}\left(|1,0\rangle+\sqrt{2}\,|1,2\rangle\right). \end{aligned} \tag{6.182}$$

The matrix representation of $m\omega^2 xy$ with respect to the subspace spanned by basis β above is

$$xy \sim \frac{1}{2}\hbar\omega \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}. \tag{6.183}$$

This diagonalizes with

$$U = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{U} \end{bmatrix} \tag{6.184a}$$

$$\tilde{U} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{6.184b}$$

$$D = \frac{1}{2}\hbar\omega \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \tag{6.184c}$$

$$xy = UDU^\dagger = UDU. \tag{6.184d}$$

The unperturbed Hamiltonian in the original basis is

$$H_0 = \hbar\omega \begin{bmatrix} 1 & 0 \\ 0 & 2I \end{bmatrix}, \tag{6.185}$$

So the transformation to the diagonal xy basis leaves the initial Hamiltonian unaltered

$$\begin{aligned} H'_0 &= U^\dagger H_0 U \\ &= \hbar\omega \begin{bmatrix} 1 & 0 \\ 0 & \tilde{U} 2I \tilde{U} \end{bmatrix} \\ &= \hbar\omega \begin{bmatrix} 1 & 0 \\ 0 & 2I \end{bmatrix}. \end{aligned} \tag{6.186}$$

Now we can compute the first order energy shifts almost by inspection. Writing the new basis as $\beta' = \{|0\rangle, |1\rangle, |2\rangle\}$ those energy shifts are just the diagonal elements from the xy operators matrix representation

$$\begin{aligned} E_0^{(1)} &= \langle 0| V |0\rangle = 0 \\ E_1^{(1)} &= \langle 1| V |1\rangle = \frac{1}{2}\hbar\omega \\ E_2^{(1)} &= \langle 2| V |2\rangle = -\frac{1}{2}\hbar\omega. \end{aligned} \tag{6.187}$$

The new energies are

$$\begin{aligned} E_0 &\rightarrow \hbar\omega \\ E_1 &\rightarrow \hbar\omega\left(2 + \delta/2\right) \\ E_2 &\rightarrow \hbar\omega\left(2 - \delta/2\right). \end{aligned} \tag{6.188}$$

Part c. For the exact solution, it's possible to rotate the coordinate system in a way that kills the explicit xy term of the perturbation. That we could do this for x, y operators wasn't obvious to me, but after doing so (and rotating the momentum operators the same way) the new operators still have the required commutators. Let

$$\begin{aligned} \begin{bmatrix} u \\ v \end{bmatrix} &= \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \\ &= \begin{bmatrix} x\cos\theta + y\sin\theta \\ -x\sin\theta + y\cos\theta \end{bmatrix}. \end{aligned} \tag{6.189}$$

Similarly, for the momentum operators, let

$$\begin{aligned} \begin{bmatrix} p_u \\ p_v \end{bmatrix} &= \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} p_x \\ p_y \end{bmatrix} \\ &= \begin{bmatrix} p_x\cos\theta + p_y\sin\theta \\ -p_x\sin\theta + p_y\cos\theta \end{bmatrix}. \end{aligned} \tag{6.190}$$

For the commutators of the new operators we have

$$\begin{aligned}
[u, p_u] &= \left[x\cos\theta + y\sin\theta, p_x\cos\theta + p_y\sin\theta\right] \\
&= [x, p_x]\cos^2\theta + \left[y, p_y\right]\sin^2\theta \\
&= i\hbar\left(\cos^2\theta + \sin^2\theta\right) \\
&= i\hbar.
\end{aligned} \tag{6.191}$$

$$\begin{aligned}
[v, p_v] &= \left[-x\sin\theta + y\cos\theta, -p_x\sin\theta + p_y\cos\theta\right] \\
&= [x, p_x]\sin^2\theta + \left[y, p_y\right]\cos^2\theta \\
&= i\hbar.
\end{aligned} \tag{6.192}$$

$$\begin{aligned}
[u, p_v] &= \left[x\cos\theta + y\sin\theta, -p_x\sin\theta + p_y\cos\theta\right] \\
&= \cos\theta\sin\theta\left(-[x, p_x] + \left[y, p_p\right]\right) \\
&= 0.
\end{aligned} \tag{6.193}$$

$$\begin{aligned}
[v, p_u] &= \left[-x\sin\theta + y\cos\theta, p_x\cos\theta + p_y\sin\theta\right] \\
&= \cos\theta\sin\theta\left(-[x, p_x] + \left[y, p_p\right]\right) \\
&= 0.
\end{aligned} \tag{6.194}$$

We see that the new operators are canonical conjugate as required. For this problem, we just want a 45 degree rotation, with

$$\begin{aligned}
x &= \frac{1}{\sqrt{2}}\left(u + v\right) \\
y &= \frac{1}{\sqrt{2}}\left(u - v\right).
\end{aligned} \tag{6.195}$$

We have

$$\begin{aligned}
x^2 + y^2 &= \frac{1}{2}\left((u+v)^2 + (u-v)^2\right) \\
&= \frac{1}{2}\left(2u^2 + 2v^2 + 2uv - 2uv\right) \\
&= u^2 + v^2,
\end{aligned} \tag{6.196}$$

$$\begin{aligned} p_x^2 + p_y^2 &= \frac{1}{2}\left((p_u + p_v)^2 + (p_u - p_v)^2\right) \\ &= \frac{1}{2}\left(2p_u^2 + 2p_v^2 + 2p_u p_v - 2p_u p_v\right) \\ &= p_u^2 + p_v^2, \end{aligned} \tag{6.197}$$

and

$$\begin{aligned} xy &= \frac{1}{2}\left((u + v)(u - v)\right) \\ &= \frac{1}{2}\left(u^2 - v^2\right). \end{aligned} \tag{6.198}$$

The perturbed Hamiltonian is

$$\begin{aligned} H_0 + \delta V &= \frac{1}{2m}\left(p_u^2 + p_v^2\right) + \frac{1}{2}m\omega^2\left(u^2 + v^2 + \delta u^2 - \delta v^2\right) \\ &= \frac{1}{2m}\left(p_u^2 + p_v^2\right) + \frac{1}{2}m\omega^2\left(u^2(1 + \delta) + v^2(1 - \delta)\right). \end{aligned} \tag{6.199}$$

In this coordinate system, the corresponding eigensystem is

$$H\left|n_1, n_2\right\rangle = \hbar\omega\left(1 + n_1\sqrt{1 + \delta} + n_2\sqrt{1 - \delta}\right)\left|n_1, n_2\right\rangle. \tag{6.200}$$

For small δ

$$n_1\sqrt{1 + \delta} + n_2\sqrt{1 - \delta} \approx n_1 + n_2 + \frac{1}{2}n_1\delta - \frac{1}{2}n_2\delta, \tag{6.201}$$

so

$$H\left|n_1, n_2\right\rangle \approx \hbar\omega\left(1 + n_1 + n_2 + \frac{1}{2}n_1\delta - \frac{1}{2}n_2\delta\right)\left|n_1, n_2\right\rangle. \tag{6.202}$$

The lowest order perturbed energy levels are

$$\left|0, 0\right\rangle \rightarrow \hbar\omega \tag{6.203}$$

$$\left|1, 0\right\rangle \rightarrow \hbar\omega\left(2 + \frac{1}{2}\delta\right) \tag{6.204}$$

$$\left|0, 1\right\rangle \rightarrow \hbar\omega\left(2 - \frac{1}{2}\delta\right) \tag{6.205}$$

The degeneracy of the $\left|0, 1\right\rangle, \left|1, 0\right\rangle$ states has been split, and to first order match the zeroth order perturbation result.

Exercise 6.12 Perturbation of two state Hamiltonian. ([11] pr. 5.11)

Given a two-state system

$$\begin{aligned} H &= H_0 + \lambda V \\ &= \begin{bmatrix} E_1 & \lambda\Delta \\ \lambda\Delta & E_2 \end{bmatrix} \end{aligned} \tag{6.206}$$

a. Solve the system exactly.
b. Find the first order perturbed states and second order energy shifts, and compare to the exact solution.
c. Solve the degenerate case for $E_1 = E_2$, and compare to the exact solution.

Answer for Exercise 6.12

Part a. The energy eigenvalues ϵ are given by

$$0 = (E_1 - \epsilon)(E_2 - \epsilon) - (\lambda\Delta)^2, \tag{6.207}$$

or

$$\epsilon^2 - \epsilon(E_1 + E_2) + E_1 E_2 = (\lambda\Delta)^2. \tag{6.208}$$

After rearranging this is

$$\epsilon = \frac{E_1 + E_2}{2} \pm \sqrt{\left(\frac{E_1 - E_2}{2}\right)^2 + (\lambda\Delta)^2}. \tag{6.209}$$

Notice that for $E_2 = E_1$ we have

$$\epsilon = E_1 \pm \lambda\Delta. \tag{6.210}$$

Since a change of basis can always put the problem in a form so that $E_1 > E_2$, let's assume that to make an approximation of the energy eigenvalues for $|\lambda\Delta| \ll (E_1 - E_2)/2$

$$\begin{aligned} \epsilon &= \frac{E_1 + E_2}{2} \pm \frac{E_1 - E_2}{2}\sqrt{1 + \frac{(2\lambda\Delta)^2}{(E_1 - E_2)^2}} \\ &\approx \frac{E_1 + E_2}{2} \pm \frac{E_1 - E_2}{2}\left(1 + 2\frac{(\lambda\Delta)^2}{(E_1 - E_2)^2}\right) \\ &= \frac{E_1 + E_2}{2} \pm \frac{E_1 - E_2}{2} \pm \frac{(\lambda\Delta)^2}{E_1 - E_2} \\ &= E_1 + \frac{(\lambda\Delta)^2}{E_1 - E_2}, E_2 + \frac{(\lambda\Delta)^2}{E_2 - E_1}. \end{aligned} \tag{6.211}$$

For the perturbed states, starting with the plus case, if

$$|+\rangle \propto \begin{bmatrix} a \\ b \end{bmatrix}, \tag{6.212}$$

we must have

$$\begin{aligned} 0 &= (E_1 - \left(E_1 + \frac{(\lambda\Delta)^2}{E_1 - E_2}\right))a + \lambda\Delta b \\ &= (-\frac{(\lambda\Delta)^2}{E_1 - E_2})a + \lambda\Delta b, \end{aligned} \tag{6.213}$$

so

$$\begin{aligned} |+\rangle &\rightarrow \begin{bmatrix} 1 \\ \frac{\lambda\Delta}{E_1 - E_2} \end{bmatrix} \\ &= |+\rangle + \frac{\lambda\Delta}{E_1 - E_2} |-\rangle \,. \end{aligned} \tag{6.214}$$

Similarly for the minus case we must have

$$\begin{aligned} 0 &= \lambda\Delta a + (E_2 - \left(E_2 + \frac{(\lambda\Delta)^2}{E_2 - E_1}\right))b \\ &= \lambda\Delta b + (-\frac{(\lambda\Delta)^2}{E_2 - E_1})b, \end{aligned} \tag{6.215}$$

for

$$|-\rangle \rightarrow |-\rangle + \frac{\lambda\Delta}{E_2 - E_1} |+\rangle \,. \tag{6.216}$$

Part b. For the perturbation the first energy shift for perturbation of the $|+\rangle$ state is

$$\begin{aligned} E_+^{(1)} &= |+\rangle\, V \,|+\rangle \\ &= \lambda\Delta \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ &= \lambda\Delta \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ &= 0. \end{aligned} \tag{6.217}$$

The first order energy shift for the perturbation of the $\left|-\right\rangle$ state is also zero. The perturbed $\left|+\right\rangle$ state is

$$\begin{aligned} \left|+\right\rangle^{(1)} &= \frac{\overline{P}_+}{E_1 - H_0} V \left|+\right\rangle \\ &= \frac{\left|-\right\rangle\left\langle-\right|}{E_1 - E_2} V \left|+\right\rangle \end{aligned} \tag{6.218}$$

The numerator matrix element is

$$\begin{aligned} \left\langle-\right| V \left|+\right\rangle &= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ &= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ \Delta \end{bmatrix} \\ &= \Delta, \end{aligned} \tag{6.219}$$

so

$$\left|+\right\rangle \rightarrow \left|+\right\rangle + \left|-\right\rangle \frac{\Delta}{E_1 - E_2}. \tag{6.220}$$

Observe that this matches the first order series expansion of the exact value above.
For the perturbation of $\left|-\right\rangle$ we need the matrix element

$$\begin{aligned} \left\langle+\right| V \left|-\right\rangle &= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} \Delta \\ 0 \end{bmatrix} \\ &= \Delta, \end{aligned} \tag{6.221}$$

so it’s clear that the perturbed ket is

$$\left|-\right\rangle \rightarrow \left|-\right\rangle + \left|+\right\rangle \frac{\Delta}{E_2 - E_1}, \tag{6.222}$$

also matching the approximation found from the exact computation. The second order energy shifts can now be calculated

$$
\begin{aligned}
\langle +|\, V \,|+\rangle' &= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} 1 \\ \frac{\Delta}{E_1 - E_2} \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\Delta^2}{E_1 - E_2} \\ \Delta \end{bmatrix} \\
&= \frac{\Delta^2}{E_1 - E_2},
\end{aligned}
\tag{6.223}
$$

and

$$
\begin{aligned}
\langle -|\, V \,|-\rangle' &= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & \Delta \\ \Delta & 0 \end{bmatrix} \begin{bmatrix} \frac{\Delta}{E_2 - E_1} \\ 1 \end{bmatrix} \\
&= \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} \Delta \\ \frac{\Delta^2}{E_2 - E_1} \end{bmatrix} \\
&= \frac{\Delta^2}{E_2 - E_1},
\end{aligned}
\tag{6.224}
$$

The energy perturbations are therefore

$$
\begin{aligned}
E_1 &\rightarrow E_1 + \frac{(\lambda\Delta)^2}{E_1 - E_2} \\
E_2 &\rightarrow E_2 + \frac{(\lambda\Delta)^2}{E_2 - E_1}.
\end{aligned}
\tag{6.225}
$$

This is what we had by approximating the exact case.

Part c. For the $E_2 = E_1$ case, we'll have to diagonalize the perturbation potential. That is

$$
\begin{aligned}
V &= U \bigwedge U^\dagger \\
\bigwedge &= \begin{bmatrix} \Delta & 0 \\ 0 & -\Delta \end{bmatrix} \\
U = U^\dagger &= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.
\end{aligned}
\tag{6.226}
$$

A change of basis for the Hamiltonian is

$$
\begin{aligned}
H' &= U^\dagger H U \\
&= U^\dagger H_0 U + \lambda U^\dagger V U \\
&= E_1 U^\dagger + \lambda U^\dagger V U \\
&= H_0 + \lambda \bigwedge .
\end{aligned}
\tag{6.227}
$$

We can now calculate the perturbation energy with respect to the new basis, say $\{|1\rangle, |2\rangle\}$. Those energy shifts are

$$
\begin{aligned}
\Delta^{(1)} &= \langle 1| V |1\rangle = \Delta \\
\Delta^{(2)} &= \langle 2| V |2\rangle = -\Delta.
\end{aligned}
\tag{6.228}
$$

The perturbed energies are therefore

$$
\begin{aligned}
E_1 &\rightarrow E_1 + \lambda\Delta \\
E_2 &\rightarrow E_2 - \lambda\Delta,
\end{aligned}
\tag{6.229}
$$

which matches eq. (6.210), the exact result.

Exercise 6.13 Expectation of spherically symmetric 3D potential derivative. ([11] pr. 5.16)

a. For a particle in a spherically symmetric potential $V(r)$ show that

$$
|\psi(0)|^2 = \frac{m}{2\pi\hbar^2}\left\langle \frac{dV}{dr} \right\rangle,
\tag{6.230}
$$

for all s-states, ground or excited.

b. Show this is the case for the 3D SHO and hydrogen wave functions.

Answer for Exercise 6.13

Part a. The text works a problem that looks similar to this by considering the commutator of an operator A, later set to $A = p_r = -i\hbar\partial/\partial r$ the radial momentum operator. First it is noted that

$$
0 = \langle nlm| [H, A] |nlm\rangle ,
\tag{6.231}
$$

since H operating to either the right or the left is the energy eigenvalue E_n. Next it appears the author uses an angular momentum factoring of the squared momentum operator. Looking earlier in the text that factoring is found to be

$$
\frac{\mathbf{p}^2}{2m} = \frac{1}{2mr^2}\mathbf{L}^2 - \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right).
\tag{6.232}
$$

With

$$R = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right). \tag{6.233}$$

we have

$$\begin{aligned}
0 &= \langle nlm| \left[H, p_r\right] |nlm\rangle \\
&= \langle nlm| \left[\frac{\mathbf{p}^2}{2m} + V(r), p_r\right] |nlm\rangle \\
&= \langle nlm| \left[\frac{1}{2mr^2}\mathbf{L}^2 + R + V(r), p_r\right] |nlm\rangle \\
&= \langle nlm| \left[\frac{-\hbar^2 l(l+1)}{2mr^2} + R + V(r), p_r\right] |nlm\rangle .
\end{aligned} \tag{6.234}$$

Let's consider the commutator of each term separately. First

$$\begin{aligned}
\left[V, p_r\right]\psi &= V p_r\psi - p_r V\psi \\
&= V p_r\psi - (p_r V)\psi - V p_r\psi \\
&= -(p_r V)\psi \\
&= i\hbar\frac{\partial V}{\partial r}\psi.
\end{aligned} \tag{6.235}$$

Setting $V(r) = 1/r^2$, we also have

$$\left[\frac{1}{r^2}, p_r\right]\psi = -\frac{2i\hbar}{r^3}\psi. \tag{6.236}$$

Finally

$$\begin{aligned}
\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}, \frac{\partial}{\partial r}\right] &= \left(\partial_{rr} + \frac{2}{r}\partial_r\right)\partial_r - \partial_r\left(\partial_{rr} + \frac{2}{r}\partial_r\right) \\
&= \partial_{rrr} + \frac{2}{r}\partial_{rr} - \left(\partial_{rrr} - \frac{2}{r^2}\partial_r + \frac{2}{r}\partial_{rr}\right) \\
&= -\frac{2}{r^2}\partial_r,
\end{aligned} \tag{6.237}$$

so

$$\begin{aligned}
\left[R, p_r\right] &= -\frac{2}{r^2}\frac{-\hbar^2}{2m}p_r \\
&= \frac{\hbar^2}{mr^2}p_r.
\end{aligned} \tag{6.238}$$

Putting all the pieces back together, we've got

$$\begin{aligned} 0 &= \langle nlm| \left[\frac{-\hbar^2 l(l+1)}{2mr^2} + R + V(r), p_r \right] |nlm\rangle \\ &= i\hbar \, \langle nlm| \left(\frac{\hbar^2 l(l+1)}{mr^3} - \frac{i\hbar}{mr^2} p_r + \frac{\partial V}{\partial r} \right) |nlm\rangle \, . \end{aligned} \tag{6.239}$$

Since s-states are those for which $l = 0$, this means

$$\begin{aligned} \left\langle \frac{\partial V}{\partial r} \right\rangle &= \frac{i\hbar}{m} \left\langle \frac{1}{r^2} p_r \right\rangle \\ &= \frac{\hbar^2}{m} \left\langle \frac{1}{r^2} \frac{\partial}{\partial r} \right\rangle \\ &= \frac{\hbar^2}{m} \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi r^2 \sin\theta \psi^*(r,\theta,\phi) \frac{1}{r^2} \frac{\partial \psi(r,\theta,\phi)}{\partial r} . \end{aligned} \tag{6.240}$$

Since s-states are spherically symmetric, this is

$$\left\langle \frac{\partial V}{\partial r} \right\rangle = \frac{4\pi\hbar^2}{m} \int_0^\infty dr \psi^* \frac{\partial \psi}{\partial r} . \tag{6.241}$$

That integral is

$$\int_0^\infty dr \psi^* \frac{\partial \psi}{\partial r} = |\psi|^2 \Big|_0^\infty - \int_0^\infty dr \frac{\partial \psi^*}{\partial r} \psi . \tag{6.242}$$

With the hydrogen atom, our radial wave functions are real valued. It's reasonable to assume that we can do the same for other real-valued spherical potentials. If that is the case, we have

$$2 \int_0^\infty dr \psi^* \frac{\partial \psi}{\partial r} = |\psi(0)|^2 , \tag{6.243}$$

and

$$\boxed{\left\langle \frac{\partial V}{\partial r} \right\rangle = \frac{2\pi\hbar^2}{m} |\psi(0)|^2 ,} \tag{6.244}$$

which completes this part of the problem.

Part b. For a hydrogen like atom, in atomic units, we have

$$
\begin{aligned}
\left\langle \frac{\partial V}{\partial r} \right\rangle &= \left\langle \frac{\partial}{\partial r}\left(-\frac{Ze^2}{r}\right)\right\rangle \\
&= Ze^2 \left\langle \frac{1}{r^2} \right\rangle \\
&= Ze^2 \frac{Z^2}{n^3 a_0^2 (l + 1/2)} \\
&= \frac{\hbar^2}{m a_0} \frac{2Z^3}{n^3 a_0^2} \\
&= \frac{2\hbar^2 Z^3}{m n^3 a_0^3}.
\end{aligned}
\tag{6.245}
$$

On the other hand for $n = 1$, we have

$$
\begin{aligned}
\frac{2\pi\hbar^2}{m} |R_{10}(0)|^2 |Y_{00}|^2 &= \frac{2\pi\hbar^2}{m} \frac{Z^3}{a_0^3} 4 \frac{1}{4\pi} \\
&= \frac{2\hbar^2 Z^3}{m a_0^3},
\end{aligned}
\tag{6.246}
$$

and for $n = 2$, we have

$$
\begin{aligned}
\frac{2\pi\hbar^2}{m} |R_{20}(0)|^2 |Y_{00}|^2 &= \frac{2\pi\hbar^2}{m} \frac{Z^3}{8a_0^3} 4 \frac{1}{4\pi} \\
&= \frac{\hbar^2 Z^3}{4 m a_0^3}.
\end{aligned}
\tag{6.247}
$$

These both match the potential derivative expectation when evaluated for the s-orbital ($l = 0$).

In sakuraiProblem5.16bSHO.nb is a verification for the 3D SHO ground state. There it was found that

$$
\begin{aligned}
\left\langle \frac{\partial V}{\partial r} \right\rangle &= \frac{2\pi\hbar^2}{m} |\psi(0)|^2 \\
&= 2\sqrt{\frac{m\omega^3\hbar}{\pi}}
\end{aligned}
\tag{6.248}
$$

Exercise 6.14 L_y perturbation. ([11] pr. 5.17(a))

Find the first non-zero energy shift for the perturbed Hamiltonian

$$\begin{aligned} H &= A\mathbf{L}^2 + BL_z + CL_y \\ &= H_0 + V. \end{aligned} \tag{6.249}$$

Answer for Exercise 6.14

The energy eigenvalues for state $|l, m\rangle$ prior to perturbation are

$$A\hbar^2 l(l+1) + B\hbar m. \tag{6.250}$$

The first order energy shift is zero

$$\begin{aligned} \Delta^1 &= \langle l, m| CL_y |l, m\rangle \\ &= \frac{C}{2i} \langle l, m| (L_+ - L_-) |l, m\rangle \\ &= 0, \end{aligned} \tag{6.251}$$

so we need the second order shift. Assuming no degeneracy to start, the perturbed state is

$$|l, m\rangle' = \sum{}' \frac{|l', m'\rangle \langle l', m'|}{E_{l,m} - E_{l',m'}} V |l, m\rangle, \tag{6.252}$$

and the next order energy shift is

$$\begin{aligned} \Delta^2 &= \langle lm| V \sum{}' \frac{|l', m'\rangle \langle l', m'|}{E_{l,m} - E_{l',m'}} V |l, m\rangle \\ &= \sum{}' \frac{\langle l, m| V |l', m'\rangle \langle l', m'|}{E_{l,m} - E_{l',m'}} V |l, m\rangle \\ &= \sum{}' \frac{|\langle l', m'| V |l, m\rangle|^2}{E_{l,m} - E_{l',m'}} \\ &= \sum_{m' \neq m} \frac{|\langle l, m'| V |l, m\rangle|^2}{E_{l,m} - E_{l,m'}} \\ &= \sum_{m' \neq m} \frac{|\langle l, m'| V |l, m\rangle|^2}{\left(A\hbar^2 l(l+1) + B\hbar m\right) - \left(A\hbar^2 l(l+1) + B\hbar m'\right)} \\ &= \frac{1}{B\hbar} \sum_{m' \neq m} \frac{|\langle l, m'| V |l, m\rangle|^2}{m - m'}. \end{aligned} \tag{6.253}$$

The sum over l' was eliminated because V only changes the m of any state $|l, m\rangle$, so the matrix element $\langle l', m'| V |l, m\rangle$ must includes a $\delta_{l',l}$ factor. Since we are now summing over $m' \neq m$, some of the matrix elements in the numerator should now be non-zero, unlike the case when the zero first order energy shift was calculated in eq. (6.251).

$$\begin{aligned}
\langle l, m' \vert C L_y \vert l, m\rangle &= \frac{C}{2i} \langle l, m' \vert (L_+ - L_-) \vert l, m\rangle \\
&= \frac{C}{2i} \langle l, m' \vert (L_+ \vert l, m\rangle - L_- \vert l, m\rangle) \\
&= \frac{C\hbar}{2i} \langle l, m' \vert \left(\sqrt{(l-m)(l+m+1)} \vert l, m+1\rangle - \sqrt{(l+m)(l-m+1)} \vert l, m-1\rangle \right) \\
&= \frac{C\hbar}{2i} \left(\sqrt{(l-m)(l+m+1)} \delta_{m',m+1} - \sqrt{(l+m)(l-m+1)} \delta_{m',m-1} \right).
\end{aligned} \tag{6.254}$$

After squaring and summing, the cross terms will be zero since they involve products of delta functions with different indices. That leaves

$$\begin{aligned}
\Delta^2 &= \frac{C^2\hbar}{4B} \sum_{m' \neq m} \frac{(l-m)(l+m+1)\delta_{m',m+1} - (l+m)(l-m+1)\delta_{m',m-1}}{m - m'} \\
&= \frac{C^2\hbar}{4B} \left(\frac{(l-m)(l+m+1)}{m-(m+1)} - \frac{(l+m)(l-m+1)}{m-(m-1)} \right) \\
&= \frac{C^2\hbar}{4B} \left(-(l^2 - m^2 + l - m) - (l^2 - m^2 + l + m) \right) \\
&= -\frac{C^2\hbar}{2B} (l^2 - m^2 + l),
\end{aligned} \tag{6.255}$$

so to first order the energy shift is

$$\boxed{A\hbar^2 l(l+1) + B\hbar m \rightarrow \hbar l(l+1)\left(A\hbar - \frac{C^2}{2B} \right) + B\hbar m + \frac{C^2 m^2 \hbar}{2B}.} \tag{6.256}$$

Exact perturbation equation If we wanted to solve the Hamiltonian exactly, we've have to diagonalize the $2m+1$ dimensional Hamiltonian

$$\begin{aligned}
\langle l, m' \vert H \vert l, m\rangle &= \Big(A\hbar^2 l(l+1) \\
&\quad + B\hbar m \Big) \delta_{m',m} + \frac{C\hbar}{2i} \left(\sqrt{(l-m)(l+m+1)} \delta_{m',m+1} - \sqrt{(l+m)(l-m+1)} \delta_{m',m-1} \right).
\end{aligned} \tag{6.257}$$

This Hamiltonian matrix has a very regular structure

$$H = (Al(l+1)\hbar^2 - B\hbar(l+1))I$$
$$+ B\hbar \begin{bmatrix} 1 & & & & \\ & 2 & & & \\ & & 3 & & \\ & & & \ddots & \\ & & & & 2l+1 \end{bmatrix}$$
$$+ \frac{C\hbar}{i} \begin{bmatrix} 0 & -\sqrt{(2l-1)(1)} & & & & \\ \sqrt{(2l-1)(1)} & 0 & -\sqrt{(2l-2)(2)} & & & \\ & \sqrt{(2l-2)(2)} & & & & \\ & & \ddots & & & \\ & & & & 0 & -\sqrt{(1)(2l-1)} \\ & & & & \sqrt{(1)(2l-1)} & 0 \end{bmatrix} \tag{6.258}$$

Solving for the eigenvalues of this Hamiltonian for increasing l in Mathematica (sakuraiProblem5.17a.nb), it appears that the eigenvalues are

$$\lambda_m = A\hbar^2(l)(l+1) + \hbar m B\sqrt{1 + \frac{4C^2}{B^2}}, \tag{6.259}$$

so to first order in C^2, these are

$$\lambda_m = A\hbar^2(l)(l+1) + \hbar m B\left(1 + \frac{2C^2}{B^2}\right). \tag{6.260}$$

We have a $C^2\hbar/B$ term in both the perturbative energy shift eq. (6.255), and the first order expansion of the exact solution eq. (6.259). Comparing this for the $l = 5$ case, the coefficients of $C^2\hbar/B$ in eq. (6.255) are all negative $-17.5, -17., -16.5, -16., -15.5, -15., -14.5, -14., -13.5, -13., -12.5$, whereas the coefficient of $C^2\hbar/B$ in the first order expansion of the exact solution eq. (6.259) are $2m$, ranging from $[-10, 10]$.

Exercise 6.15 Quadratic Zeeman effect. ([11] *pr. 5.18*)

Work out the quadratic Zeeman effect for the ground state hydrogen atom due to the usually neglected $e^2\mathbf{A}^2/2m_ec^2$ term in the Hamiltonian.

Answer for Exercise 6.15

The first order energy shift is
For a z-oriented magnetic field we can use

$$\mathbf{A} = \frac{B}{2}(-y, x, 0), \tag{6.261}$$

so the perturbation potential is

$$\begin{aligned} V &= \frac{e^2\mathbf{A}^2}{2m_e c^2} \\ &= \frac{e^2\mathbf{B}^2(x^2+y^2)}{8m_e c^2} \\ &= \frac{e^2\mathbf{B}^2 r^2 \sin^2\theta}{8m_e c^2} \end{aligned} \tag{6.262}$$

The ground state wave function is

$$\begin{aligned} \psi_0 &= \langle \mathbf{x} | 0 \rangle \\ &= \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}, \end{aligned} \tag{6.263}$$

so the energy shift is

$$\begin{aligned} \Delta &= \langle 0 | V | 0 \rangle \\ &= \frac{1}{\pi a_0^3} 2\pi \frac{e^2\mathbf{B}^2}{8m_e c^2} \int_0^\infty r^2 \sin\theta e^{-2r/a_0} r^2 \sin^2\theta dr d\theta \\ &= \frac{e^2\mathbf{B}^2}{4a_0^3 m_e c^2} \int_0^\infty r^4 e^{-2r/a_0} dr \int_0^\pi \sin^3\theta d\theta \\ &= -\frac{e^2\mathbf{B}^2}{4a_0^3 m_e c^2} \frac{4!}{(2/a_0)^{4+1}} \left(u - \frac{u^3}{3} \right)\Big|_1^{-1} \\ &= \frac{e^2 a_0^2 \mathbf{B}^2}{4m_e c^2}. \end{aligned} \tag{6.264}$$

If this energy shift is written in terms of a diamagnetic susceptibility χ defined by

$$\Delta = -\frac{1}{2}\chi\mathbf{B}^2, \tag{6.265}$$

the diamagnetic susceptibility is

$$\chi = -\frac{e^2 a_0^2}{2m_e c^2}. \tag{6.266}$$

Part II

APPENDICES

A

USEFUL FORMULAS AND REVIEW

Trig

$$1 + \cos x = 2\cos^2\frac{x}{2} \tag{A.1}$$

$$1 - \cos x = 2\sin^2\frac{x}{2} \tag{A.2}$$

$$\sin x = 2\sin\frac{x}{2}\cos\frac{x}{2} \tag{A.3}$$

$$2\cos a\cos b = \cos(a+b) + \cos(a-b) \tag{A.4}$$

$$2\sin a\sin b = \cos(a-b) - \cos(a-b) \tag{A.5}$$

$$2\cos a\sin b = \sin(a+b) - \sin(a-b) \tag{A.6}$$

$$2\sin a\cos b = \sin(a-b) + \sin(a+b) \tag{A.7}$$

$$\cos(a \pm b) = \cos a\cos b \mp \sin a\sin b \tag{A.8}$$

$$\sin(a \pm b) = \sin a\cos b \pm \cos a\sin b \tag{A.9}$$

Basics

$$\langle x|p\rangle \propto e^{ipx/\hbar} \tag{A.10}$$

$$|\Psi(t)\rangle = U\,|\Psi(0)\rangle \tag{A.11}$$

$$U = e^{-iHt/\hbar}, \qquad \text{for time independent } H \tag{A.12}$$

$$p = -i\hbar\frac{\partial}{\partial x} \tag{A.13}$$

$$x = i\hbar \frac{\partial}{\partial p} \tag{A.14}$$

$$H = i\hbar \frac{\partial}{\partial t} \tag{A.15}$$

$$A \sim (\langle a_{\text{row}} | A | a_{\text{column}} \rangle) \tag{A.16}$$

$$\begin{aligned} \rho &= \psi^* \psi \\ \mathbf{j} &= \frac{\hbar}{m} \operatorname{Im} \left(\psi^* \boldsymbol{\nabla} \psi \right) = -\frac{i\hbar}{2m} \left(\psi^* \boldsymbol{\nabla} \psi - \psi \boldsymbol{\nabla} \psi^* \right) \end{aligned} \tag{A.17}$$

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{j} = 0 \tag{A.18}$$

Commutators

$$[x, p] = i\hbar \tag{A.19}$$

$$\begin{aligned} \left[x_j, F(\mathbf{p}) \right] &= i\hbar \frac{\partial F}{\partial p_j} \\ \left[p_j, G(\mathbf{x}) \right] &= -i\hbar \frac{\partial G}{\partial x_j} \end{aligned} \tag{A.20}$$

$$e^{A\mu} B e^{-A\mu} = B + \mu [A, B] + \frac{\mu^2}{2!} [A, [A, B]] + \cdots \tag{A.21}$$

$$[A, B]_{\text{classical}} = \frac{\partial A}{\partial q} \frac{\partial B}{\partial p} - \frac{\partial A}{\partial p} \frac{\partial B}{\partial q} \tag{A.22}$$

Heisenberg picture

$$A_{\mathrm{H}} = U^\dagger A U \tag{A.23}$$

$$\frac{dA_{\mathrm{H}}}{dt} = \frac{1}{i\hbar} [A_{\mathrm{H}}, H] \tag{A.24}$$

$$\frac{d}{dt} \langle \mathbf{x} \cdot \mathbf{p} \rangle = \left\langle \frac{\mathbf{p}^2}{m} \right\rangle - \langle \mathbf{x} \cdot \boldsymbol{\nabla} V \rangle \tag{A.25}$$

Density operator

$$\rho = \sum_i w_i \left|\alpha^i\right\rangle \left\langle\alpha^i\right|, \qquad \sum_i w_i = 1. \tag{A.26}$$

$$[A] = \sum_i w_i \left\langle\alpha^i\right| A \left|\alpha^i\right\rangle = \mathrm{tr}(\rho A). \tag{A.27}$$

$$S = -\,\mathrm{tr}(\rho \ln \rho) = -\,\mathrm{tr}(\rho_{kk} \ln \rho_{kk}) \tag{A.28}$$

$$\begin{aligned}
|\psi_{mn}\rangle &= |a_m\rangle_1 \otimes |a_n\rangle \\
|\psi\rangle &= \sum_{mn} c_{mn} |\psi_{mn}\rangle \\
\rho &= |\psi\rangle \langle\psi| \\
\mathrm{tr}_2(\rho) = \rho_2 &= \sum_a {}_2\langle a|\rho\, |a\rangle_2 \\
\sum_a {}_1\langle a|\, \mathrm{tr}_2(\rho)\, |a\rangle_1 &= \sum_n |c_{mn}|^2
\end{aligned} \tag{A.29}$$

Pauli matrices

$$\begin{aligned}
\sigma_x &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\
\sigma_y &= \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \\
\sigma_z &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}
\end{aligned} \tag{A.30}$$

$$\left[\sigma_a, \sigma_b\right] = 2i\epsilon_{abc}\sigma_c \tag{A.31}$$

$$|S_x; \pm\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm 1 \end{bmatrix} \tag{A.32a}$$

$$\left|S_y; \pm\right\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm i \end{bmatrix} \tag{A.32b}$$

$$|S_z;\pm\rangle = \begin{bmatrix}1\\0\end{bmatrix}, \begin{bmatrix}0\\1\end{bmatrix} \tag{A.32c}$$

For $\hat{\mathbf{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, the eigenkets of $\mathbf{S}\cdot\hat{\mathbf{n}}$ are

$$|\hat{\mathbf{n}};+\rangle = \begin{bmatrix}\cos(\theta/2)\,e^{-i\phi/2}\\ \sin(\theta/2)\,e^{i\phi/2}\end{bmatrix} = e^{-i\sigma_z\phi/2}e^{-i\sigma_y\theta/2}\,|\hat{\mathbf{z}};+\rangle \tag{A.33}$$

$$|\hat{\mathbf{n}};-\rangle = \begin{bmatrix}-\sin(\theta/2)\,e^{-i\phi/2}\\ \cos(\theta/2)\,e^{i\phi/2}\end{bmatrix} = e^{-i\sigma_z\phi/2}e^{-i\sigma_y(\theta+\pi)/2}\,|\hat{\mathbf{z}};+\rangle \tag{A.34}$$

$$H = -\frac{e}{mc}\mathbf{S}\cdot\mathbf{B} = -\frac{eB}{mc}S_z \tag{A.35}$$

Harmonic oscillator

$$x_0^2 = \frac{\hbar}{m\omega} \tag{A.36}$$

$$p_0^2 = m\omega\hbar \tag{A.37}$$

$$x(t) = \frac{x_0}{\sqrt{2}}\left(ae^{-i\omega t} + a^\dagger e^{i\omega t}\right) \tag{A.38}$$

$$p(t) = \frac{i\hbar}{\sqrt{2}x_0}\left(a^\dagger e^{i\omega t} - ae^{-i\omega t}\right) \tag{A.39}$$

$$a, a^\dagger = \frac{1}{\sqrt{2}x_0}\left(x \mp x_0^2\frac{d}{dx}\right) \tag{A.40}$$

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle \tag{A.41}$$

$$a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{A.42}$$

$$x(t) = x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t \tag{A.43}$$

$$p(t) = p(0)\cos\omega t - m\omega x(0)\sin\omega t \tag{A.44}$$

$$x(t)^2 = \frac{\hbar\omega}{2}\left(ae^{-i\omega t} + a^\dagger e^{i\omega t}\right)^2 \tag{A.45}$$

$$p(t)^2 = \frac{\hbar\omega}{2}\left(ae^{-i\omega t} - a^\dagger e^{i\omega t}\right)\left(a^\dagger e^{i\omega t} - ae^{-i\omega t}\right) \tag{A.46}$$

$$N = a^\dagger a \tag{A.47}$$

$$N|n\rangle = n|n\rangle \tag{A.48}$$

$$[N, a] = -a \tag{A.49}$$

$$\left[N, a^\dagger\right] = a^\dagger \tag{A.50}$$

$$H = \hbar\omega\left(N + \frac{1}{2}\right) \tag{A.51}$$

$$\left[a, a^\dagger\right] = 1 \tag{A.52}$$

$$a = \frac{1}{x_0\sqrt{2}}\left(x + \frac{ip}{m\omega}\right) \tag{A.53}$$

$$\langle x|n\rangle = \frac{1}{\pi^{1/4}\sqrt{2^n n!}} x_0^{-(n+1/2)}\left(x - x_0^2\frac{d}{dx}\right)^n e^{-(x/x_0)^2/2} \tag{A.54}$$

$$|n\rangle = \frac{\left(a^\dagger\right)^n}{\sqrt{n!}}|0\rangle \tag{A.55}$$

Coherent states

$$a\,|z\rangle = z\,|z\rangle \tag{A.56}$$

$$|z\rangle = e^{-|z|^2/2 + z a^\dagger}\,|0\rangle \tag{A.57}$$

$$\langle z|\, a a^\dagger \,|z\rangle = \langle z|\, 1 + a^\dagger a \,|z\rangle \tag{A.58}$$

$$\begin{aligned} \langle x\rangle(0) &= x_0 \equiv \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}\, z = \sqrt{\frac{\hbar}{2m\omega}}\,(z + z^*) \\ \langle p\rangle(0) &= p_0 \equiv \sqrt{2m\hbar\omega}\,\mathrm{Im}\, z = -i\sqrt{\frac{m\hbar\omega}{2}}\,(z - z^*)\,. \end{aligned} \tag{A.59}$$

Electromagnetism

$$(\mathbf{A}', \phi') = (\mathbf{A} + \boldsymbol{\nabla}\chi, \phi - \partial_t \chi) \tag{A.60}$$

$$\begin{aligned} \mathbf{E} &= -\frac{\partial \mathbf{A}}{\partial t} - \boldsymbol{\nabla}\phi \\ \mathbf{B} &= \boldsymbol{\nabla} \times \mathbf{A} \end{aligned} \tag{A.61}$$

$$\mathbf{A} = \begin{cases} \frac{B\rho_a^2}{2\rho}\hat{\boldsymbol{\phi}} & \text{if } \rho \geq \rho_a \implies \mathbf{B} = 0 \\ \frac{B\rho}{2}\hat{\boldsymbol{\phi}} & \text{if } \rho < \rho_a \implies \mathbf{B} = B\hat{\mathbf{z}} \end{cases} \tag{A.62}$$

$$\Phi \equiv \oint \mathbf{A} \cdot d\mathbf{l} \tag{A.63}$$

Aharonov-Bohm and Magnetic fields

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right) + q\phi \tag{A.64}$$

$$\begin{aligned}
\mathbf{\Pi} &= \mathbf{p} - \frac{e}{c}\mathbf{A} \\
[\Pi_x, \Pi_y] &= \frac{ie\hbar}{c} B_z \\
H &= \frac{1}{2m}\mathbf{\Pi}^2 = \hbar\omega\left(b^\dagger b + \frac{1}{2}\right) \\
\omega &= \frac{eB_0}{mc} \\
b &= \frac{1}{\sqrt{2m\omega\hbar}}\left(\Pi_x + i\Pi_y\right)
\end{aligned} \tag{A.65}$$

$$\mathbf{A} = \frac{B_0}{2}\left(-y, x, 0\right), \mathbf{A} = B_0\left(0, x, 0\right) \implies \mathbf{B} = B_0\hat{\mathbf{z}} \tag{A.66}$$

Dirac equation

$$H = \begin{bmatrix} \hat{p}c + V & mc^2 \\ mc^2 & -\hat{p}c + V \end{bmatrix} = \hat{p}c\sigma_z + mc^2\sigma_x + V \tag{A.67}$$

$$\begin{aligned}
\psi &= e^{\pm ikx - iEt/\hbar} \\
|+k; \pm\epsilon\rangle &= \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}, \begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix} \\
|-k; \pm\epsilon\rangle &= \begin{bmatrix} \sin\theta \\ \cos\theta \end{bmatrix}, \begin{bmatrix} -\cos\theta \\ \sin\theta \end{bmatrix} \\
\tan(2\theta) &= mc/\hbar|k| \\
\epsilon^2 &= \left(mc^2\right)^2 + (\hbar kc)^2
\end{aligned} \tag{A.68}$$

$$\begin{aligned}
\psi &= e^{\mp kx - iEt/\hbar} \\
|\pm\rangle &= \frac{1}{\sqrt{2}}\begin{bmatrix} \pm e^{\pm i\phi/2} \\ e^{\mp i\phi/2} \end{bmatrix} \\
\epsilon^2 &= \left(mc^2\right)^2 - (\hbar kc)^2 \\
e^{i\phi} &= \frac{\epsilon \pm ik\hbar c}{mc^2}
\end{aligned} \tag{A.69}$$

$$j = c\Psi^\dagger\sigma_z\Psi \tag{A.70}$$

Generators

$$T_{\mathbf{a}} = e^{-i\mathbf{p}\cdot\mathbf{a}/\hbar} \tag{A.71}$$

$$T_{\tilde{\mathbf{p}}} = e^{i\tilde{\mathbf{p}}\cdot\mathbf{x}/\hbar} \tag{A.72}$$

$$\mathcal{D}(\hat{\mathbf{n}}, \phi) = \exp\left(-i\mathbf{J}\cdot\hat{\mathbf{n}}\phi/\hbar\right) \tag{A.73}$$

Calculus

$$\nabla^2\psi = \frac{1}{\rho}\partial_\rho\left(\rho\partial_\rho\psi\right) + \frac{1}{\rho^2}\partial_{\phi\phi}\psi + \partial_{zz}\psi \tag{A.74}$$

$$\nabla^2\psi = \frac{1}{r^2}\partial_r\left(r^2\partial_r\psi\right) + \frac{1}{r^2\sin\theta}\partial_\theta\left(\sin\theta\partial_\theta\psi\right) + \frac{1}{r^2\sin^2\theta}\partial_{\phi\phi} \tag{A.75}$$

$$\int_{-\infty}^{\infty}\exp(ax^2)dx = \sqrt{\frac{-\pi}{a}} \tag{A.76}$$

$$\Gamma(t) = \int_0^\infty x^{t-1}e^{-x}dx = (t-1)! \tag{A.77}$$

$$\int_0^\infty e^{-\alpha r}r^n dr = \frac{n!}{\alpha^{n+1}} \tag{A.78}$$

$$\lim_{N\to\infty}\left(1+\frac{x}{N}\right)^N = e^x \tag{A.79}$$

Symmetries

$$\begin{aligned}\pi^\dagger &= \pi \\ &= \pi^{-1}\end{aligned} \tag{A.80}$$

$$\pi^\dagger\mathbf{x}\pi = -\mathbf{x} \tag{A.81}$$

$$\pi^\dagger\mathbf{p}\pi = -\mathbf{p} \tag{A.82}$$

$$\pi |\mathbf{x}\rangle = |-\mathbf{x}\rangle \tag{A.83}$$

$$\langle \mathbf{x}| \pi |\psi\rangle = \langle -\mathbf{x}|\psi\rangle = \psi(-\mathbf{x}) \tag{A.84}$$

$$[\pi, \mathbf{J}] = 0 \tag{A.85}$$

$$\Theta H = H\Theta \tag{A.86}$$

$$\Theta \mathbf{p} \Theta^{-1} = -\mathbf{p} \tag{A.87}$$

$$\Theta \mathbf{J} \Theta^{-1} = -\mathbf{J} \tag{A.88}$$

$$\Theta \mathbf{x} \Theta^{-1} = \mathbf{x} \tag{A.89}$$

$$\langle \mathbf{x}| \Theta |\alpha\rangle = \langle \alpha|\mathbf{x}\rangle \tag{A.90}$$

$$\Theta |j, m\rangle = i^{2m} |j, -m\rangle \tag{A.91}$$

$$\Theta^2 = (-1)^{2j} \tag{A.92}$$

$$\begin{aligned} &\Theta = -i\sigma_y \eta K, \qquad \eta = i \\ &Ki = -i \\ &\Theta |\hat{\mathbf{n}}; +\rangle = \eta |\hat{\mathbf{n}}; -\rangle \\ &\Theta |\hat{\mathbf{n}}; -\rangle = -\eta |\hat{\mathbf{n}}; +\rangle \end{aligned} \tag{A.93}$$

Spin

$$\left[J_x, J_y\right] = i\hbar J_z \tag{A.94}$$

$$[J_r, J_s] = i\hbar \epsilon_{rst} J_t \tag{A.95}$$

$$\left[\mathbf{J}^2, J_\pm\right] = 0 \tag{A.96}$$

$$[J_z, J_\pm] = \pm\hbar J_\pm \tag{A.97}$$

$$[J_+, J_-] = 2\hbar J_z \tag{A.98}$$

$$\begin{aligned} \mathbf{J} &= \mathbf{L} \otimes 1 + 1 \otimes \mathbf{S} \\ &= \mathbf{L} + \mathbf{S} \end{aligned} \tag{A.99}$$

$$J_z |j, m\rangle = m\hbar |j, m\rangle \tag{A.100}$$

$$\mathbf{J}^2 |j, m\rangle = j(j+1)\hbar^2 |j, m\rangle \tag{A.101}$$

$$J_\pm |j, m\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}\, |j, m\rangle \tag{A.102}$$

$$\mathcal{D}(R) = \exp(-i\mathbf{L} \cdot \hat{\mathbf{n}}\phi/\hbar) \otimes \exp(-i\mathbf{S} \cdot \hat{\mathbf{n}}\phi/\hbar) \tag{A.103}$$

Spin one representation

$$J_x = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{A.104}$$

$$J_y = \frac{\hbar i}{\sqrt{2}} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \tag{A.105}$$

$$J_z = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \tag{A.106}$$

Angular momentum

$$\begin{aligned} \mathbf{L}^2 &= L_z^2 + \frac{1}{2}\left(L_+L_- + L_-L_+\right) \\ &= -\hbar^2 \left(\frac{1}{\sin^2\theta} \partial_{\phi\phi} + \frac{1}{\sin\theta} \partial_\theta \left(\sin\theta\partial_\theta\right) \right) \\ &= \mathbf{x}^2\mathbf{p}^2 - (\mathbf{x}\cdot\mathbf{p})^2 + i\hbar\mathbf{x}\cdot\mathbf{p} \\ &= r^2\mathbf{p}^2 + \hbar^2\left(r^2\partial_{rr} + 2r\partial_r\right) \end{aligned} \tag{A.107}$$

$$\begin{aligned} L_x &= -i\hbar\left(-\sin\phi\partial_\theta - \cot\theta\cos\phi\partial_\phi\right) \\ L_y &= -i\hbar\left(\cos\phi\partial_\theta - \cot\theta\sin\phi\partial_\phi\right) \\ L_z &= -i\hbar\partial_\phi \end{aligned} \tag{A.108}$$

$$\left[L_x, L_y\right] = i\hbar L_z \tag{A.109}$$

$$\{L_+, L_-\} = 2(L_x^2 + L_y^2) = 2(\mathbf{L}^2 - L_z^2) \tag{A.110}$$

$$L_\pm = -i\hbar e^{\pm i\phi}\left(\pm i\partial_\theta - \cot\theta\partial_\phi\right) = L_x \pm iL_y \tag{A.111}$$

$$L_{\pm}\,|l,m\rangle = \hbar\sqrt{(l \mp m)(l \pm m + 1)}\,|l, m \pm 1\rangle \tag{A.112}$$

$$\mathbf{L}^2\,|l,m\rangle = l(l+1)\,\hbar^2\,|l,m\rangle \tag{A.113}$$

$$L_z\,|l,m\rangle = m\,\hbar\,|l,m\rangle \tag{A.114}$$

Spherical harmonics

$$\begin{aligned}
Y_{00} &= \frac{1}{2\sqrt{\pi}} \\
Y_{10} &= \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos(\theta) \\
Y_{20} &= \frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3\cos^2(\theta) - 1\right) \\
Y_{30} &= \frac{1}{4}\sqrt{\frac{7}{\pi}}\left(5\cos^3(\theta) - 3\cos(\theta)\right) \\
Y_{40} &= \frac{3\left((35\cos^4(\theta) - 30\cos^2(\theta) + 3\right)}{16\sqrt{\pi}} \\
Y_{50} &= \frac{1}{16}\sqrt{\frac{11}{\pi}}\left(63\cos^5(\theta) - 70\cos^3(\theta) + 15\cos(\theta)\right) \\
Y_{60} &= \frac{1}{32}\sqrt{\frac{13}{\pi}}\left(231\cos^6(\theta) - 315\cos^4(\theta) + 105\cos^2(\theta) - 5\right) \\
Y_{70} &= \frac{1}{32}\sqrt{\frac{15}{\pi}}\left(429\cos^7(\theta) - 693\cos^5(\theta) + 315\cos^3(\theta) - 35\cos(\theta)\right) \\
Y_{80} &= \frac{1}{256}\sqrt{\frac{17}{\pi}}\left(6435\cos^8(\theta) - 12012\cos^6(\theta) + 6930\cos^4(\theta) - 1260\cos^2(\theta) + 35\right)
\end{aligned} \tag{A.115}$$

$$Y_{l,-m} = (-1)^m Y^*_{lm} \tag{A.116}$$

FIXME: complete this table.

Hydrogen wavefunctions From [14], with the a_0 factors added in.

$$\psi_{1s} = \psi_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0} \tag{A.117a}$$

$$\psi_{2s} = \psi_{200} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{rZ}{a_0}\right) e^{-Zr/2a_0} \tag{A.117b}$$

$$\psi_{2p_x} = \frac{1}{\sqrt{2}} \left(\psi_{2,1,-1} - \psi_{2,1,1}\right) = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{rZ}{a_0} e^{-rZ/2a_0} \sin\theta\cos\phi \tag{A.117c}$$

$$\psi_{2p_y} = \frac{i}{\sqrt{2}} \left(\psi_{2,1,-1} + \psi_{2,1,1}\right) = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{rZ}{a_0} e^{-rZ/2a_0} \sin\theta\sin\phi \tag{A.117d}$$

$$\psi_{2p_z} = \psi_{210} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{rZ}{a_0} e^{-rZ/2a_0} \cos\theta. \tag{A.117e}$$

I looked to [7] to see where to add in the a_0 factors.
Energy levels are n dependent only

$$E_n = -\frac{Z^2 e^2}{2n^2 a_0}. \tag{A.118}$$

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \tag{A.119}$$

Perturbation

$$H = H_0 + \lambda V \tag{A.120a}$$

$$|n\rangle = \sum_{j=0} \lambda^j \left|n_j\right\rangle \tag{A.120b}$$

$$\Delta_n = \sum_{j=1} \lambda^j \Delta_{n_j} \tag{A.120c}$$

$$\bar{P}_n = \sum_{m \neq n} |m\rangle \langle m| \tag{A.120d}$$

$$\begin{aligned}
|n_0\rangle &= \left|n^{(0)}\right\rangle \\
|n_1\rangle &= \frac{\bar{P}_n}{E_n^{(0)} - H_0} V |n_0\rangle \\
|n_2\rangle &= \frac{\bar{P}_n}{E_n^{(0)} - H_0} \left(V - \Delta_{n_1}\right) |n_1\rangle \\
|n_3\rangle &= \frac{\bar{P}_n}{E_n^{(0)} - H_0} \left(V |n_2\rangle - \Delta_{n_1} |n_2\rangle - \Delta_{n_2} |n_1\rangle\right) \\
\left|n_j\right\rangle &= \frac{\bar{P}_n}{E_n^{(0)} - H_0} \left(V \left|n_{j-1}\right\rangle - \sum_{k=1}^{j-1} \Delta_{n_k} \left|n_{j-k}\right\rangle\right)
\end{aligned} \tag{A.121}$$

$$\Delta_{n_j} = \langle n_0| V \left|n_{j-1}\right\rangle \tag{A.122}$$

$$f(|x|) = \Theta(x) f(x) + \Theta(-x) f(-x) \tag{A.123}$$

$$\frac{d}{dx}\delta(x) = -\frac{\delta(x)}{x} \tag{A.124}$$

Clebsch Ex. $l_1 = 2,\ l_2 = 1$

$$\begin{aligned}
|3,3\rangle &= |2,2\rangle \otimes |1,1\rangle \\
|3,2\rangle &= \frac{1}{\langle 3,2| L_- |3,3\rangle} \left((L_- |2,2\rangle) \otimes |1,1\rangle + |2,2\rangle \otimes L_- |1,1\rangle\right) \\
|2,2\rangle &: a|1\rangle + b|2\rangle \rightarrow -b|1\rangle + a|2\rangle \\
|1,1\rangle &= |3,1\rangle \times |2,1\rangle
\end{aligned} \tag{A.125}$$

B

ODDS AND ENDS

B.1 SCHWARTZ INEQUALITY IN BRA-KET NOTATION

Motivation In [11] the Schwartz inequality

$$\boxed{\langle a|a\rangle \langle b|b\rangle \ge |\langle a|b\rangle|^2,} \tag{B.1}$$

is used in the derivation of the uncertainty relation. The proof of the Schwartz inequality uses a sneaky substitution that doesn't seem obvious, and is even less obvious since there is a typo in the value to be substituted. Let's understand where that sneakiness is coming from.

Without being sneaky My ancient first year linear algebra text [8] contains a non-sneaky proof, but it only works for real vector spaces. Recast in bra-ket notation, this method examines the bounds of the norms of sums and differences of unit state vectors (i.e. $\langle a|a\rangle = \langle b|b\rangle = 1$.)

$$\langle a - b|a - b\rangle = \langle a|a\rangle + \langle b|b\rangle - \langle a|b\rangle - \langle b|a\rangle = 2 - 2\,\mathrm{Re}\,\langle a|b\rangle \ge 0, \tag{B.2}$$

so

$$1 \ge \mathrm{Re}\,\langle a|b\rangle\,. \tag{B.3}$$

Similarly

$$\langle a + b|a + b\rangle = \langle a|a\rangle + \langle b|b\rangle + \langle a|b\rangle + \langle b|a\rangle = 2 + 2\,\mathrm{Re}\,\langle a|b\rangle \ge 0, \tag{B.4}$$

so

$$\mathrm{Re}\,\langle a|b\rangle \ge -1. \tag{B.5}$$

This means that for normalized state vectors

$$-1 \le \mathrm{Re}\,\langle a|b\rangle \le 1, \tag{B.6}$$

or

$$|\mathrm{Re}\,\langle a|b\rangle| \le 1. \tag{B.7}$$

Writing out the unit vectors explicitly, that last inequality is

$$\left|\operatorname{Re}\left\langle \frac{a}{\sqrt{\langle a|a\rangle}} \middle| \frac{b}{\sqrt{\langle b|b\rangle}} \right\rangle\right| \le 1, \tag{B.8}$$

squaring and rearranging gives

$$|\operatorname{Re}\langle a|b\rangle|^2 \le \langle a|a\rangle \langle b|b\rangle . \tag{B.9}$$

This is similar to, but not identical to the Schwartz inequality. Since $|\operatorname{Re}\langle a|b\rangle| \le |\langle a|b\rangle|$ the Schwartz inequality cannot be demonstrated with this argument. This first year algebra method works nicely for demonstrating the inequality for real vector spaces, so a different argument is required for a complex vector space (i.e. quantum mechanics state space.)

Arguing with projected and rejected components Notice that the equality condition holds when the vectors are colinear, and the largest inequality ($0 \le 1$) holds when the vectors are normal to each other. Given those geometrical observations, it seems reasonable to examine the norms of projected or rejected components of a vector. To do so in bra-ket notation, the correct form of a projection operation must be determined. Care is required to get the ordering of the bra-kets right when expressing such a projection (or rejection)

Suppose we wish to calculation the rejection of $|a\rangle$ from $|b\rangle$, that is $|b - \alpha a\rangle$, such that

$$\begin{aligned} 0 &= \langle a|b - \alpha a\rangle \\ &= \langle a|b\rangle - \alpha \langle a|a\rangle , \end{aligned} \tag{B.10}$$

or

$$\alpha = \frac{\langle a|b\rangle}{\langle a|a\rangle}. \tag{B.11}$$

Therefore, the projection of $|b\rangle$ on $|a\rangle$ is

$$\mathrm{Proj}_{|a\rangle} |b\rangle = \frac{\langle a|b\rangle}{\langle a|a\rangle} |a\rangle = \frac{\langle b|a\rangle^*}{\langle a|a\rangle} |a\rangle . \tag{B.12}$$

The conventional way to write this in QM is in the operator form

$$\mathrm{Proj}_{|a\rangle} |b\rangle = \frac{|a\rangle \langle a|}{\langle a|a\rangle} |b\rangle . \tag{B.13}$$

In this form the rejection of $|a\rangle$ from $|b\rangle$ can be expressed as

$$\mathrm{Rej}_{|a\rangle} |b\rangle = |b\rangle - \frac{|a\rangle \langle a|}{\langle a|a\rangle} |b\rangle . \tag{B.14}$$

This state vector is normal to $|a\rangle$ as desired

$$\left\langle a \middle| b - \frac{\langle a|b\rangle}{\langle a|a\rangle} a \right\rangle = \langle a|b\rangle - \frac{\langle a|b\rangle}{\cancel{\langle a|a\rangle}} \cancel{\langle a|a\rangle} = 0. \tag{B.15}$$

How about it's length? That is

$$\begin{aligned} \left\langle b - \frac{\langle a|b\rangle}{\langle a|a\rangle} a \middle| b - \frac{\langle a|b\rangle}{\langle a|a\rangle} a \right\rangle &= \langle b|b\rangle - 2\frac{|\langle a|b\rangle|^2}{\langle a|a\rangle} + \frac{|\langle a|b\rangle|^2}{\langle a|a\rangle^2} \langle a|a\rangle \\ &= \langle b|b\rangle - \frac{|\langle a|b\rangle|^2}{\langle a|a\rangle}. \end{aligned} \tag{B.16}$$

Observe that this must be greater to or equal to zero, so

$$\langle b|b\rangle \geq \frac{|\langle a|b\rangle|^2}{\langle a|a\rangle}. \tag{B.17}$$

Rearranging this gives eq. (B.1) as desired. The Schwartz proof in [11] obscures the geometry involved and starts with

$$\langle b + \lambda a|b + \lambda a\rangle \geq 0, \tag{B.18}$$

where the "proof" is nothing more than a statement that one can "pick" $\lambda = -\langle b|a\rangle / \langle a|a\rangle$. The Pythagorean context of the Schwartz inequality is not mentioned, and without thinking about it, one is left wondering what sort of magic hat that λ selection came from.

B.2 AN OBSERVATION ABOUT THE GEOMETRY OF PAULI X,Y MATRICES

Motivation The conventional form for the Pauli matrices is

$$\begin{aligned} \sigma_x &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \sigma_y &= \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \\ \sigma_z &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \end{aligned}. \tag{B.19}$$

In [2] these forms are derived based on the commutation relations

$$[\sigma_r, \sigma_s] = 2i\epsilon_{rst}\sigma_t, \tag{B.20}$$

by defining raising and lowering operators $\sigma_\pm = \sigma_x \pm i\sigma_y$ and figuring out what form the matrix must take. I noticed an interesting geometrical relation hiding in that derivation if σ_+ is not assumed to be real.

Derivation For completeness, I'll repeat the argument of [2], which builds on the commutation relations of the raising and lowering operators. Those are

$$\begin{aligned}[\sigma_z, \sigma_\pm] &= \sigma_z \left(\sigma_x \pm i\sigma_y\right) - \left(\sigma_x \pm i\sigma_y\right)\sigma_z \\ &= [\sigma_z, \sigma_x] \pm i\left[\sigma_z, \sigma_y\right] \\ &= 2i\sigma_y \pm i(-2i)\sigma_x \\ &= \pm 2\left(\sigma_x \pm i\sigma_y\right) \\ &= \pm 2\sigma_\pm,\end{aligned} \tag{B.21}$$

and

$$\begin{aligned}[\sigma_+, \sigma_-] &= \left(\sigma_x + i\sigma_y\right)\left(\sigma_x - i\sigma_y\right) - \left(\sigma_x - i\sigma_y\right)\left(\sigma_x + i\sigma_y\right) \\ &= -i\sigma_x\sigma_y + i\sigma_y\sigma_x - i\sigma_x\sigma_y + i\sigma_y\sigma_x \\ &= 2i\left[\sigma_y, \sigma_x\right] \\ &= 2i(-2i)\sigma_z \\ &= 4\sigma_z\end{aligned} \tag{B.22}$$

From these a matrix representation containing unknown values can be assumed. Let

$$\sigma_+ = \begin{bmatrix} a & b \\ c & d \end{bmatrix}. \tag{B.23}$$

The commutator with σ_z can be computed

$$\begin{aligned}[\sigma_z, \sigma_+] &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} a & b \\ c & d \end{bmatrix} - \begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ &= \begin{bmatrix} a & b \\ -c & -d \end{bmatrix} - \begin{bmatrix} a & -b \\ c & -d \end{bmatrix} \\ &= 2\begin{bmatrix} 0 & b \\ -c & 0 \end{bmatrix}\end{aligned} \tag{B.24}$$

Now compare this with eq. (B.21)

$$\begin{aligned}2\begin{bmatrix} 0 & b \\ -c & 0 \end{bmatrix} &= 2\sigma_+ \\ &= 2\begin{bmatrix} a & b \\ d & d \end{bmatrix}.\end{aligned} \tag{B.25}$$

This shows that $a = 0$, and $d = 0$. Similarly the σ_z commutator with the lowering operator is

$$\begin{aligned}
[\sigma_z, \sigma_-] &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & -c^* \\ b^* & 0 \end{bmatrix} - \begin{bmatrix} 0 & -c^* \\ b^* & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\
&= \begin{bmatrix} 0 & -c^* \\ -b^* & 0 \end{bmatrix} - \begin{bmatrix} 0 & c^* \\ b^* & 0 \end{bmatrix} \\
&= -2 \begin{bmatrix} 0 & c^* \\ b^* & 0 \end{bmatrix}
\end{aligned} \tag{B.26}$$

Again comparing to eq. (B.21), we have

$$\begin{aligned}
-2 \begin{bmatrix} 0 & c^* \\ b^* & 0 \end{bmatrix} &= -2\sigma_- \\
&= -2 \begin{bmatrix} 0 & -c^* \\ b^* & 0 \end{bmatrix},
\end{aligned} \tag{B.27}$$

so $c = 0$. Computing the commutator of the raising and lowering operators fixes b

$$\begin{aligned}
[\sigma_+, \sigma_-] &= \begin{bmatrix} 0 & b \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ b^* & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ b^* & 0 \end{bmatrix} \begin{bmatrix} 0 & b \\ 0 & 0 \end{bmatrix} \\
&= \begin{bmatrix} |b|^2 & 0 \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 00 & -|b|^2 \end{bmatrix} \\
&= |b|^2 \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\
&= |b|^2 \sigma_z.
\end{aligned} \tag{B.28}$$

From eq. (B.22) it must be that $|b|^2 = 4$, so the most general form of the raising operator is

$$\sigma_+ = 2 \begin{bmatrix} 0 & e^{i\phi} \\ 0 & 0 \end{bmatrix}. \tag{B.29}$$

Observation The conventional choice is to set $\phi = 0$, but I found it interesting to see the form of σ_x, σ_y without that choice. That is

$$\begin{aligned}\sigma_x &= \frac{1}{2}(\sigma_+ + \sigma_-) \\ &= \begin{bmatrix} 0 & e^{i\phi} \\ e^{-i\phi} & 0 \end{bmatrix}\end{aligned} \tag{B.30}$$

$$\begin{aligned}\sigma_y &= \frac{1}{2i}(\sigma_+ - \sigma_-) \\ &= \begin{bmatrix} 0 & -ie^{i\phi} \\ -ie^{-i\phi} & 0 \end{bmatrix} \\ &= \begin{bmatrix} 0 & e^{i(\phi-\pi/2)} \\ e^{-i(\phi-\pi/2)} & 0 \end{bmatrix}.\end{aligned} \tag{B.31}$$

Notice that the Pauli matrices σ_x and σ_y actually both have the same form as σ_x, but the phase of the complex argument of each differs by 90°. That 90° separation isn't obvious in the standard form eq. (B.19).

It's a small detail, but I thought it was kind of cool that the orthogonality of these matrix unit vector representations is built directly into the structure of their matrix representations.

B.3 OPERATOR MATRIX ELEMENT

Weird dreams I woke up today having a dream still in my head from the night, but it was a strange one. I was expanding out the Dirac notation representation of an operator in matrix form, but the symbols in the kets were elaborate pictures of Disney princesses that I was drawing with forestry scenery in the background, including little bears. At the point that I woke up from the dream, I noticed that I'd gotten the proportion of the bears wrong in one of the pictures, and they looked like they were ready to eat one of the princess characters.

Guts As a side effect of this weird dream I actually started thinking about matrix element representation of operators.

When forming the matrix element of an operator using Dirac notation the elements are of the form $\langle \text{row}| A |\text{column}\rangle$. I've gotten that mixed up a couple of times, so I thought it would be helpful to write this out explicitly for a 2×2 operator representation for clarity.

To start, consider a change of basis for a single matrix element from basis $\{|q\rangle, |r\rangle\}$, to basis $\{|a\rangle, |b\rangle\}$

$$
\begin{aligned}
\langle q| A |r\rangle &= \langle q|a\rangle \langle a| A |r\rangle + \langle q|b\rangle \langle b| A |r\rangle \\
&= \langle q|a\rangle \langle a| A |a\rangle \langle a|r\rangle + \langle q|a\rangle \langle a| A |b\rangle \langle b|r\rangle \\
&+ \langle q|b\rangle \langle b| A |a\rangle \langle a|r\rangle + \langle q|b\rangle \langle b| A |b\rangle \langle b|r\rangle \\
&= \langle q|a\rangle \begin{bmatrix} \langle a| A |a\rangle & \langle a| A |b\rangle \end{bmatrix} \begin{bmatrix} \langle a|r\rangle \\ \langle b|r\rangle \end{bmatrix} + \langle q|b\rangle \begin{bmatrix} \langle b| A |a\rangle & \langle b| A |b\rangle \end{bmatrix} \begin{bmatrix} \langle a|r\rangle \\ \langle b|r\rangle \end{bmatrix} \\
&= \begin{bmatrix} \langle q|a\rangle & \langle q|b\rangle \end{bmatrix} \begin{bmatrix} \langle a| A |a\rangle & \langle a| A |b\rangle \\ \langle b| A |a\rangle & \langle b| A |b\rangle \end{bmatrix} \begin{bmatrix} \langle a|r\rangle \\ \langle b|r\rangle \end{bmatrix}.
\end{aligned}
\tag{B.32}
$$

Suppose the matrix representation of $|q\rangle$, $|r\rangle$ are respectively

$$
\begin{aligned}
|q\rangle &\sim \begin{bmatrix} \langle a|q\rangle \\ \langle b|q\rangle \end{bmatrix}, \\
|r\rangle &\sim \begin{bmatrix} \langle a|r\rangle \\ \langle b|r\rangle \end{bmatrix}
\end{aligned}
\tag{B.33}
$$

then

$$
\begin{aligned}
\langle q| &\sim \begin{bmatrix} \langle a|q\rangle \\ \langle b|q\rangle \end{bmatrix}^\dagger \\
&= \begin{bmatrix} \langle q|a\rangle & \langle q|b\rangle \end{bmatrix}.
\end{aligned}
\tag{B.34}
$$

The matrix element is then

$$
\langle q| A |r\rangle \sim \langle q| \begin{bmatrix} \langle a| A |a\rangle & \langle a| A |b\rangle \\ \langle b| A |a\rangle & \langle b| A |b\rangle \end{bmatrix} |r\rangle ,
\tag{B.35}
$$

and the corresponding matrix representation of the operator is

$$
A \sim \begin{bmatrix} \langle a| A |a\rangle & \langle a| A |b\rangle \\ \langle b| A |a\rangle & \langle b| A |b\rangle \end{bmatrix}.
\tag{B.36}
$$

B.4 GENERALIZED GAUSSIAN INTEGRALS

Both [11] and [16] use Gaussian integrals with both (negative) real, and imaginary arguments, which give the impression that the following is true:

$$
\int_{-\infty}^{\infty} \exp\left(ax^2\right) dx = \sqrt{\frac{-\pi}{a}},
\tag{B.37}
$$

even when a is not a real negative constant, and in particular, with values $a = \pm i$. Clearly this doesn't follow by just making a substitution $x \rightarrow x/\sqrt{a}$, since that moves the integration range onto a rotated path in the complex plane when a is $\pm i$. However, with some care, it can be shown that eq. (B.37) holds provided $\operatorname{Re} a \leq 0$.

To show this, this integral will be considered for the pure real case, purely imaginary, and finally the complex case with non-zero real and imaginary parts for a.

Real (negative) case. The first special case is $\int_{-\infty}^{\infty} \exp\left(-x^2\right) dx = \sqrt{\pi}$ which is easy to derive using the usual square it and integrate in circular coordinates trick.

Purely imaginary cases. Let's handle the $a = \pm i$ cases next. These can be evaluated by considering integrals over the contours of fig. B.1, where the upper plane contour is used for $a = i$ and the lower plane contour for $a = -i$.

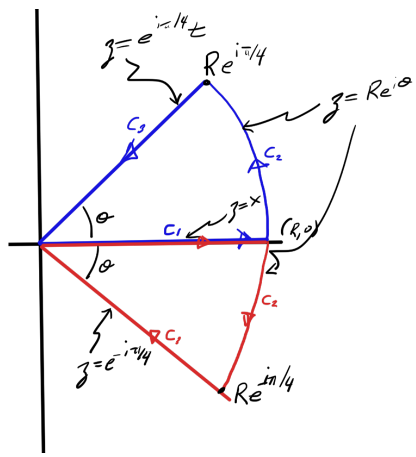

Figure B.1: Contours for $a = \pm i$.

Since there are no poles, the integral over either such contour is zero. Credit for figuring out how to tackle that integral and what contour to use goes to Dr MV, on stackexchange [6].

For the upper plane contour we have

$$
\begin{aligned}
0 &= \oint \exp\left(iz^2\right) dz \\
&= \int_0^R \exp\left(ix^2\right) dx + \int_0^{\pi/4} \exp\left(iR^2 e^{2i\theta}\right) Rie^{i\theta} d\theta + \int_R^0 \exp\left(i^2 t^2\right) e^{i\pi/4} dt.
\end{aligned}
\tag{B.38}
$$

Observe that $ie^{2i\theta} = i\cos(2\theta) - \sin(2\theta)$ which has a negative real part for all values of $\theta \neq 0$. Provided the contour is slightly deformed from the axis, that second integral has a term of the form $\sim Re^{-R^2}$ which tends to zero as $R \rightarrow \infty$. So in the limit, this is

$$\int_0^\infty \exp\left(ix^2\right) dx = \sqrt{\pi} e^{i\pi/4}/2, \tag{B.39}$$

or

$$\int_{-\infty}^\infty \exp\left(ix^2\right) dx = \sqrt{i\pi}, \tag{B.40}$$

a special case of eq. (B.37) as desired. For $a = -i$ integrating around the lower plane contour, we have

$$\begin{aligned} 0 &= \oint \exp\left(-iz^2\right) dz \\ &= \int_0^R \exp\left(ix^2\right) dx + \int_0^{-\pi/4} \exp\left(-iR^2 e^{2i\theta}\right) Rie^{i\theta} d\theta + \int_R^0 \exp\left(-i(-i)t^2\right) e^{-i\pi/4} dt. \end{aligned} \tag{B.41}$$

This time, in the second integral we also have $-iR^2 e^{2i\theta} = iR^2 \cos(2\theta) + \sin(2\theta)$, which also has a negative real part for $\theta \in (0, \pi/4]$. Again the contour needs to be infinitesimally deformed[1], placed just lower than the axis.

This time we find

$$\int_{-\infty}^\infty \exp\left(-ix^2\right) dx = \sqrt{-i\pi}, \tag{B.42}$$

another special case of eq. (B.37).

Completely complex case. A similar trick can be used to evaluate the more general cases, but a bit of thought is required to figure out the contours required. More precisely, while these contours will still have a wedge of pie shape, as sketched in fig. B.2, we have to figure out the angle subtended by the edge of this piece of pie.

To evaluate an integral consider

$$\begin{aligned} 0 &= \oint \exp\left(e^{i\phi} z^2\right) dz \\ &= \int_0^R \exp\left(e^{i\phi} x^2\right) dx + \int_0^\theta \exp\left(e^{i\phi} R^2 e^{2i\mu}\right) Rie^{i\mu} d\mu + \int_R^0 \exp\left(e^{i\phi} e^{2i\theta} t^2\right) e^{i\theta} dt, \end{aligned} \tag{B.43}$$

where $\phi \in (\pi/2, \pi) \cup (\pi, 3\pi/2)$. We have a hope of evaluating this last integral if $\phi + 2\theta = \pi$, or

$$\theta = (\pi - \phi)/2, \tag{B.44}$$

1 Distorting the contour in this fashion seems somewhat like handwaving. A better approach would probably follow [5] where Jordan's lemma is covered. It doesn't look like Jordan's lemma applies as is to this case, but the arguments look like they could be adapted appropriately.

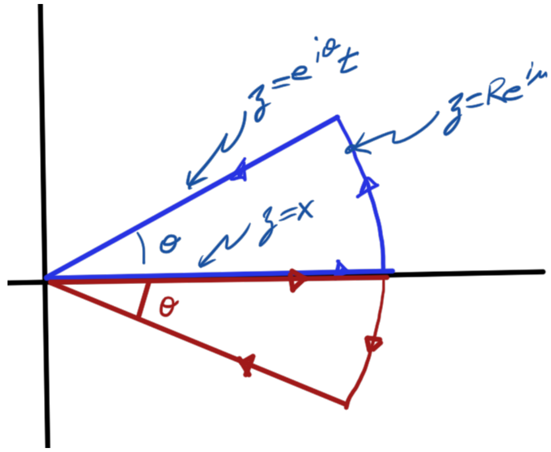

Figure B.2: Contours for complex a.

giving

$$\int_0^R \exp\left(e^{i\phi}x^2\right)dx = e^{i(\pi-\phi)/2}\int_0^R \exp\left(-t^2\right)dt - \int_0^\theta \exp\left(R^2\left(\cos\left(\phi+2\mu\right)+i\sin\left(\phi+2\mu\right)\right)\right)Rie^{i\mu}d\mu. \tag{B.45}$$

If the cosine is always negative on the chosen contours, then that integral will vanish in the $R \to \infty$ limit. This turns out to be the case, which can be confirmed by considering each of the contours in sequence. If the upper plane contour is used to evaluate eq. (B.43) for the $\phi \in (\pi/2, \pi)$ case, we have

$$\theta \in (0, \pi/4). \tag{B.46}$$

Since $\phi + 2\theta = \pi$, we have

$$\phi + 2\mu \in (\pi/2, \pi), \tag{B.47}$$

and find that the cosine is strictly negative on that contour for that range of ϕ. Picking the lower plane contour for the $\phi \in (\pi, 3\pi/2)$ range, we have

$$\theta \in (-\pi/4, 0), \tag{B.48}$$

and so

$$\phi + 2\mu \in (\pi/2, 3\pi/2). \tag{B.49}$$

For this range of ϕ the cosine on the lower plane contour is again negative as desired, so in the infinite R limit we have

$$\int_0^\infty \exp\left(e^{i\phi}x^2\right)dx = \frac{1}{2}\sqrt{-\pi e^{-i\phi}}. \tag{B.50}$$

The points at $\phi = \pi/2, \pi, 3\pi/2$ were omitted, but we've found the same result at those points, completing the verification of eq. (B.37) for all $\operatorname{Re} a \le 0$.

B.5 A CURIOUS PROOF OF THE BAKER-CAMPBELL-HAUSDORFF FORMULA

Equation (39) of [3] states the Baker-Campbell-Hausdorff formula for two operators a, b that commute with their commutator $\left[a, b\right]$

$$e^a e^b = e^{a+b+[a,b]/2}, \tag{B.51}$$

and provides the outline of an interesting method of proof. That method is to consider the derivative of

$$f(\lambda) = e^{\lambda a} e^{\lambda b} e^{-\lambda(a+b)}, \tag{B.52}$$

That derivative is

$$\begin{aligned}
\frac{df}{d\lambda} &= e^{\lambda a} a e^{\lambda b} e^{-\lambda(a+b)} + e^{\lambda a} b e^{\lambda b} e^{-\lambda(a+b)} - e^{\lambda a} b e^{\lambda b} (a+b) e^{-\lambda(a+b)} \\
&= e^{\lambda a} \left(a e^{\lambda b} + b e^{\lambda b} - e^{\lambda b} (a+b) \right) e^{-\lambda(a+b)} \\
&= e^{\lambda a} \left(\left[a, e^{\lambda b} \right] + \cancel{\left[b, e^{\lambda b} \right]} \right) e^{-\lambda(a+b)} \\
&= e^{\lambda a} \left[a, e^{\lambda b} \right] e^{-\lambda(a+b)}.
\end{aligned} \tag{B.53}$$

The commutator above is proportional to $\left[a, b\right]$

$$\begin{aligned}
\left[a, e^{\lambda b} \right] &= \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} \left[a, b^k \right] \\
&= \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} k b^{k-1} \left[a, b \right] \\
&= \lambda \sum_{k=1}^{\infty} \frac{\lambda^{k-1}}{(k-1)!} b^{k-1} \left[a, b \right] \\
&= \lambda e^{\lambda b} \left[a, b \right],
\end{aligned} \tag{B.54}$$

so

$$\frac{df}{d\lambda} = \lambda \left[a, b \right] f. \tag{B.55}$$

To get the above, we should also do the induction demonstration for $\left[a, b^k\right] = k b^{k-1} \left[a, b\right]$. This clearly holds for $k = 0, 1$. For any other k we have

$$
\begin{aligned}
\left[a, b^{k+1}\right] &= ab^{k+1} - b^{k+1}a \\
&= \left(\left[a, b^k\right] + b^k a\right) b - b^{k+1} a \\
&= kb^{k-1}\left[a, b\right] b + b^k \left(\left[a, b\right] + \cancel{ba}\right) - \cancel{b^{k+1}} a \\
&= kb^k \left[a, b\right] + b^k \left[a, b\right] \\
&= (k+1) b^k \left[a, b\right] \qquad \square
\end{aligned}
\tag{B.56}
$$

Observe that eq. (B.55) is solved by

$$
f = e^{\lambda^2 [a,b]/2},
\tag{B.57}
$$

which gives

$$
e^{\lambda^2 [a,b]/2} = e^{\lambda a} e^{\lambda b} e^{-\lambda(a+b)}.
\tag{B.58}
$$

Right multiplication by $e^{\lambda(a+b)}$ which commutes with $e^{\lambda^2 [a,b]/2}$ and setting $\lambda = 1$ recovers eq. (B.51) as desired.

What I wonder looking at this, is what thought process led to trying this in the first place? This is not what I would consider an obvious approach to demonstrating this identity.

B.6 POSITION OPERATOR IN MOMENTUM SPACE REPRESENTATION

A derivation of the position space representation of the momentum operator $-i\hbar\partial_x$ is made in [2], starting with the position-momentum commutator. Here I'll repeat that argument for the momentum space representation of the position operator.

What we want to do is expand the matrix element of the commutator. First using the definition of the commutator

$$
\begin{aligned}
\left\langle p' \middle| XP - PX \middle| p'' \right\rangle &= i\hbar \left\langle p' \middle| p'' \right\rangle \\
&= i\hbar \delta p' - p'',
\end{aligned}
\tag{B.59}
$$

and then by inserting an identity operation in a momentum space basis

$$
\begin{aligned}
\left\langle p' \middle| XP - PX \middle| p'' \right\rangle &= \int dp \left\langle p' \middle| X \middle| p \right\rangle \left\langle p \middle| P \middle| p'' \right\rangle - \int dp \left\langle p' \middle| P \middle| p \right\rangle \left\langle p \middle| X \middle| p'' \right\rangle \\
&= \int dp \left\langle p' \middle| X \middle| p \right\rangle p \delta(p - p'') - \int dp p \delta(p' - p) \left\langle p \middle| X \middle| p'' \right\rangle \\
&= \left\langle p' \middle| X \middle| p'' \right\rangle p'' - p' \left\langle p' \middle| X \middle| p'' \right\rangle.
\end{aligned}
\tag{B.60}
$$

So we have

$$\langle p' \big| X \big| p'' \rangle p'' - p' \langle p' \big| X \big| p'' \rangle = i\hbar\delta p' - p''. \tag{B.61}$$

Because the RHS is zero whenever $p' \neq p''$, the matrix element $\langle p' | X | p'' \rangle$ must also include a delta function. Let

$$\langle p' \big| X \big| p'' \rangle = \delta(p' - p'')X(p''). \tag{B.62}$$

Because eq. (B.61) is an operator equation that really only takes on meaning when applied to a wave function and integrated, we do that

$$\int dp''\delta(p' - p'')X(p'')p''\psi(p'') - \int dp'' p'\delta(p' - p'')X(p'')\psi(p'') = \int dp'' i\hbar\delta p' - p''\psi(p''), \tag{B.63}$$

or

$$i\hbar\psi(p') = X(p')p'\psi(p') - p'X(p')\psi(p'). \tag{B.64}$$

Provided $X(p')$ operates on everything to its right, this equation is solved by setting

$$\boxed{X(p') = i\hbar\frac{\partial}{\partial p'}.} \tag{B.65}$$

B.7 EXPANSION OF THE SQUARED ANGULAR MOMENTUM OPERATOR

In [11] eq. 6.16 is

$$\mathbf{L}^2 = \mathbf{x}^2\mathbf{p}^2 - (\mathbf{x}\cdot\mathbf{p})^2 + i\hbar\mathbf{x}\cdot\mathbf{p}, \tag{B.66}$$

and a derivation of the same. The derivation is clear right until the end, where the details for the last steps are left off. When I attempted those last steps I got a different sign for the $\mathbf{x}\cdot\mathbf{p}$ term. I also get that same difference in sign if I do this expansion myself:

$$\begin{aligned}
\mathbf{L}^2 &= \epsilon_{ijk}x_i p_j \epsilon_{rsk} x_r p_s \\
&= \delta_{ij}^{[rs]} x_i p_j x_r p_s \\
&= x_i p_j x_i p_j - x_i p_j x_j p_i \\
&= x_i \left(x_i p_j - i\hbar\delta_{ij}\right) p_j - x_i p_j \left(p_i x_j + i\hbar\delta_{ij}\right) \\
&= \mathbf{x}^2\mathbf{p}^2 - i\hbar\mathbf{x}\cdot\mathbf{p} - x_i p_j p_i x_j - i\hbar\mathbf{x}\cdot\mathbf{p} \\
&= \mathbf{x}^2\mathbf{p}^2 - 2i\hbar\mathbf{x}\cdot\mathbf{p} - x_i p_i p_j x_j \\
&= \mathbf{x}^2\mathbf{p}^2 - 2i\hbar\mathbf{x}\cdot\mathbf{p} - (\mathbf{x}\cdot\mathbf{p})\left(x_j p_j - i\hbar\right) \\
&= \mathbf{x}^2\mathbf{p}^2 - i\hbar\mathbf{x}\cdot\mathbf{p} - (\mathbf{x}\cdot\mathbf{p})^2.
\end{aligned} \tag{B.67}$$

I couldn't spot an error anywhere above, but Prof Paramekanti spotted it when I asked. The error is in the second last step above, since $p_j x_j = p_1 x_1 + p_2 x_2 + p_3 x_3$ and flipping the order must be done to each.

$$\begin{aligned} \mathbf{L}^2 &= \mathbf{x}^2\mathbf{p}^2 - 2i\hbar\mathbf{x}\cdot\mathbf{p} - (\mathbf{x}\cdot\mathbf{p})\left(x_j p_j - 3i\hbar\right) \\ &= \mathbf{x}^2\mathbf{p}^2 + i\hbar\mathbf{x}\cdot\mathbf{p} - (\mathbf{x}\cdot\mathbf{p})^2. \end{aligned} \tag{B.68}$$

The text is correct.

C

JULIA NOTEBOOKS

These Julia notebooks, can be found in
https://github.com/peeterjoot/julia.

These notebooks are text files. The julia program, available freely at www.julialang.org, is required to execute them. Some Julia code can also be evaluated with Matlab.

- Sep 24, 2015 phy1520/vectorSolenoid.jl

  Plot of solenoid potential for constant interior magnetic field
- Nov 15, 2015 phy1520/rodbalancing.jl

  Plug in some numbers for uncertainty time rod balancing calculation.

D

MATHEMATICA NOTEBOOKS

These Mathematica notebooks, some just trivial ones used to generate figures, others more elaborate, and perhaps some even polished, can be found in

https://github.com/peeterjoot/mathematica/tree/master/.

The free Wolfram CDF player, is capable of read-only viewing these notebooks to some extent.

- Sep 28, 2015 phy1520/anticommutingWithZeroEigenvalue.nb

  Construct and verify an example of a pair of anticommuting matrices each having a zero eigenvalue, and a shared eigenvector. This was for Sakurai p.1.17, and includes some numeric commutator expansions to verify the example constructions done with that problem.

- Oct 25, 2015 phy1520/energyVsMomentumForDiracStepPotentialWaveFunctions.nb

  A Manipulate to explore the energy vs momentum curves for a stepped potential barrier and the Dirac Hamiltonian.

- Nov 1, 2015 phy1520/spinOneHalfSymbolicManipulation.nb

  For a spin one-half system Sakurai leaves it to the reader (and also to problem 3.10) to verify that knowledge of the three ensemble averages $\langle S_x \rangle, \left\langle S_y \right\rangle, \langle S_z \rangle$ is sufficient to reconstruct the density operator. Showing that is algebraically messy, and well suited to do in Mathematica.

- Nov 2, 2015 phy1520/eulerAngleVsNormalRotationPauliMatrices.nb

  Comparing a unimodular transformation to an arbitrary rotation matrix was trivial. To do the same for an Euler angle rotation matrix and arbitrary matrix is less so because of sign differences. Here is a dumb symbol expansion of the full rotation on a general vector in Pauli matrix form to have a look at the two results and see if there is anything striking. It turns out there is not anything striking. Both expressions are messy even after FullSimplify.

- Nov 16, 2015 phy1520/spinOneOperatorRepresentation.nb

  Spin one operators. Sakurai only seems to list the S_y spin one matrix representation. See these in Desai, but need to verify that all my corrections to Desai eq. (27.117) are correct.

- Nov 19, 2015 phy1520/diracDeltaFunctionIntegrals.nb

  Double check the integral done in the Dirac delta function problem, and perform the first Fourier transformation.

- Nov 24, 2015 phy1520/spinOneDensityOperatorRepresentationInTermsOfEnsembleAverages.nb

  Solution for Sakurai problem 3.12: What must we know in addition to the ensemble averages of the spin operators to completely characterize the density matrix of a spin 1 system? I guessed that we also needed the ensemble averages of at least the squares, but that and the unit trace, was not enough, since those relations do not provide nine equations, for the nine unknowns. Omitting the trace requirement, but also introducing variables for the other second order products was enough to solve the problem. Printing out all those products is helpful to show why this is the case: you can see visually that these products appear to span the space of 3×3 matrices.

- Nov 24, 2015 phy1520/squareOfAngularMomentumOperatorSphericalCoordinates.nb

  Expand out $\mathbf{L}$ in spherical coordinates in terms of L_x, L_y, L_z operators and compare to stated result (Sakurai (6.15)).

- Nov 26, 2015 phy1520/lecture19integralsAndPlots.nb

  Confirm some of the lecture 19 (variational method) integrals, and plot the energy distribution.

- Dec 2, 2015 phy1520/visualizationOfEigenvaluesOfTwoByTwoHermitianMatrix.nb

  Dynamic visualization of eigenvalues of 2×2 Hermitian matrix, as sketched in lecture 20, plus some plots with specific values.

- Dec 3, 2015 phy1520/lecture21someSphericalHarmonicsAndTheirIntegrals.nb

  Lecture 21. Print out some spherical harmonic functions and their integrals, to look at the conditions for the integral of $Y_{lm}z$ to be zero. Also evaluate the z and z^2 brakets mentioned in the lecture.

- Dec 6, 2015 phy1520/sakuraiProblem5.13c.nb

  Sakurai. Problem 5.11 (c). Verify hand calculations (diagonalization).

- Dec 8, 2015 phy1520/vanDerWalls.nb

  Do a second order expansion of the van der Walls potential to compare to value stated. Did not figure out how to get Mathematica to simplify this gracefully and did it by hand manually instead.

- Dec 10, 2015 phy1520/lecture22Integrals.nb

  Integrals from lecture 22 (van der Walls potential).

- Dec 11, 2015 phy1520/sakuraiProblem3.17.nb

  sakuraiProblem3.17

- Dec 13, 2015 phy1520/sakuraiProblem5.17a.nb

  Sakurai pr. 5.17 (a): Find energy eigenvalues for $H = AL^2 + BL_z + CL_y$.

- Dec 14, 2015 phy1520/commutatorOfRadialPortionOfMomentumSquaredOperator.nb

  Compute the commutator $\left[-\frac{\hbar^2}{2mr^2}\partial_r(r^2\partial_r), -i\hbar\partial_r\right] = -\frac{\hbar^2}{2mr^2}p_r$. The first operator is a component of $\mathbf{p}^2/2m$ with the $\mathbf{L}^2$ contribution removed.

- Dec 14, 2015 phy1520/sakuraiProblem5.16bSHO.nb

  Verify the relation from Sakurai pr. 5.16(a) using the ground state of the 3D SHO. Verification of the potential derivative expectations for higher values of n do not complete in reasonable times.

- Dec 15, 2015 phy1520/sakuraiProblem3.33.nb

  Spin three halves operator question (Sakurai 3.33). Implement operators for S_+, S_-, S_z that act on kets $|\pm 3/2\rangle, |\pm 1/2\rangle$. These operators act on only a single basis element, but are used to construct the matrix representations for these operators (which are more general). Use those matrices to compute the representation of the Hamiltonian for the problem and compute its energy eigenvalues. Display the end result and the representations for all of $S_+, S_-, S_x, S_y, S_z, H = A(3S_z^2 - \mathbf{S}^2) + B(S_+^2 + S_-^2)$.

- Dec 15, 2015 phy1520/spinMatrices.nb

  Compute and display $S_+, S_-, S_x, S_y, S_z, S^2$ for a given spin (with $\hbar = 1$). Use this to display the matrix representations of these operators for each of: spin 1/2, spin 1, spin 3/2, spin 2, spin 5/2. Use this to solve the (spin one) eigensystem in Sakurai pr. 4.12.

Part III

INDEX

INDEX

Part IV

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BIBLIOGRAPHY

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