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QUANTUM MECHANICS I

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Notes and problems from UofT PHY356H1F 2010

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DOCUMENT VERSION

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

PREFACE

These are my personal lecture notes for the Fall 2010, University of Toronto Quantum mechanics I course (PHY356H1F), taught by Prof. Vatche Deyirmenjian.

The official description of this course was:

The general structure of wave mechanics; eigenfunctions and eigenvalues; operators; orbital angular momentum; spherical harmonics; central potential; separation of variables, hydrogen atom; Dirac notation; operator methods; harmonic oscillator and spin.

This document contains a few things

- My lecture notes.

  Typos, if any, are probably mine (Peeter), and no claim nor attempt of spelling or grammar correctness will be made. The first four lectures I had chosen not to take notes for since they followed the text [3] very closely.

- Notes from reading of the text. This includes observations, notes on what seem like errors, and some solved problems. None of these problems have been graded. Note that my informal errata sheet [7] for the text has been separated out from this document.

- Some assigned problems. I have corrected some the errors after receiving grading feedback, and where I have not done so I at least recorded some of the grading comments as a reference.

- Some worked problems associated with exam preparation.

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CONTENTS

LIST OF FIGURES

Part I

NOTES AND PROBLEMS

1 BASIC FORMALISM

1.1 DIRAC ADJOINT NOTES

I have got the textbook [3] now for the QM I course I will be taking in the fall, and have started some light perusing. Starting things off is the Dirac bra ket notation. Some aspects of that notation, or the explanation in the text, are not quite obvious to me so here I try to make sense of things.

There are a pair of relations given to define the Dirac adjoint. These are 1.26 and 1.27 respectively:

$$\begin{aligned}\left(A\left|\alpha\right\rangle\right)^* &= \left\langle\alpha\right| A^\dagger \\ \left\langle\beta\right| A \left|\alpha\right\rangle^* &= \left\langle\alpha\right| A^\dagger \left|\beta\right\rangle\end{aligned} \tag{1.1}$$

Is there some redundancy to these definitions. Namely is 1.27 a consequence of 1.26?

Since the ket was defined as the conjugate of the bra, we can probably rewrite 1.26 as

$$\left\langle\alpha\right| A^* = \left\langle\alpha\right| A^\dagger \tag{1.2}$$

The operational word here is "probably". This seems somewhat dubious. For example with the identity operator this would mean

$$\left(\left|\alpha\right\rangle\right)^* = \left\langle\alpha\right|, \tag{1.3}$$

and I am unsure that this makes sense. If one assumes that it does, then one can find that 1.26 implies 1.27, as follows.

Left “multiplication”, by the ket $\left|\beta\right\rangle$ gives

$$\begin{aligned}(\left\langle\alpha\right| A^\dagger)\left|\beta\right\rangle &= (\left\langle\alpha\right| A^*)\left|\beta\right\rangle \\ &= \left\langle\beta\right| (A\left|\alpha\right\rangle)^*\end{aligned} \tag{1.4}$$

Again the dubious operation $\left\langle\alpha\right|^* = \left|\alpha\right\rangle$ has been employed implicitly.

Also note that I have added and retained parenthesis to retain the operational direction. Is that operational direction not important? For example, given an operator like $p = -i\hbar\partial_x$, it makes a big difference whether the operator operates to the left or to the right. In the text, this last relation is equation 1.27 once the parens are dropped, so it does appear that 1.27 is a consequence of 1.26. This also then seems to imply that in a bra operator ket sandwich, the operator implicitly operates on the ket (to the right), while an adjoint operator implicitly operates on the bra (to the left).

Let us compare this to the simpler and more pedestrian notation found in an old fashioned book like Bohm's [1]. His expectation values explicitly use an integral definition, and his adjoint definition is very explicit about order of operations. Namely

$$\int \phi^* (A\psi) \equiv \int \psi (A^\dagger \phi^*) \tag{1.5}$$

Starting with a concrete definition like this seems a bit easier. Suppose we also define the bra ket sandwich based on the integral as follows

$$\begin{aligned} \langle \phi | A | \psi \rangle &\equiv \langle \phi | (A | \psi \rangle) \\ &\equiv \int \phi^* (A\psi) \end{aligned} \tag{1.6}$$

Now, we can rewrite eq. (1.5), as

$$\begin{aligned} \int \phi^* (A\psi) &\equiv \int \psi (A^\dagger \phi^*) \\ &\Longrightarrow \\ \langle \phi | (A | \psi \rangle) &= \left\langle \psi^* \right| (A^\dagger \left| \phi^* \right\rangle) \\ &\Longrightarrow \\ \left(\langle \phi | (A | \psi \rangle) \right)^* &= (\langle \phi | A^\dagger) | \psi \rangle \end{aligned} \tag{1.7}$$

When starting off with the integral we see the notational requirement for non-adjoint operators to operate implicitly to the right, and the adjoint operators to operate implicitly to the left. With that notation requirement we can drop the parens and recover 1.27.

A couple clarification goals are now complete. The first is seeing how equation 1.26 in the text implies 1.27 (provided the plain old conjugation of a bra creates a ket). We also have reconciled the Dirac notation with the familiar integral inner product notation, and seen two different ways that clarify the implicit operator directionality in the bra operator ket sandwiches.

Update. Vatche, my professor for the course, also had trouble with 1.26. He feels it ought to be

$$\left(A | \alpha \rangle \right)^\dagger = \langle \alpha | A^\dagger. \tag{1.8}$$

Matrix notation was used to demonstrate this, since conjugation only changes the element values and does not transpose the matrix. Use of the identity operator makes his point particularly clear.

1.2 LECTURE NOTES: REVIEW

Information about systems comes from vectors and operators. Express the vector $|\phi\rangle$ describing the system in terms of eigenvectors $|a_n\rangle, n \in 1, 2, 3, \cdots$ of some operator A.

$$|\phi\rangle = \sum_n c_n |a_n\rangle = \sum_n |c_n a_n\rangle \tag{1.9}$$

What are the coefficients c_n? Act on both sides by $\langle a_m|$ to find

$$\begin{aligned}
\langle a_m|\phi\rangle &= \sum_n \langle a_m| |c_n a_n\rangle \\
&= \sum_n c_n \langle a_m|a_n\rangle \\
&= \sum_n c_n \overbrace{\boxed{\langle a_m|a_n\rangle}}^{\text{Kronecker delta}} \\
&= \sum c_n \delta_{mn} \\
&= c_m
\end{aligned} \tag{1.10}$$

So our coefficients are

$$c_m = \langle a_m|\phi\rangle . \tag{1.11}$$

The complete decomposition in terms of the chosen basis of A is then

$$|\phi\rangle = \sum_n \langle a_n|\phi\rangle |a_n\rangle = \left(\sum_n |a_n\rangle \langle a_n| \right) |\phi\rangle . \tag{1.12}$$

Note carefully the physics convention for this complex inner product. We have linearity in the <u>second</u> argument

$$\langle \psi|a\phi\rangle = a \langle \psi|\phi\rangle , \tag{1.13}$$

whereas the normal mathematics convention is to define complex inner products as linear in the first argument

$$\langle a\psi, \phi \rangle = a\langle \psi, \phi \rangle. \tag{1.14}$$

We can make an analogy with 3D Euclidean inner products easily

$$\mathbf{v} = \sum_i v_i \mathbf{e}_i \tag{1.15}$$

$$\mathbf{e}_1 \cdot \mathbf{v} = \sum_i v_i \mathbf{e}_1 \cdot \mathbf{e}_i = v_1 \tag{1.16}$$

Physical information comes from the probability for obtaining a measurement of the physical entity associated with operator A. The probability of obtaining outcome a_m, an eigenvalue of A, is $|c_m|^2$

1.3 PROBLEMS

Exercise 1.1 *([3] pr 1.1)*

FIXME: description?

Answer for Exercise 1.1

With

$$\begin{aligned}
|\alpha_1\rangle &\equiv \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\
|\alpha_2\rangle &\equiv \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\
\langle\alpha_1| &\equiv \begin{bmatrix} 1 & 0 \end{bmatrix} \\
\langle\alpha_2| &\equiv \begin{bmatrix} 0 & 1 \end{bmatrix}
\end{aligned} \tag{1.17}$$

i. Orthonormal Straight multiplication is sufficient to show this and we get

$$\begin{aligned}
\langle\alpha_1|\alpha_1\rangle &= \begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}1\end{bmatrix}\\
\langle\alpha_2|\alpha_2\rangle &= \begin{bmatrix}0 & 1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}1\end{bmatrix}\\
\langle\alpha_1|\alpha_2\rangle &= \begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}0\end{bmatrix}\\
\langle\alpha_2|\alpha_1\rangle &= \begin{bmatrix}0 & 1\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}0\end{bmatrix}
\end{aligned} \tag{1.18}$$

ii. Linear combinations for state vectors

$$\begin{bmatrix}a\\b\end{bmatrix} = a\,|\alpha_1\rangle + b\,|\alpha_2\rangle \tag{1.19}$$

iii. Outer products We have

$$\begin{aligned}
|\alpha_1\rangle\langle\alpha_2| &= \begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix} = \begin{bmatrix}0 & 1\\0 & 0\end{bmatrix}\\
|\alpha_2\rangle\langle\alpha_1| &= \begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} = \begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}\\
|\alpha_1\rangle\langle\alpha_1| &= \begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}\\
|\alpha_2\rangle\langle\alpha_2| &= \begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix} = \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix}
\end{aligned} \tag{1.20}$$

iv. Completeness relation From the above outer products, summation over just the diagonal terms we have

$$|\alpha_1\rangle\langle\alpha_1| + |\alpha_2\rangle\langle\alpha_2| = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} + \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix} = I \tag{1.21}$$

v. Arbitrary matrix as sum of outer products By inspection

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = a \left|\alpha_1\right\rangle \left\langle\alpha_1\right| + b \left|\alpha_1\right\rangle \left\langle\alpha_2\right| + c \left|\alpha_2\right\rangle \left\langle\alpha_1\right| + d \left|\alpha_2\right\rangle \left\langle\alpha_2\right| \tag{1.22}$$

vi. Spin matrix Given

$$\begin{aligned} A \left|\alpha_1\right\rangle &= + \left|\alpha_1\right\rangle \\ A \left|\alpha_2\right\rangle &= - \left|\alpha_1\right\rangle \end{aligned} \tag{1.23}$$

Our matrix elements are

$$\begin{aligned} \left\langle\alpha_1\right| A \left|\alpha_1\right\rangle &= 1 \\ \left\langle\alpha_2\right| A \left|\alpha_1\right\rangle &= 0 \\ \left\langle\alpha_1\right| A \left|\alpha_2\right\rangle &= 0 \\ \left\langle\alpha_2\right| A \left|\alpha_2\right\rangle &= -1 \end{aligned} \tag{1.24}$$

Thus the matrix representation of the operator A with respect to basis $\{\alpha_1, \alpha_2\}$ is

$$\{A\} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1.25}$$

Exercise 1.2 Derivative of inverse operator (*[3] pr 1.2*)

FIXME: describe.

Answer for Exercise 1.2

We take derivatives of the identity operator, giving

$$\begin{aligned} 0 &= \frac{dI}{d\lambda} \\ &= \frac{d(AA^{-1})}{d\lambda} \\ &= \frac{dA}{d\lambda} A^{-1} + A \frac{dA^{-1}}{d\lambda} \end{aligned} \tag{1.26}$$

left multiplication by A^{-1} and rearranging we have

$$\frac{dA^{-1}}{d\lambda} = -A^{-1} \frac{dA}{d\lambda} A^{-1} \tag{1.27}$$

as desired.

Exercise 1.3 Unitary representations ([3] *pr 1.3*)

Show that a unitary operator U can be written

$$U = \frac{1 + iK}{1 - iK}, \tag{1.28}$$

where K is a Hermitian operator.

Answer for Exercise 1.3

A commutation assumption for the numerator and denominator Before tackling the problem, note that with the fraction written this way, and not as

$$U = (1 + iK)\frac{1}{1 - iK}, \tag{1.29}$$

or

$$U = \frac{1}{1 - iK}(1 + iK), \tag{1.30}$$

there appears to be an implicit assumption that the numerator and denominator commute. How can that be justified?

Suppose that the denominator can be expanded in Taylor series

$$\frac{1}{1 - iK} = 1 + iK + (iK)^2 + (iK)^3 + \cdots \tag{1.31}$$

If this converges, this series does in fact commute with the numerator since both are polynomials in K. Another way of looking at this would be to apply a spectral decomposition to the operators (assumed to be matrices now) where using $K = V\Sigma V^\dagger$ for a unitary V and diagonal Σ, we can write

$$U = \frac{1}{1 - iK}(1 + iK) = \frac{1}{1 - i\Sigma}(1 + i\Sigma) \tag{1.32}$$

Both the numerator and denominator are now diagonal and thus commute. Generalizing either of these commutation justifications to infinite dimensional Hilbert operators or where that inverse power series in K does not converge would take further thought.

That this representation is unitary From eq. (1.29) we have

$$\begin{aligned} UU^\dagger &= (1+iK)\frac{1}{1-iK}\frac{1}{1+iK}(1-iK) \\ &= \frac{1+K^2}{1+K^2} \\ &= 1 \end{aligned} \tag{1.33}$$

So this operator is unitary for all Hermitian K. However, is there a K for any unitary U that is Hermitian and for which this identity holds true? We can rearrange for K to get

$$K = i\frac{U-1}{U+1} \tag{1.34}$$

Is this Hermitian? If so then $K - K^\dagger = 0$, so let us evaluate that.

$$K - K^\dagger = i\frac{U-1}{U+1} + i\frac{U^\dagger - 1}{U^\dagger + 1} \tag{1.35}$$

Multiplying by $-i(U+1)(U^\dagger+1)$ we have

$$\begin{aligned} -i(U+1)(U^\dagger+1)(K-K^\dagger) &= (U-1)(U^\dagger+1) + (U^\dagger-1)(U+1) \\ &= UU^\dagger - 1 - U^\dagger + U + U^\dagger U - U + U^\dagger - 1 \\ &= 0. \end{aligned} \tag{1.36}$$

Therefore, provided $2 + U + U^\dagger \neq 0$ (if it does we only showed that $0 = 0$), the operator K is Hermitian. The expression eq. (1.34) then allows any unitary operator to be expressed as the fraction eq. (1.29).

An exponential representation Show that one can also write

$$U = e^{iC}, \tag{1.37}$$

where C is Hermitian. Utilizing the power series we have

$$\begin{aligned} (e^{iC})^\dagger &= \sum_{k=0}^{\infty} \frac{1}{k!}((iC)^k)^\dagger \\ &= \sum_{k=0}^{\infty} \frac{1}{k!}((-iC)^k) \\ &= e^{-iC}. \end{aligned} \tag{1.38}$$

The operators iC and $-iC$ commute, so we can write

$$(e^{iC})^\dagger e^{iC} = e^{-iC+iC} = 1, \tag{1.39}$$

which shows that this exponential construction is in fact unitary for any Hermitian C. The remainder of the exercise requires a demonstration that we can find such an operator C for any given unitary operator U. Rearranging, we have

$$C = -i \ln(U). \tag{1.40}$$

How can we give this some meaning? One way, with the presumption that working with the matrix representation of the operator is allowable, is to utilize the spectral theorem for normal matrices. Normal here means that the matrix and its Hermitian conjugate commute, which is implied by $UU^\dagger = 1 = U^\dagger U$. So we can write, for a diagonal matrix Σ, and a unitary matrix V,

$$U = V\Sigma V^\dagger, \tag{1.41}$$

so the logarithm of eq. (1.40) can be reduced, and we are left with

$$C = -iV \ln(\Sigma) V^\dagger. \tag{1.42}$$

Here the logarithm of the diagonal matrix is nothing more than the diagonal matrix of the eigenvalues.

We still have to show that C as defined in eq. (1.42) is Hermitian. At a glance it looks like this may be anti Hermitian $C^\dagger = -C$, but we really need a characterization of the eigenvalues to say. That conjugate is

$$C^\dagger = iV(\ln(\Sigma))^\dagger V^\dagger. \tag{1.43}$$

It seems worthwhile to work an example to see if we are even on the right track. Let us pick the 2 dimensional rotation matrix, and express it using its eigenvalue decomposition. That is

$$U = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}, \tag{1.44}$$

with decomposition

$$\begin{aligned}
V &= \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} \\
\Sigma &= \begin{bmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{bmatrix} \\
U &= V\Sigma V^\dagger .
\end{aligned} \tag{1.45}$$

We have

$$\ln \Sigma = \begin{bmatrix} i\theta & 0 \\ 0 & -i\theta \end{bmatrix}. \tag{1.46}$$

Ah. This is purely imaginary, and accounts for the Hermiticity of C in this specific example. Are the logs of the eigenvalues of unitary matrices all purely imaginary? That seems like a lot to ask for.

Incidentally, for this example, $C = -iV \ln \Sigma V^\dagger$ gives us

$$\begin{aligned}
C &= i\theta \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \\
&= \theta\sigma_2 ,
\end{aligned} \tag{1.47}$$

So, in a rather neat way, we have an matrix exponential expression for the standard planar rotation matrix, in terms of one of the Pauli matrices. It is straight forward to verify that

$$U = e^{i\sigma_2\theta}, \tag{1.48}$$

does in fact recover eq. (1.44). This follows directly from $(i\sigma_2)^2 = -I$, allowing us to write

$$U = \cos\theta I + i\sigma_2 \sin\theta. \tag{1.49}$$

Okay. With that example worked out, we come to the conclusion that the operator specified in eq. (1.42), can be Hermitian.

Having worked an example, we are left to prove the more general case. To do this we have only to note that the eigenvalues of a Unitary matrix have unit norm, so they must all be of the form $e^{i\alpha}$. Suppose we write for the diagonal matrix

$$\Sigma = \left[e^{i\alpha_k} \delta_{kj} \right]_k . \tag{1.50}$$

The logarithm and its conjugate are then

$$\begin{aligned} \ln \Sigma &= \left[i\alpha_k \delta_{kj} \right]_k \\ (\ln \Sigma)^\dagger &= - \ln \Sigma. \end{aligned} \tag{1.51}$$

This completes the required proof, showing that the matrix C is Hermitian

$$C = -iV \ln(\Sigma) V^\dagger = C^\dagger . \tag{1.52}$$

I initially relied on wikipedia [15] for the hint that Unitary matrices have unit norm eigenvalues (and the wiki article references Shankar, which I do not have). However, this is straightforward to show. Suppose that x is an eigenvector for U with eigenvalue λ, then we have

$$\begin{aligned} \langle Ux | Ux \rangle &= \left\langle U^\dagger U x | x \right\rangle \\ &= \langle x | x \rangle , \end{aligned} \tag{1.53}$$

but we also have

$$\begin{aligned} \langle Ux | Ux \rangle &= \langle \lambda x | \lambda x \rangle \\ &= |\lambda|^2 \langle x | x \rangle . \end{aligned} \tag{1.54}$$

We must then have $|\lambda|^2 = 1$, or $\lambda = e^{i\alpha}$ for some real α.

Commuting real and imaginary parts If

$$U = A + iB, \tag{1.55}$$

show that A and B commute.

We can form the matrices A, and B with the usual real and imaginary decomposition, but using Hermitian conjugation. That is

$$\begin{aligned} A &= \frac{1}{2}(U + U^\dagger) \\ B &= \frac{1}{2i}(U - U^\dagger). \end{aligned} \tag{1.56}$$

Then the commutation question essentially just requires that we show the commutator is zero

$$\begin{aligned} AB - BA &= \frac{1}{4i}\left((U + U^\dagger)(U - U^\dagger) - (U - U^\dagger)(U + U^\dagger)\right) \\ &= \frac{1}{4i}\left(U^2 + (U^\dagger)^2 + 1 - 1 - (U^2 + (U^\dagger)^2 - 1 + 1)\right) \\ &= 0. \qquad \square \end{aligned} \tag{1.57}$$

Now, if $U = e^{iC} = A + iB$, we can expand U trigonometrically, with the typical power series expansions, and can also write

$$\begin{aligned} A &= \cos C \\ B &= \sin C \end{aligned} \tag{1.58}$$

We can also use the spectral decomposition of U and C above in eq. (1.42), to write

$$\begin{aligned} A &= V \cosh(\ln \Sigma) V^\dagger \\ B &= -V \sinh(\ln \Sigma) V^\dagger, \end{aligned} \tag{1.59}$$

and again here the functions of matrices are nothing more than diagonal evaluation of the respective functions to each of the eigenvalues of Σ.

Exercise 1.4 Determinant of exponential in terms of trace. (*[3] pr 1.4*)

Show

$$\det(e^A) = e^{\operatorname{Tr} A}. \tag{1.60}$$

The problem does not put constraints (ie: no statement that A is Hermitian), so we can not assume a Unitary diagonalization is possible. We can however assume an upper triangular similarity transformation of the form

$$A = W J W^{-1}, \tag{1.61}$$

where W is invertible, but not necessarily unitary, and J is in Jordan Canonical form. That form is upper triangular with the eigenvalues on the diagonal, and only ones or zeros above the diagonal (however, for the purposes of this problem we only need to know that it is upper triangular).

Answer for Exercise 1.4

The determinant of e^A is then

$$\begin{aligned}\det(e^A) &= \det(W)\det(e^J)\det(W^{-1}) \\ &= \det(e^J).\end{aligned} \tag{1.62}$$

Note that the exponential of a triangular matrix has the exponentials of the eigenvalues along the diagonal. We can see this by computing the square of an upper triangular matrix in block form. A general proof of this is straightforward, but one gets the idea by considering the two by two case

$$\begin{bmatrix} a & c \\ 0 & b \end{bmatrix}\begin{bmatrix} a & c \\ 0 & b \end{bmatrix} = \begin{bmatrix} a^2 & (a+b)c \\ 0 & b^2 \end{bmatrix}. \tag{1.63}$$

Forming the exponential series, one is left with exponentials of the eigenvalues along the diagonal. So we have for our determinant

$$\begin{aligned}\det(e^A) &= \det(e^J) \\ &= \prod_k e^{\lambda_k} \\ &= e^{\sum_k \lambda_k} \\ &= e^{\mathrm{Tr}(A)}. \qquad \square\end{aligned} \tag{1.64}$$

Exercise 1.5 Trace of an outer product operator ([3] pr 1.5)

Show that

$$\mathrm{Tr}(\lvert\alpha\rangle\langle\beta\rvert) = \langle\beta\vert\alpha\rangle\,. \tag{1.65}$$

Answer for Exercise 1.5

Let $A = |\alpha\rangle\langle\beta|$, and introduce a complete basis $|e_k\rangle$. The trace with respect to this basis (or any) is thus

$$\begin{aligned}
\mathrm{Tr}(A) &= \sum_k \langle e_k| A |e_k\rangle \\
&= \sum_k \langle e_k| \left(|\alpha\rangle\langle\beta|\right) |e_k\rangle \\
&= \sum_k \langle\beta|e_k\rangle \langle e_k|\alpha\rangle \\
&= \langle\beta| \left(\sum_k |e_k\rangle\langle e_k| \right) |\alpha\rangle \\
&= \langle\beta| I |\alpha\rangle \\
&= \langle\beta|\alpha\rangle . \qquad \square
\end{aligned} \tag{1.66}$$

Exercise 1.6 eigen calculation ([3] pr 1.6)

For operator(s)

$$A = |\alpha\rangle\langle\alpha| + \lambda |\beta\rangle\langle\alpha| + \lambda^* |\alpha\rangle\langle\beta| \pm |\beta\rangle\langle\beta| , \tag{1.67}$$

where $\langle\alpha|\beta\rangle = 0$, and $\langle\alpha|\alpha\rangle = \langle\beta|\beta\rangle = 1$, find the eigenvalues and vectors for (i) $\lambda = 1$, and (ii) $\lambda = i$.

Answer for Exercise 1.6

Without using matrix representation Our eigenvector must be some linear combination of the two kets, so lets look for one of the form $|e\rangle = |\alpha\rangle + a|\beta\rangle$, and use this to find eigenvalues for

$$A|e\rangle = b|e\rangle . \tag{1.68}$$

This means we seek solutions to

$$|\alpha\rangle + \lambda|\beta\rangle + a\lambda^* |\alpha\rangle \pm a|\beta\rangle = b(|\alpha\rangle + a|\beta\rangle). \tag{1.69}$$

This supplies a pair of simultaneous equations

$$\begin{aligned}
1 + a\lambda^* &= b \\
\lambda \pm a &= ba.
\end{aligned} \tag{1.70}$$

We have our eigenvalue b in terms of the constant a immediately, so for a we wish to solve the quadratic

$$\lambda \pm a = (1 + a\lambda^*)a \tag{1.71}$$

Let us treat these four cases separately, starting the two $\lambda = 1$ operators. Those quadratics are

$$\begin{aligned} 1 + a &= (1 + a)a \\ 1 - a &= (1 + a)a \end{aligned} \tag{1.72}$$

with respective solutions

$$\begin{aligned} a &= \pm 1 \\ a &= \pm\sqrt{2} - 1 \end{aligned} \tag{1.73}$$

Summarizing the operator, eigenvalue, and eigenvector triplets for this $\lambda = 1$ case we have

$$\begin{aligned} A &= |\alpha\rangle\langle\alpha| + |\beta\rangle\langle\alpha| + |\alpha\rangle\langle\beta| + |\beta\rangle\langle\beta| \\ |e\rangle_\pm &= |\alpha\rangle \pm |\beta\rangle \\ \lambda_\pm &= 1 \pm 1 \end{aligned} \tag{1.74a}$$

and

$$\begin{aligned} A &= |\alpha\rangle\langle\alpha| + |\beta\rangle\langle\alpha| + |\alpha\rangle\langle\beta| - |\beta\rangle\langle\beta| \\ |e\rangle_\pm &= |\alpha\rangle + (\pm\sqrt{2} - 1)\,|\beta\rangle \\ \lambda_\pm &= \pm\sqrt{2} \end{aligned} \tag{1.75a}$$

Now for the pair of $\lambda = i$ operators, our quadratic is

$$i \pm a = (1 - ia)a, \tag{1.76}$$

or separately

$$\begin{aligned} a^2 + 1 &= 0 \\ (a + i)^2 + 2 &= 0 \end{aligned} \tag{1.77}$$

The respective solutions are

$$\begin{aligned} a &= \pm i \\ a &= i(-1 \pm \sqrt{2}), \end{aligned} \tag{1.78}$$

with eigenvalues $b = 1 - ia$, which are respectively

$$\begin{aligned} b &= 1 \pm 1 \\ b &= \pm \sqrt{2}. \end{aligned} \tag{1.79}$$

Summarizing the results, we have

$$\begin{aligned} A &= |\alpha\rangle \langle\alpha| + i\,|\beta\rangle \langle\alpha| - i\,|\alpha\rangle \langle\beta| + |\beta\rangle \langle\beta| \\ |e\rangle_\pm &= |\alpha\rangle \pm i\,|\beta\rangle \\ \lambda_\pm &= 2, 0 \end{aligned} \tag{1.80a}$$

and

$$\begin{aligned} A &= |\alpha\rangle \langle\alpha| + i\,|\beta\rangle \langle\alpha| - i\,|\alpha\rangle \langle\beta| + |\beta\rangle \langle\beta| \\ |e\rangle_\pm &= |\alpha\rangle + i(-1 \pm \sqrt{2})\,|\beta\rangle \\ \lambda_\pm &= \pm \sqrt{2} \end{aligned} \tag{1.81a}$$

So it appears we got the same eigenvalues and vectors for both $\lambda = 1$ and $\lambda = i$. Is there a higher order principle that this follows from? Perhaps the fact that both terms with λ coefficients were conjugate pairs? That is something perhaps worth thinking about.

Using matrix representation In the matrix notation with basis $\{\sigma_1, \sigma_2\} = \{(1, 0), (0, 1)\}$, and $A_{mn} = \langle\sigma_m| A |\sigma_n\rangle$, we have

$$\begin{aligned} A_{11} &= \langle\sigma_1| A |\sigma_1\rangle = \langle\alpha|\alpha\rangle = 1 \\ A_{22} &= \langle\sigma_2| A |\sigma_2\rangle = \mu \langle\beta|\beta\rangle = \mu \\ A_{12} &= \langle\sigma_1| A |\sigma_2\rangle = \lambda^* \\ A_{21} &= \langle\sigma_2| A |\sigma_1\rangle = \lambda \end{aligned} \tag{1.82}$$

Or in whole matrix notation, we have

$$\{A\} = \begin{bmatrix} 1 & \lambda^* \\ \lambda & \mu \end{bmatrix}. \tag{1.83}$$

Finding the eigenvalues and vectors becomes a straightforward, albeit somewhat tedious, algebraic job, solving for $|A - \sigma I| = 0$, for eigenvalues σ. Doing this, I get

- $\lambda = 1, \mu = 1$

$$
\begin{aligned}
\sigma &= 2, 0 \\
|\sigma_2\rangle &= \frac{1}{\sqrt{2}}(1, 1) \\
|\sigma_0\rangle &= \frac{1}{\sqrt{2}}(1, -1)
\end{aligned} \tag{1.84}
$$

  Alternatively, for the $\sigma = 2$ case we have

$$
|\sigma_2\rangle = \frac{1}{\sqrt{2}} \left(|\alpha\rangle + |\beta\rangle \right), \tag{1.85}
$$

  and for the $\sigma = 0$ case we have

$$
|\sigma_0\rangle = \frac{1}{\sqrt{2}} \left(|\alpha\rangle - |\beta\rangle \right). \tag{1.86}
$$

  Ignoring the normalization constant used here, this is consistent with eq. (1.74) as it should be.

- $\lambda = 1, \mu = -1$

$$
\begin{aligned}
\sigma &= \pm \sqrt{2} \\
|\sigma_\pm\rangle &\propto (1, -1 \pm \sqrt{2})
\end{aligned} \tag{1.87}
$$

  Normalization was not bothered with this time due to pesky $\sqrt{2}$ terms. The eigenstates expressed in terms of the original basis vectors are

$$
|\sigma_\pm\rangle = |\alpha\rangle + (-1 \pm \sqrt{2}) |\beta\rangle \tag{1.88}
$$

  This is consistent with eq. (1.75) as expected.

- $\lambda = i, \mu = 1$

$$\begin{aligned}\sigma &= 2, 0 \\ |\sigma_0\rangle &= \frac{1}{\sqrt{2}}(i, 1) \\ |\sigma_2\rangle &= \frac{1}{\sqrt{2}}(-i, 1)\end{aligned} \tag{1.89}$$

In terms of the original basis vectors this is

$$|\sigma_0\rangle = \frac{1}{\sqrt{2}}\left(i\,|\alpha\rangle + |\beta\rangle\right) \tag{1.90}$$

$$|\sigma_2\rangle = \frac{1}{\sqrt{2}}\left(-i\,|\alpha\rangle + |\beta\rangle\right) \tag{1.91}$$

Checking against eq. (1.80) shows that $|\sigma_2\rangle$ above only differs by a constant as expected.

- $\lambda = i, \mu = -1$

$$\begin{aligned}\sigma &= \pm\sqrt{2} \\ |\sigma_\pm\rangle &\propto (1, -i(1 \mp \sqrt{2}))\end{aligned} \tag{1.92}$$

Or, in terms of the original basis,

$$|\sigma_\pm\rangle = |\alpha\rangle + i(-1 \pm \sqrt{2})\,|\beta\rangle\,. \tag{1.93}$$

This matches the previous calculation summarized by eq. (1.81).

Exercise 1.7 problem set 1.

Assume that X and $P = -i\hbar\partial/\partial x$ are the x-direction position and momentum operators. Show that $\left[X, P\right] = i\hbar\mathbf{1}$. Find $\langle x|\,(XP - PX)\,|x'\rangle$ using the above definitions. What is the physical meaning of this expression?

Answer for Exercise 1.7

Avoiding Dirac notation We can get a rough idea where we are going by temporarily avoiding the Dirac notation that complicates things. To do so, consider the commutator action on an arbitrary wave function $\psi(x)$

$$\begin{aligned}(xP - Px)\psi &= xP\psi + i\hbar\frac{\partial}{\partial x}(x\psi) \\ &= xP\psi + i\hbar\left(\psi + \frac{\partial\psi}{\partial x}\right) \\ &= xP\psi + i\hbar\psi - xP\psi \\ &= i\hbar\psi\end{aligned} \tag{1.94}$$

Since this is true for all $\psi(x)$ we can make the identification

$$xP - Px = i\hbar\mathbf{1} \tag{1.95}$$

Having evaluated the commutator, the matrix element is simple to compute. It is

$$\begin{aligned}\langle x| XP - PX \left|x'\right\rangle &= \langle x| i\hbar\mathbf{1} \left|x'\right\rangle \\ &= i\hbar \left\langle x|x'\right\rangle.\end{aligned} \tag{1.96}$$

This braket has a delta function action, so this matrix element reduces to

$$\langle x| XP - PX \left|x'\right\rangle = i\hbar\delta(x - x'). \tag{1.97}$$

This could perhaps be considered the end of the problem (barring the physical meaning interpretation requirement to come). However, given that the Dirac notation that is so central to the lecture notes and course text, it seems like cheating to avoid it. It seems reasonable to follow this up with the same procedure utilizing the trickier Dirac notation, and this will be done next. If nothing else, this should provide some experience with what sort of manipulations are allowed.

Using Dirac notation Intuition says that we need to consider the action of the commutator within a matrix element of the form

$$\langle x| XP - PX |\psi\rangle = \int dx' \langle x| XP - PX \left|x'\right\rangle \left\langle x'|\psi\right\rangle = \int dx' \langle x| XP - PX \left|x'\right\rangle \psi(x'). \tag{1.98}$$

Observe above that with the introduction of an identity operation, such an expression also includes the matrix element to be evaluated in the second part of this problem. Because of this, if we can show that $\langle x| XP - PX |\psi\rangle = i\hbar\psi(x)$, then as a side effect we will also have shown that the matrix element $\langle x| XP - PX |x'\rangle = i\hbar\delta(x - x')$, as well as demonstrated the commutator relation $XP - PX = i\hbar\mathbf{1}$.

Proceeding with a reduction of the right most integral in eq. (1.98) above, we have

$$
\begin{aligned}
\int dx' \langle x| XP - PX \left|x'\right\rangle \psi(x') &= \int dx' \langle x| xP - Px' \left|x'\right\rangle \psi(x') \\
&= \int dx' \langle x| xP\psi(x') - Px'\psi(x') \left|x'\right\rangle \\
&= -i\hbar \int dx' \langle x| x\frac{\partial\psi(x')}{\partial x} - \frac{\partial}{\partial x}(x'\psi(x')) \left|x'\right\rangle \\
&= i\hbar \int dx' \langle x| - x\frac{\partial\psi(x')}{\partial x} + \frac{\partial x'}{\partial x}\psi(x') + x'\frac{\partial\psi(x')}{\partial x} \left|x'\right\rangle \\
&= i\hbar \int dx' \left(-x\frac{\partial\psi(x')}{\partial x} + \frac{\partial x'}{\partial x}\psi(x') + x'\frac{\partial\psi(x')}{\partial x}\right) \langle x|x'\rangle \\
&= i\hbar \int dx' \left(-x\frac{\partial\psi(x')}{\partial x} + \frac{\partial x'}{\partial x}\psi(x') + x'\frac{\partial\psi(x')}{\partial x}\right) \delta(x - x') \\
&= \left(i\hbar\frac{\partial x'}{\partial x}\psi(x') + i\hbar(x' - x)\frac{\partial\psi(x')}{\partial x}\right)\Bigg|_{x'=x} \\
&= i\hbar\frac{\partial x}{\partial x}\psi(x) + i\hbar(x - x)\frac{\partial\psi(x)}{\partial x} \\
&= i\hbar\psi(x)
\end{aligned}
\tag{1.99}
$$

The convolution with the delta function leaves us with only functions of x, allowing all the derivatives to be evaluated. In the manipulations above the wave function $\psi(x')$ could be brought into the braket since it is just a (complex) scalar. What was a bit sneaky, is the restriction of the action of the operator P to $\psi(x')$, and $x'\psi(x')$, but not to $|x'\rangle$. That was a key step in the reduction since it allows all the resulting terms to be brought out of the braket, leaving the delta function.

What is a good justification for not allowing P to act on the ket? A pragmatic one is that the desired result would not have been obtained otherwise. After the fact I also see that this is consistent with [11], which states (without citation) that $-i\hbar\boldsymbol{\nabla}|\psi\rangle$ is an abuse of notation since the operator should be viewed as operating on projections (ie: wave functions).

Another point to follow up on later is the justification for the order of operations. If the derivatives had been evaluated first before the evaluation at $x = x'$, then we would have nothing left due to the $\partial x'/\partial x = 0$. Perhaps a good answer for that is that the zero times delta function is not well behaved. One has to eliminate the delta function first to see if the magnitudes of the zero of that we would have from a pre-evaluated $\partial x'/\partial x$ is "more zero", than the infinity of the delta function at $x = x'$. This procedure still screams out ad-hoc, and the only real resolution is likely in the framework of distribution theory.

Anyways, assuming the correctness of all the manipulations above, let us return to the problem. We refer back to eq. (1.98) and see that we now have

$$
\begin{aligned}
\langle x| XP - PX |\psi\rangle &= i\hbar\psi(x) \\
&= i\hbar \langle x|\psi\rangle \\
&= \langle x| i\hbar\mathbf{1} |\psi\rangle \\
\implies & \\
0 &= \langle x| XP - PX - i\hbar\mathbf{1} |\psi\rangle
\end{aligned}
\tag{1.100}
$$

Since this is true for all $\langle x|$, and $|\psi\rangle$, we must have $XP - PX = i\hbar\mathbf{1}$ as desired.
Also referring back to eq. (1.98) we can write

$$
\begin{aligned}
\int dx' \langle x| XP - PX \left|x'\right\rangle \psi(x') &= i\hbar\psi(x) \\
&= \int dx' i\hbar\delta(x - x')\psi(x').
\end{aligned}
\tag{1.101}
$$

Taking differences we have for all $\psi(x')$

$$
\int dx' \left(\langle x| XP - PX \left|x'\right\rangle - i\hbar\delta(x - x')\right)\psi(x') = 0,
\tag{1.102}
$$

which we utilize to produce the identification

$$
\langle x| XP - PX \left|x'\right\rangle = i\hbar\delta(x - x')
\tag{1.103}
$$

This completes all the non-interpretation parts of this problem.

The physical meaning of this expression The remaining part of this question ties the mathematics to some reality.

One nice description of a general matrix element can be found in [10], where the author states "We see that the "matrix element" of an operator with respect to a continuous basis is nothing but the kernel of the integral transform that represents the action of that operator in the given basis."

While that characterizes this sort of continuous matrix element nicely, it does not provide any physical meaning, so we have to look further.

The most immediate observation that we can make of this matrix element is not one that assigns physical meaning, but instead points out a non-physical characteristic. Note that in the

LHS when $x = x'$ this is an expectation value for the commutator. Because this expectation "value" is purely imaginary (an $i\hbar$ scaled delta function, with the delta function presumed to be a positive real infinity), we are able to note that this position momentum commutator operator cannot itself represent an observable. It must also be non-Hermitian as a consequence, and that is easy enough to verify directly. Perhaps it would be more interesting to ask the question what the meaning of the matrix element of the Hermitian operator $-i\left[X, P\right]$ is? That operator (an $\hbar$ scaled identity) would at least represent an observable.

How about asking the question of what physical meaning we have for a general commutator, before considering the matrix element of such a commutator. Given two operators A, and B representing observables, a non-zero commutator $\left[A, B\right]$ of these operators means that simultaneous precise measurement of the two observables is not possible. This property can also be thought of as a meaning for the matrix element $\langle x'| \left[A, B\right] |x\rangle$ of such a commutator. For the position momentum commutator, this matrix element $\langle x| \left[X, P\right] |x'\rangle = i\hbar\delta(x - x')$ would also be zero if simultaneous measurement of the operators was possible.

Because this matrix element of this commutator is non-zero (despite the fact that the delta function is zero almost everywhere) we know that a measurement of position will disturb the momentum of the particle, and conversely, a measurement of momentum will disturb the position. An illustration of this is in the slit diffraction experiment. Narrowing an initial wide slot to "measure" the position of the photon or electron passing through the slit slit more accurately, has an effect of increasing the scattering range of the particle (ie: reducing the uncertainty in the position measurement imparts momentum in the scattering plane).

Exercise 1.8 problem set 1.

The state of a one-dimensional system is given by $|x_0\rangle$. Does this system obey the position-momentum uncertainty relation? Explain your answer.

Answer for Exercise 1.8

Yes, the system obeys the position-momentum uncertainty relation. Note that in long form the uncertainty relation takes the following form:

$$\sqrt{\left\langle (X - \langle X\rangle)^2 \right\rangle} \sqrt{\left\langle (P - \langle P\rangle)^2 \right\rangle} \ge \frac{\hbar}{2}. \tag{1.104}$$

Each of these expectation values is with respect to some specific state

$$\langle X\rangle \equiv \langle\psi| X |\psi\rangle, \tag{1.105}$$

so one could write this out in still longer form:

$$\sqrt{\langle\psi| (X - \langle\psi| X |\psi\rangle)^2 |\psi\rangle} \sqrt{\langle\psi| (P - \langle\psi| P |\psi\rangle)^2 |\psi\rangle} \ge \frac{\hbar}{2}. \tag{1.106}$$

This inequality holds for all states $|\psi\rangle$ that the system could be observed in. This includes the state $|x_0\rangle$ of this problem, associated with a specific observation of the system.

My grade I completely misunderstood this, and got only 0.5/5 on it. What he was looking for was that if $|x_0\rangle$ is a position eigenstate in a continuous vector space, then one cannot form the expectation with respect to this state, let alone the variance. For example with respect to this state we have

$$\begin{aligned}\langle X\rangle &= \langle x_0|\, X\, |x_0\rangle \\ &= x_0 \langle x_0|x_0\rangle \\ &= x_0\delta(x_0 - x_0)\end{aligned} \tag{1.107}$$

We cannot evaluate this delta function, since it blows up at zero. The implication would be that we have complete uncertainty of position in the one dimensional continuous vector space with respect to this state. Despite bombing on the question, it is a nice one, since it points out some of the implicit assumptions for the uncertainty relation. We can only say that the uncertainty relation applies with respect to normalizable states. That said, is it a fair question? I think the original question was fairly vague, and I would not consider the question well posed.

Exercise 1.9 Parity operator (2007 PHY355H1F 1b)

If Π is the parity operator, defined by $\Pi\,|x\rangle = |-x\rangle$, where $|x\rangle$ is the eigenket of the position operator X with eigenvalue x), and P is the momentum operator conjugate to X, show (carefully) that $\Pi P \Pi = -P$.

Answer for Exercise **1.10**

Consider the matrix element $\langle -x' | [\Pi, P] | x \rangle$. This is

$$\begin{aligned}
\left\langle -x' \right| [\Pi, P] \left| x \right\rangle &= \left\langle -x' \right| \Pi P - P \Pi \left| x \right\rangle \\
&= \left\langle -x' \right| \Pi P \left| x \right\rangle - \left\langle -x \right| P \Pi \left| x \right\rangle \\
&= \left\langle x' \right| P \left| x \right\rangle - \left\langle -x \right| P \left| -x \right\rangle \\
&= -i\hbar \left(\delta(x' - x) \frac{\partial}{\partial x} - \overbrace{\boxed{\delta(-x - (-x'))}}^{= \delta(x' - x) = \delta(x - x')} \frac{\partial}{\partial -x} \right) \\
&= -2i\hbar \delta(x' - x) \frac{\partial}{\partial x} \\
&= 2 \left\langle x' \right| P \left| x \right\rangle \\
&= 2 \left\langle -x' \right| \Pi P \left| x \right\rangle
\end{aligned} \tag{1.108}$$

We have taken advantage of the Hermitian property of P and Π here, and can rearrange for

$$\left\langle -x' \right| \Pi P - P \Pi - 2 \Pi P \left| x \right\rangle = 0 \tag{1.109}$$

Since this is true for all $\langle -x|$ and $|x\rangle$ we have

$$\Pi P + P \Pi = 0. \tag{1.110}$$

Right multiplication by Π and rearranging we have

$$\Pi P \Pi = -P \Pi \Pi = -P. \tag{1.111}$$

Exercise 1.10 Trace invariance for unitary transformation (2008 PHY355H1F final 1b.)

Show that the trace of an operator is invariant under unitary transforms, i.e. if $A' = U^\dagger A U$, where U is a unitary operator, prove $\mathrm{Tr}(A') = \mathrm{Tr}(A)$.

Answer for Exercise 1.10

The bulk of this question is really to show that commutation of operators leaves the trace invariant (unless this is assumed). To show that we start with the definition of the trace

$$
\begin{aligned}
\mathrm{Tr}(AB) &= \sum_n \langle n| AB |n\rangle \\
&= \sum_{nm} \langle n| A |m\rangle \langle m| B |n\rangle \\
&= \sum_{nm} \langle m| B |n\rangle \langle n| A |m\rangle \\
&= \sum_{m} \langle m| BA |m\rangle .
\end{aligned}
\tag{1.112}
$$

Thus we have

$$
\mathrm{Tr}(AB) = \mathrm{Tr}(BA). \tag{1.113}
$$

For the unitarily transformed operator we have

$$
\begin{aligned}
\mathrm{Tr}(A') &= \mathrm{Tr}(U^\dagger A U) \\
&= \mathrm{Tr}(U^\dagger (A U)) \\
&= \mathrm{Tr}((A U) U^\dagger) \\
&= \mathrm{Tr}(A (U U^\dagger)) \\
&= \mathrm{Tr}(A) \qquad \square
\end{aligned}
\tag{1.114}
$$

Exercise 1.11 Determinant of an exponential operator in terms of trace (2008 PHY355H1F final 1d.

If A is an Hermitian operator, show that

$$
\det(\exp A) = \exp(\mathrm{Tr}(A)) \tag{1.115}
$$

where the determinant (det) of an operator is the product of all its eigenvectors.

Answer for Exercise 10.9

The eigenvalues clue in the question provides the starting point. We write the exponential in its series form

$$
e^A = 1 + \sum_{k=1}^{\infty} \frac{1}{k!} A^k \tag{1.116}
$$

Now, suppose that we have the following eigenvalue relationships for A

$$A|n\rangle = \lambda_n |n\rangle . \tag{1.117}$$

From this the exponential is

$$\begin{aligned} e^A |n\rangle &= |n\rangle + \sum_{k=1}^{\infty} \frac{1}{k!} A^k |n\rangle \\ &= |n\rangle + \sum_{k=1}^{\infty} \frac{1}{k!} (\lambda_n)^k |n\rangle \\ &= e^{\lambda_n} |n\rangle . \end{aligned} \tag{1.118}$$

We see that the eigenstates of e^A are those of A, with eigenvalues e^{λ_n}.
By the definition of the determinant given we have

$$\begin{aligned} \det(e^A) &= \prod_n e^{\lambda_n} \\ &= e^{\sum_n \lambda_n} \\ &= e^{\mathrm{Tr}(A)}. \qquad \square \end{aligned} \tag{1.119}$$

2 COMMUTATOR AND TIME EVOLUTION

2.1 ROTATIONS USING MATRIX EXPONENTIALS

In [3] it is noted in problem 1.3 that any Unitary operator can be expressed in exponential form

$$U = e^{iC}, \tag{2.1}$$

where C is Hermitian. This is a powerful result hiding away in this problem. I have not actually managed to prove this yet to my satisfaction, but working through some examples is highly worthwhile. In particular it is interesting to compute the matrix C for a rotation matrix. One finds that the matrix for such a rotation operator is in fact one of the Pauli spin matrices, and I found it interesting that this falls out so naturally. Additionally, it is rather slick that one is able to so concisely express the rotation in exponential form, something that is natural and powerful in complex variable algebra, and also possible using Geometric Algebra using exponentials of bivectors. Here we can do it after all with nothing more than the plain old matrix algebra that everybody is already comfortable with.

The logarithm of the Unitary matrix By inspection we can invert eq. (2.1) for C, by taking the logarithm

$$C = -i \ln U. \tag{2.2}$$

The problem becomes one of evaluating the logarithm, or even giving meaning to it. I will assume that the functions of matrices that we are interested in are all polynomial in powers of the matrix, as in

$$f(U) = \sum_k \alpha_k U^k, \tag{2.3}$$

and that such series are convergent. Then using a spectral decomposition, possible since Unitary matrices are normal, we can write for diagonal $\Sigma = \left[\lambda_i\right]_i$

$$U = V \Sigma V^\dagger, \tag{2.4}$$

and

$$f(U) = V \left(\sum_k \alpha_k \Sigma^k \right) V^\dagger = V \Big[f(\lambda_i) \Big]_i V^\dagger. \tag{2.5}$$

Provided the logarithm has a convergent power series representation for U, we then have for our Hermitian matrix C

$$C = -iV(\ln \Sigma)V^\dagger \tag{2.6}$$

Evaluate this logarithm for an x, y plane rotation Given the rotation matrix

$$U = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}, \tag{2.7}$$

We find that the eigenvalues are $e^{\pm i\theta}$, with eigenvectors proportional to $(1, \pm i)$ respectively. Our decomposition for U is then given by eq. (2.4), and

$$\begin{aligned} V &= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} \\ \Sigma &= \begin{bmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{bmatrix}. \end{aligned} \tag{2.8}$$

Taking logs we have

$$\begin{aligned} C &= \frac{1}{2} \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} \begin{bmatrix} \theta & 0 \\ 0 & -\theta \end{bmatrix} \begin{bmatrix} 1 & -i \\ 1 & i \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} \begin{bmatrix} \theta & -i\theta \\ -\theta & -i\theta \end{bmatrix} \\ &= \begin{bmatrix} 0 & -i\theta \\ i\theta & 0 \end{bmatrix}. \end{aligned} \tag{2.9}$$

With the Pauli matrix

$$\sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \tag{2.10}$$

we then have for an x, y plane rotation matrix just:

$$C = \theta\sigma_2 \tag{2.11}$$

and

$$U = e^{i\theta\sigma_2}. \tag{2.12}$$

Immediately, since $\sigma_2^2 = I$, this also provides us with a trigonometric expansion

$$U = I\cos\theta + i\sigma_2\sin\theta. \tag{2.13}$$

By inspection one can see that this takes us full circle back to the original matrix form eq. (2.7) of the rotation. The exponential form of eq. (2.12) has a beauty that is however far superior to the plain old trigonometric matrix that we are comfortable with. All without any geometric algebra or bivector exponentials.

Three dimensional exponential rotation matrices By inspection, we can augment our matrix C for a three dimensional rotation in the x, y plane, or a y, z rotation, or a x, z rotation. Those are, respectively

$$\begin{aligned}
U_{x,y} &= \exp\begin{bmatrix} 0 & \theta & 0 \\ -\theta & 0 & 0 \\ 0 & 0 & i \end{bmatrix} \\
U_{y,z} &= \exp\begin{bmatrix} i & 0 & 0 \\ 0 & 0 & \theta \\ 0 & -\theta & 0 \end{bmatrix} \\
U_{x,z} &= \exp\begin{bmatrix} 0 & 0 & \theta \\ 0 & i & 0 \\ -\theta & 0 & 0 \end{bmatrix}
\end{aligned} \tag{2.14}$$

Each of these matrices can be related to each other by similarity transformation using the permutation matrices

$$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \tag{2.15}$$

and

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}. \tag{2.16}$$

Exponential matrix form for a Lorentz boost The next obvious thing to try with this matrix representation is a Lorentz boost.

$$L = \begin{bmatrix} \cosh\alpha & -\sinh\alpha \\ -\sinh\alpha & \cosh\alpha \end{bmatrix}, \tag{2.17}$$

where $\cosh\alpha = \gamma$, and $\tanh\alpha = \beta$.
This matrix has a spectral decomposition given by

$$\begin{aligned} V &= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \\ \Sigma &= \begin{bmatrix} e^{\alpha} & 0 \\ 0 & e^{-\alpha} \end{bmatrix}. \end{aligned} \tag{2.18}$$

Taking logs and computing C we have

$$\begin{aligned} C &= -\frac{i}{2} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} \alpha & 0 \\ 0 & -\alpha \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \\ &= -\frac{i}{2} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} \alpha & -\alpha \\ -\alpha & -\alpha \end{bmatrix} \\ &= i\alpha \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \end{aligned} \tag{2.19}$$

Again we have one of the Pauli spin matrices. This time it is

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{2.20}$$

So we can write our Lorentz boost eq. (2.17) as just

$$L = e^{-\alpha\sigma_1} = I\cosh\alpha - \sigma_1 \sinh\alpha. \tag{2.21}$$

By inspection again, we can come full circle by inspection from this last hyperbolic representation back to the original explicit matrix representation. Quite nifty!

It occurred to me after the fact that the Lorentz boost is not Unitary. The fact that the eigenvalues are not a purely complex phase term, like those of the rotation is actually a good hint that looking at how to characterize the eigenvalues of a unitary matrix can be used to show that the matrix $C = -iV \ln \Sigma V^\dagger$ is Hermitian.

2.2 ON COMMUTATION OF EXPONENTIALS

Previously while working a Liboff problem, I wondered about what the conditions were required for exponentials to commute. In those problems the exponential arguments were operators. Exponentials of bivectors as in quaternion like spatial or Lorentz boosts are also good examples of (sometimes) non-commutative exponentials. It appears likely that the key requirement is that the exponential arguments commute, but how does one show this? Here this is explored a bit.

If one could show that it was true that

$$e^x e^y = e^{x+y}. \tag{2.22}$$

Then it would also imply that

$$e^x e^y = e^y e^x. \tag{2.23}$$

Let us perform the school boy exercise to prove eq. (2.22) and explore the restrictions for such a proof. We assume a power series definition of the exponential operator, and do not assume the values x, y are numeric, instead just that they can be multiplied. A commutative multiplication will not be assumed.

By virtue of the power series exponential definition we have

$$e^x e^y = \sum_{k=0}^{\infty} \frac{1}{k!} x^k \sum_{m=0}^{\infty} \frac{1}{m!} y^m. \tag{2.24}$$

To attempt to put this into e^{x+y} form we will need to change the order that we evaluate the double sum, and here a picture fig. 2.1 is helpful.

For somebody who has seen this summation trick before the picture probably says it all. We want to iterate over all pairs (k, m), and could do so in $\{(k, 0), (k, 1), \cdots (k, \infty), k \in [0, \infty]\}$ order as in our sum. This is all the pairs of points in the upper right hand side of the grid. We can also cover these grid coordinates in a different order. In particular, these can be iterated over the

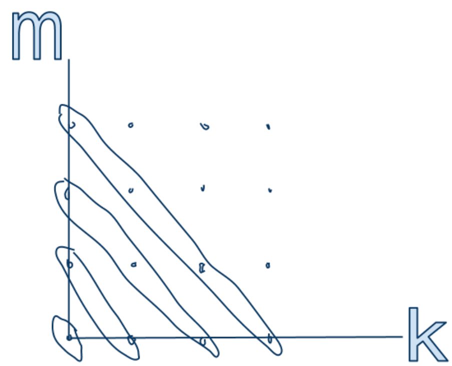

Figure 2.1: Double sum diagonal ordering

diagonals. The first diagonal having the point $(0, 0)$, the second with the points $\{(0, 1), (1, 0)\}$, the third with the points $\{(0, 2), (1, 1), (2, 0)\}$.

Observe that along each diagonal the sum of the coordinates is constant, and increases by one. Also observe that the number of points in each diagonal is this sum. These observations provide a natural way to index the new grid traversal. Labeling each of these diagonals with index j, and points on that subset with $n = 0, 1, \cdots, j$, we can express the original loop indices k and m in terms of these new (coupled) loop indices j and n as follows

$$k = j - n \tag{2.25}$$

$$m = n. \tag{2.26}$$

Our sum becomes

$$e^x e^y = \sum_{j=0}^{\infty} \sum_{n=0}^{j} \frac{1}{(j-n)!} x^{j-n} \frac{1}{n!} y^n. \tag{2.27}$$

With one small rearrangement, by introducing a $j!$ in both the numerator and the denominator, the goal is almost reached.

$$e^x e^y = \sum_{j=0}^{\infty} \frac{1}{j!} \sum_{n=0}^{j} \frac{j!}{(j-n)!\,n!} x^{j-n} y^n = \sum_{j=0}^{\infty} \frac{1}{j!} \sum_{n=0}^{j} \binom{n}{j} x^{j-n} y^n. \tag{2.28}$$

This shows where we have a requirement that x and y commute, because only in that case do we have a binomial expansion

$$(x+y)^j = \sum_{n=0}^{j} \binom{n}{j} x^{j-n} y^n, \tag{2.29}$$

in the interior sum. This reduced the problem to a consideration of the implication of possible non-commutation have on the binomial expansion. Consider the simple special case of $(x+y)^2$. If x and y do not necessarily commute, then we have

$$(x+y)^2 = x^2 + xy + yx + y^2 \tag{2.30}$$

whereas the binomial expansion formula has no such allowance for non-commutative multiplication and just counts the number of times a product can occur in any ordering as in

$$(x+y)^2 = x^2 + 2xy + y^2 = x^2 + 2yx + y^2. \tag{2.31}$$

One sees the built in requirement for commutative multiplication here. Now this does not prove that $e^x e^y != e^y e^x$ unconditionally if x and y do not commute, but we do see that a requirement for commutative multiplication is sufficient if we want equality of such commuted exponentials. In particular, the end result of the Liboff calculation where we had

$$e^{i\hat{f}} e^{-i\hat{f}}, \tag{2.32}$$

and was assuming this to be unity even for the differential operators $\hat{f}$ under consideration is now completely answered (since we have $(i\hat{f})(-i\hat{f})\psi = (-i\hat{f})(i\hat{f})\psi$).

2.3 CANONICAL COMMUTATOR

Based on the canonical relationship $[X, P] = i\hbar$, and $\langle x' | x \rangle = \delta(x' - x)$, Desai determines the form of the P operator in continuous space. A consequence of this is that the matrix element of the momentum operator is found to have a delta function specification

$$\langle x' \big| P \,| x \rangle = \delta(x - x') \left(-i\hbar \frac{d}{dx} \right). \tag{2.33}$$

In particular the matrix element associated with the state $|\phi\rangle$ is found to be

$$\langle x' \big| P |\phi\rangle = -i\hbar \frac{d}{dx'}\phi(x'). \tag{2.34}$$

Compare this to [9], where this last is taken as the definition of the momentum operator, and the relationship to the delta function is not spelled out explicitly. This canonical commutator approach, while more abstract, seems to have less black magic involved in the setup. We do require the commutator relationship $[X, P] = i\hbar$ to be pulled out of a magic hat, but at least the magic show is a structured one based on a small set of core assumptions.

It will likely be good to come back to this later when trying to reconcile this new (for me) Dirac notation with the more basic notation I am already comfortable with. When trying to compare the two, it will be good to note that there is a matrix element that is implied in the more old fashioned treatment in a book such as [1].

There is one fundamental assumption that appears to be made in this section that is not justified by anything except the end result. That is the assumption that P is a derivative like operator, acting with a product rule action. That is used to obtain (2.28) and is a fairly black magic operation. This same assumption, is also hiding, somewhat sneakily, in the manipulation for (2.44).

If one has to make that assumption that P is a derivative like operator, I do not feel this method of introducing it is any less arbitrary seeming. It is still pulled out of a magic hat, only because the answer is known ahead of time. The approach of [1], where the derivative nature is presented as consequence of transforming (via Fourier transforms) from the position to the momentum representation, seems much more intuitive and less arbitrary.

2.4 GENERALIZED MOMENTUM COMMUTATOR

It is stated that

$$[P, X^n] = -ni\hbar X^{n-1}. \tag{2.35}$$

Let us prove this. The $n = 1$ case is the canonical commutator, which is assumed. Is there any good way to justify that from first principles, as presented in the text? We have to prove this for n, given the relationship for $n-1$. Expanding the nth power commutator we have

$$\begin{aligned} [P, X^n] &= PX^n - X^n P \\ &= PX^{n-1}X - X^n P \end{aligned} \tag{2.36}$$

Rearranging the $n-1$ result we have

$$PX^{n-1} = X^{n-1}P - (n-1)i\hbar X^{n-2}, \tag{2.37}$$

and can insert that in our $[P, X^n]$ expansion for

$$\begin{aligned}
[P, X^n] &= \left(X^{n-1}P - (n-1)i\hbar X^{n-2}\right)X - X^n P \\
&= X^{n-1}(PX) - (n-1)i\hbar X^{n-1} - X^n P \\
&= X^{n-1}(XP - i\hbar) - (n-1)i\hbar X^{n-1} - X^n P \\
&= -X^{n-1}i\hbar - (n-1)i\hbar X^{n-1} \\
&= -ni\hbar X^{n-1} \qquad \square
\end{aligned} \tag{2.38}$$

2.5 UNCERTAINTY PRINCIPLE

The origin of the statement $[\Delta A, \Delta B] = [A, B]$ is not something that seemed obvious. Expanding this out however is straightforward, and clarifies things. That is

$$\begin{aligned}
[\Delta A, \Delta B] &= (A - \langle A \rangle)(B - \langle B \rangle) - (B - \langle B \rangle)(A - \langle A \rangle) \\
&= \left(AB - \langle A \rangle B - \langle B \rangle A + \langle A \rangle \langle B \rangle\right) - \left(BA - \langle B \rangle A - \langle A \rangle B + \langle B \rangle \langle A \rangle\right) \\
&= AB - BA \\
&= [A, B] \qquad \square
\end{aligned} \tag{2.39}$$

2.6 SIZE OF A PARTICLE

I found it curious that using $\Delta x \Delta p \approx \hbar$ instead of $\Delta x \Delta p \geq \hbar/2$, was sufficient to obtain the hydrogen ground state energy $E_{\text{min}} = -e^2/2a_0$, without also having to do any factor of two fudging.

2.7 SPACE DISPLACEMENT OPERATOR

Initial notes I had be curious to know if others find the loose use of equality for approximation after approximation slightly disturbing too?

I also find it curious that (2.140) is written

$$D(x) = \exp\left(-i\frac{P}{\hbar}x\right), \tag{2.40}$$

and not

$$D(x) = \exp\left(-ix\frac{P}{\hbar}\right). \tag{2.41}$$

Is this intentional? It does not seem like P ought to be acting on x in this case, so why order the terms that way?

Expanding the application of this operator, or at least its first order Taylor series, is helpful to get an idea about this. Doing so, with the original $\Delta x'$ value used in the derivation of the text we have to start

$$\begin{aligned} D(\Delta x') \left|\phi\right\rangle &\approx \left(1 - i\frac{P}{\hbar}\Delta x'\right)\left|\phi\right\rangle \\ &= \left(1 - i\left(-i\hbar\delta(x-x')\frac{\partial}{\partial x}\right)\frac{1}{\hbar}\Delta x'\right)\left|\phi\right\rangle \end{aligned} \tag{2.42}$$

This shows that the Δx factor can be commuted with the momentum operator, as it is not a function of x', so the question of Px, vs xP above appears to be a non-issue.

Regardless of that conclusion, it seems worthy to continue an attempt at expanding this shift operator action on the state vector. Let us do so, but do so by computing the matrix element $\left\langle x'\right| D(\Delta x') \left|\phi\right\rangle$. That is

$$\begin{aligned} \left\langle x'\right| D(\Delta x') \left|\phi\right\rangle &\approx \left\langle x' | \phi\right\rangle - \left\langle x'\right| \delta(x-x')\frac{\partial}{\partial x}\Delta x' \left|\phi\right\rangle \\ &= \phi(x') - \int \left\langle x'\right| \delta(x-x')\frac{\partial}{\partial x}\Delta x' \left|x'\right\rangle \left\langle x' | \phi\right\rangle dx' \\ &= \phi(x') - \Delta x' \int \delta(x-x')\frac{\partial}{\partial x} \left\langle x' | \phi\right\rangle dx' \\ &= \phi(x') - \Delta x' \frac{\partial}{\partial x'} \left\langle x' | \phi\right\rangle \\ &= \phi(x') - \Delta x' \frac{\partial}{\partial x'}\phi(x') \end{aligned} \tag{2.43}$$

This is consistent with the text. It is interesting, and initially surprising that the space displacement operator when applied to a state vector introduces a negative shift in the wave function associated with that state vector. In the derivation of the text, this was associated with the use of integration by parts (ie: due to the sign change in that integration). Here we see it sneak back in, due to the i^2 once the momentum operator is expanded completely.

As last note and question. The first order Taylor approximation of the momentum operator was used. If the higher order terms are retained, as in

$$\exp\left(-i\Delta x'\frac{P}{\hbar}\right) = 1 - \Delta x'\delta(x-x')\frac{\partial}{\partial x} + \frac{1}{2}\left(-\Delta x'\delta(x-x')\frac{\partial}{\partial x}\right)^2 + \cdots, \tag{2.44}$$

then how does one evaluate a squared delta function (or Nth power)?

Talked to Vatche about this after class. The key to this is sequential evaluation. Considering the simple case for P^2, we evaluate one operator at a time, and never actually square the delta function

$$\langle x' \big| P^2 |\phi\rangle \tag{2.45}$$

I was also questioned why I was including the delta function at this point. Why would I do that. Thinking further on this, I see that is not a reasonable thing to do. That delta function only comes into the mix when one takes the matrix element of the momentum operator as in

$$\langle x' \big| P |x\rangle = -i\hbar\delta(x - x')\frac{d}{dx'}. \tag{2.46}$$

This is very much like the fact that the delta function only shows up in the continuous representation in other context where one has matrix elements. The most simple example of which is just

$$\langle x'|x\rangle = \delta(x - x'). \tag{2.47}$$

I also see now that the momentum operator is directly identified with the derivative (no delta function) in two other places in the text. These are equations (2.32) and (2.46) respectively:

$$\begin{aligned} P(x) &= -i\hbar\frac{d}{dx} \\ P &= -i\hbar\frac{d}{dX}. \end{aligned} \tag{2.48}$$

In the first, (2.32), I thought the $P(x)$ was somehow different, just a helpful expression found along the way, but now it occurs to me that this was intended to be an unambiguous representation of the momentum operator itself.

A second try Getting a feel for this Dirac notation takes a bit of adjustment. Let us try evaluating the matrix element for the space displacement operator again, without abusing the notation, or thinking that we have a requirement for squared delta functions and other weirdness. We start with

$$
\begin{aligned}
D(\Delta x') \left|\phi\right\rangle &= e^{-\frac{iP\Delta x'}{\hbar}} \left|\phi\right\rangle \\
&= \int dx e^{-\frac{iP\Delta x'}{\hbar}} \left|x\right\rangle \left\langle x|\phi\right\rangle \\
&= \int dx e^{-\frac{iP\Delta x'}{\hbar}} \left|x\right\rangle \phi(x).
\end{aligned}
\tag{2.49}
$$

Now, to evaluate $e^{-\frac{iP\Delta x'}{\hbar}} \left|x\right\rangle$, we can expand in series

$$
e^{-\frac{iP\Delta x'}{\hbar}} \left|x\right\rangle = \left|x\right\rangle + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{-i\Delta x'}{\hbar}\right)^k P^k \left|x\right\rangle .
\tag{2.50}
$$

It is tempting to left multiply by $\left\langle x'\right|$ and commute that past the P^k, then write $P^k = -i\hbar d/dx$. That probably produces the correct result, but is abusive of the notation. We can still left multiply by $\left\langle x'\right|$, but to be proper, I think we have to leave that on the left of the P^k operator. This yields

$$
\begin{aligned}
\left\langle x'\right| D(\Delta x') \left|\phi\right\rangle &= \int dx \left(\left\langle x'|x\right\rangle + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{-i\Delta x'}{\hbar}\right)^k \left\langle x'\right| P^k \left|x\right\rangle \right) \phi(x) \\
&= \int dx \delta(x' - x)\phi(x) + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{-i\Delta x'}{\hbar}\right)^k \int dx \left\langle x'\right| P^k \left|x\right\rangle \phi(x).
\end{aligned}
\tag{2.51}
$$

The first integral is just $\phi(x')$, and we are left with integrating the higher power momentum matrix elements, applied to the wave function $\phi(x)$. We can proceed iteratively to expand those integrals

$$
\int dx \left\langle x'\right| P^k \left|x\right\rangle \phi(x) = \iint dx dx'' \left\langle x'\right| P^{k-1} \left|x''\right\rangle \left\langle x''\right| P \left|x\right\rangle \phi(x)
\tag{2.52}
$$

Now we have a matrix element that we know what to do with. Namely, $\left\langle x''\right| P \left|x\right\rangle = -i\hbar\delta(x'' - x)\partial/\partial x$, which yields

$$
\begin{aligned}
\int dx \left\langle x'\right| P^k \left|x\right\rangle \phi(x) &= -i\hbar \iint dx dx'' \left\langle x'\right| P^{k-1} \left|x''\right\rangle \delta(x'' - x) \frac{\partial}{\partial x}\phi(x) \\
&= -i\hbar \int dx \left\langle x'\right| P^{k-1} \left|x\right\rangle \frac{\partial \phi(x)}{\partial x}.
\end{aligned}
\tag{2.53}
$$

Each similar application of the identity operator brings down another $-i\hbar$ and derivative yielding

$$\int dx \left\langle x' \right| P^k \left| x \right\rangle \phi(x) = (-i\hbar)^k \frac{\partial^k \phi(x')}{\partial x'^k}. \tag{2.54}$$

Going back to our displacement operator matrix element, we now have

$$\begin{aligned}\left\langle x' \right| D(\Delta x') \left| \phi \right\rangle &= \phi(x') + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{-i\Delta x'}{\hbar} \right)^k (-i\hbar)^k \frac{\partial^k \phi(x')}{\partial x'^k} \\ &= \phi(x') + \sum_{k=1}^{\infty} \frac{1}{k!} \left(-\Delta x' \frac{\partial}{\partial x'} \right)^k \phi(x') \\ &= \phi(x' - \Delta x').\end{aligned} \tag{2.55}$$

This shows nicely why the sign goes negative and it is no longer surprising when one observes that this can be obtained directly by using the adjoint relationship

$$\begin{aligned}\left\langle x' \right| D(\Delta x') \left| \phi \right\rangle &= (D^\dagger(\Delta x') \left| x' \right\rangle)^\dagger \left| \phi \right\rangle \\ &= (D(-\Delta x') \left| x' \right\rangle)^\dagger \left| \phi \right\rangle \\ &= \left| x' - \Delta x' \right\rangle^\dagger \left| \phi \right\rangle \\ &= \left\langle x' - \Delta x' | \phi \right\rangle \\ &= \phi(x' - \Delta x')\end{aligned} \tag{2.56}$$

That is a whole lot easier than the integral manipulation, but at least shows that we now have a feel for the notation, and have confirmed the exponential formulation of the operator nicely.

2.8 TIME EVOLUTION OPERATOR

The phrase "we identify time evolution with the Hamiltonian". What a magic hat maneuver! Is there a way that this would be logical without already knowing the answer?

2.9 DISPERSION DELTA FUNCTION REPRESENTATION

The Principle part notation here I found a bit unclear. He writes

$$\lim_{\epsilon \to 0} \frac{(x' - x)}{(x' - x)^2 + \epsilon^2} = P\left(\frac{1}{x' - x} \right). \tag{2.57}$$

In complex variables the principle part is the negative power series terms. For example for $f(z) = \sum a_k z^k$, the principle part is

$$\sum_{k=-\infty}^{-1} a_k z^k \tag{2.58}$$

This does not vanish at $z = 0$ as the principle part in this section is stated to. In (2.202) he pulls the P out of the integral, but I think the intention is really to keep this associated with the $1/(x' - x)$, as in

$$\lim_{\epsilon \to 0} \frac{1}{\pi} \int_0^\infty dx' \frac{f(x')}{x' - x - i\epsilon} = \frac{1}{\pi} \int_0^\infty dx' f(x') P\left(\frac{1}{x' - x}\right) + i f(x) \tag{2.59}$$

Will this even have any relevance in this text?

2.10 UNITARY EXPONENTIAL SANDWICH

One of the chapter II exercises in [3] involves a commutator exponential sandwich of the form

$$e^{iF} B e^{-iF} \tag{2.60}$$

where F is Hermitian. Asking about commutators on physicsforums I was told that such sandwiches (my term) preserve expectation values, and also have a Taylor series like expansion involving the repeated commutators. Let us derive the commutator relationship.

Let us expand a sandwich of this form in series, and shuffle the summation order so that we sum over all the index plane diagonals $k + m =$ constant. That is

$$\begin{aligned}
e^A B e^{-A} &= \sum_{k,m=0}^{\infty} \frac{1}{k!\, m!} A^k B (-A)^m \\
&= \sum_{r=0}^{\infty} \sum_{m=0}^{r} \frac{1}{(r-m)!\, m!} A^{r-m} B (-A)^m \\
&= \sum_{r=0}^{\infty} \frac{1}{r!} \sum_{m=0}^{r} \frac{r!}{(r-m)!\, m!} A^{r-m} B (-A)^m \\
&= \sum_{r=0}^{\infty} \frac{1}{r!} \sum_{m=0}^{r} \binom{r}{m} A^{r-m} B (-A)^m .
\end{aligned} \tag{2.61}$$

Assuming that these interior sums can be written as commutators, we will shortly have an induction exercise. Let us write these out for a couple values of r to get a feel for things.

- $r = 1$

$$\binom{1}{0} AB + \binom{1}{1} B(-A) = [A, B] \tag{2.62}$$

- $r = 2$

$$\binom{2}{0} A^2 B + \binom{2}{1} AB(-A) + \binom{2}{2} B(-A)^2 = A^2 B - 2ABA + BA \tag{2.63}$$

This compares exactly to the double commutator:

$$\begin{aligned} [A, [A, B]] &= A(AB - BA) - (AB - BA)A \\ &= A^2 B - ABA - ABA + BA^2 \\ &= A^2 B - 2ABA + BA^2 \end{aligned} \tag{2.64}$$

- $r = 3$

$$\binom{3}{0} A^3 B + \binom{3}{1} A^2 B(-A) + \binom{3}{2} AB(-A)^2 + \binom{3}{3} B(-A)^3 = A^3 B - 3A^2 BA + 3ABA^2 - BA^3. \tag{2.65}$$

And this compares exactly to the triple commutator

$$\begin{aligned} [A, [A, [A, B]]] &= A^3 B - 2A^2 BA + ABA^2 - (A^2 BA - 2ABA^2 + BA^3) \\ &= A^3 B - 3A^2 BA + 3ABA^2 - BA^3 \end{aligned} \tag{2.66}$$

The induction pattern is clear. Let us write the r fold commutator as

$$C_r(A, B) \equiv \overbrace{[A, [A, \cdots, [A,}^{r \text{ times}} B]] \cdots] = \sum_{m=0}^{r} \binom{r}{m} A^{r-m} B(-A)^m, \tag{2.67}$$

and calculate this for the $r+1$ case to verify the induction hypothesis. We have

$$\begin{aligned}
C_{r+1}(A,B) &= \sum_{m=0}^{r}\binom{r}{m}\Big(A^{r-m+1}B(-A)^m - A^{r-m}B(-A)^m A\Big) \\
&= \sum_{m=0}^{r}\binom{r}{m}\Big(A^{r-m+1}B(-A)^m + A^{r-m}B(-A)^{m+1}\Big) \\
&= A^{r+1}B + \sum_{m=1}^{r}\binom{r}{m}A^{r-m+1}B(-A)^m + \sum_{m=0}^{r-1}\binom{r}{m}A^{r-m}B(-A)^{m+1} + B(-A)^{r+1} \\
&= A^{r+1}B + \sum_{k=0}^{r-1}\binom{r}{k+1}A^{r-k}B(-A)^{k+1} + \sum_{m=0}^{r-1}\binom{r}{m}A^{r-m}B(-A)^{m+1} + B(-A)^{r+1} \\
&= A^{r+1}B + \sum_{k=0}^{r-1}\left(\binom{r}{k+1} + \binom{r}{k}\right)A^{r-k}B(-A)^{k+1} + B(-A)^{r+1}
\end{aligned} \tag{2.68}$$

We now have to sum those binomial coefficients. I like the search and replace technique for this, picking two visibly distinct numbers for r, and k that are easy to manipulate without abstract confusion. How about $r = 7$, and $k = 3$. Using those we have

$$\begin{aligned}
\binom{7}{3+1} + \binom{7}{3} &= \frac{7!}{(3+1)!\,(7-3-1)!} + \frac{7!}{3!\,(7-3)!} \\
&= \frac{7!\,(7-3)}{(3+1)!\,(7-3)!} + \frac{7!\,(3+1)}{(3+1)!\,(7-3)!} \\
&= \frac{7!\,\big(7-3+3+1\big)}{(3+1)!\,(7-3)!} \\
&= \frac{(7+1)!}{(3+1)!\,((7+1)-(3+1))!}.
\end{aligned} \tag{2.69}$$

Straight text replacement of 7 and 3 with r and k respectively now gives the harder to follow, but more general identity

$$\begin{aligned}\binom{r}{k+1}+\binom{r}{k} &= \frac{r!}{(k+1)!\,(r-k-1)!}+\frac{r!}{k!\,(r-k)!} \\ &= \frac{r!\,(r-k)}{(k+1)!\,(r-k)!}+\frac{r!\,(k+1)}{(k+1)!\,(r-k)!} \\ &= \frac{r!\,\big(r-k+k+1\big)}{(k+1)!\,(r-k)!} \\ &= \frac{(r+1)!}{(k+1)!\,((r+1)-(k+1))!} \\ &= \binom{r+1}{k+1}\end{aligned} \tag{2.70}$$

For our commutator we now have

$$\begin{aligned}C_{r+1}(A,B) &= A^{r+1}B+\sum_{k=0}^{r-1}\binom{r+1}{k+1}A^{r-k}B(-A)^{k+1}+B(-A)^{r+1} \\ &= A^{r+1}B+\sum_{s=1}^{r}\binom{r+1}{s}A^{r+1-s}B(-A)^{s}+B(-A)^{r+1} \\ &= \sum_{s=0}^{r+1}\binom{r+1}{s}A^{r+1-s}B(-A)^{s} \qquad \square\end{aligned} \tag{2.71}$$

That completes the inductive proof and allows us to write

$$e^{A}Be^{-A} = \sum_{r=0}^{\infty}\frac{1}{r!}C_r(A,B), \tag{2.72}$$

Or, in explicit form

$$e^{A}Be^{-A} = B+\frac{1}{1!}\,[A,B]+\frac{1}{2!}\,[A,[A,B]]+\cdots \tag{2.73}$$

2.11 LECTURE NOTES: REVIEW

Deal with operators that have continuous eigenvalues and eigenvectors. We now express

$$|\phi\rangle = \int dk \overbrace{\boxed{f(k)}}^{\text{coefficients analogous to } c_n} |k\rangle \tag{2.74}$$

Now if we project onto k'

$$\begin{aligned} \langle k'|\phi\rangle &= \int dk f(k) \overbrace{\boxed{\langle k'|k\rangle}}^{\text{Dirac delta}} \\ &= \int dk f(k)\delta(k'-k) \\ &= f(k') \end{aligned} \tag{2.75}$$

Unlike the discrete case, this is not a probability. Probability density for obtaining outcome k' is $|f(k')|^2$.

Example 2.

$$|\phi\rangle = \int dk f(k) |k\rangle \tag{2.76}$$

Now if we project x onto both sides

$$\langle x|\phi\rangle = \int dk f(k) \langle x|k\rangle \tag{2.77}$$

With $\langle x|k\rangle = u_k(x)$

$$\begin{aligned} \phi(x) &\equiv \langle x|\phi\rangle \\ &= \int dk f(k) u_k(x) \\ &= \int dk f(k) \frac{1}{\sqrt{L}} e^{ikx} \end{aligned} \tag{2.78}$$

This is with periodic boundary value conditions for the normalization. The infinite normalization is also possible.

$$\phi(x) = \frac{1}{\sqrt{L}} \int dk f(k) e^{ikx} \tag{2.79}$$

Multiply both sides by $e^{-ik'x}/\sqrt{L}$ and integrate. This is analogous to multiplying $|\phi\rangle = \int f(k) |k\rangle \, dk$ by $\langle k'|$. We get

$$\begin{aligned}
\int \phi(x) \frac{1}{\sqrt{L}} e^{-ik'x} dx &= \frac{1}{L} \iint dk f(k) e^{i(k-k')x} dx \\
&= \int dk f(k) \Big(\frac{1}{L} \int e^{i(k-k')x}\Big) \\
&= \int dk f(k) \delta(k - k') \\
&= f(k')
\end{aligned} \tag{2.80}$$

$$f(k') = \int \phi(x) \frac{1}{\sqrt{L}} e^{-ik'x} dx \tag{2.81}$$

We can talk about the state vector in terms of its position basis $\phi(x)$ or in the momentum space via Fourier transformation. This is the equivalent thing, but just expressed different. The question of interpretation in terms of probabilities works out the same. Either way we look at the probability density.

The quantity

$$|\phi\rangle = \int dk f(k) |k\rangle \tag{2.82}$$

is also called a wave packet state since it involves a superposition of many stats $|k\rangle$. Example: See Fig 4.1 (Gaussian wave packet, with $|\phi|^2$ as the height). This wave packet is a snapshot of the wave function amplitude at one specific time instant. The evolution of this wave packet is governed by the Hamiltonian, which brings us to chapter 3.

2.12 PROBLEMS

Exercise 2.1 Cauchy-Schwartz identity (*[3] pr 2.1*)

FIXME: describe.

Answer for Exercise 2.1

We wish to find the value of λ that is just right to come up with the desired identity. The starting point is the expansion of the inner product

$$\langle a + \lambda b | a + \lambda b \rangle = \langle a|a\rangle + \lambda\lambda^* \langle b|b\rangle + \lambda \langle a|b\rangle + \lambda^* \langle b|a\rangle \tag{2.83}$$

There is a trial and error approach to this problem, where one magically picks $\lambda \propto \langle b|a\rangle / \langle b|b\rangle^n$, and figures out the proportionality constant and scale factor for the denominator to do the job. A nicer way is to set up the problem as an extreme value exercise. We can write this inner product as a function of λ, and proceed with setting the derivative equal to zero

$$f(\lambda) = \langle a|a\rangle + \lambda\lambda^* \langle b|b\rangle + \lambda \langle a|b\rangle + \lambda^* \langle b|a\rangle \tag{2.84}$$

Its derivative is

$$\begin{aligned}\frac{df}{d\lambda} &= \left(\lambda^* + \lambda\frac{d\lambda^*}{d\lambda}\right)\langle b|b\rangle + \langle a|b\rangle + \frac{d\lambda^*}{d\lambda}\langle b|a\rangle \\ &= \lambda^* \langle b|b\rangle + \langle a|b\rangle + \frac{d\lambda^*}{d\lambda}\left(\lambda \langle b|b\rangle + \langle b|a\rangle\right)\end{aligned} \tag{2.85}$$

Now, we have a bit of a problem with $d\lambda^*/d\lambda$, since that does not actually exist. However, that problem can be side stepped if we insist that the factor that multiplies it is zero. That provides a value for λ that also kills of the remainder of $df/d\lambda$. That value is

$$\lambda = -\frac{\langle b|a\rangle}{\langle b|b\rangle}. \tag{2.86}$$

Back substitution yields

$$\langle a + \lambda b | a + \lambda b \rangle = \langle a|a\rangle - \langle a|b\rangle \langle b|a\rangle / \langle b|b\rangle \geq 0. \tag{2.87}$$

This is easily rearranged to obtain the desired result:

$$\langle a|a\rangle \langle b|b\rangle \geq \langle b|a\rangle \langle a|b\rangle . \tag{2.88}$$

Exercise 2.2 Uncertainty relation (*[3] pr 2.2*)

FIXME: describe.

Answer for Exercise 2.2

Using the Schwartz inequality of problem 1, and a symmetric and antisymmetric (anticommutator and commutator) sum of products that

$$|\Delta A \Delta B|^2 \geq \frac{1}{4}\left|[A, B]\right|^2, \tag{2.89}$$

and that this result implies

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{2.90}$$

The solution This problem seems somewhat misleading, since the Schwartz inequality appears to have nothing to do with showing eq. (2.89), but only with the split of the operator product into symmetric and antisymmetric parts. Another possible tricky thing about this problem is that there is no mention of the anticommutator in the text at this point that I can find, so if one does not know what it is defined as, it must be figured out by context.

I have also had an interpretation problem with this since $\Delta x \Delta p$ in eq. (2.90) cannot mean the operators as is the case of eq. (2.89). My assumption is that in eq. (2.90) these deltas are really absolute expectation values, and that we really want to show

$$|\langle \Delta X \rangle||\langle \Delta P \rangle| \geq \frac{\hbar}{2}. \tag{2.91}$$

However, I am unable to demonstrate this. Instead I am able to show two things:

$$\begin{aligned} \left\langle (\Delta X)^2 \right\rangle \left\langle (\Delta P)^2 \right\rangle &\geq \frac{\hbar^2}{4} \\ |\langle \Delta X \Delta P \rangle| &\geq \frac{\hbar}{2} \end{aligned} \tag{2.92}$$

Is one of these the result to be shown? Note that only the first of these required the Schwartz inequality. Also, it seems strange that we want the expectation of the operator $\Delta X \Delta P$?

Starting with the first part of the problem, note that we can factor any operator product into a linear combination of two Hermitian operators using the commutator and anticommutator. That is

$$\begin{aligned} CD &= \frac{1}{2}\left(CD + DC\right) + \frac{1}{2}\left(CD - DC\right) \\ &= \frac{1}{2}\left(CD + DC\right) + \frac{1}{2i}\left(CD - DC\right) i \\ &\equiv \frac{1}{2}\{C, D\} + \frac{1}{2i}\left[C, D\right] i \end{aligned} \tag{2.93}$$

For Hermitian operators C, and D, using $(CD)^\dagger = D^\dagger C^\dagger = DC$, we can show that the two operator factors are Hermitian,

$$\begin{aligned}\left(\frac{1}{2}\{C,D\}\right)^\dagger &= \frac{1}{2}\left(CD+DC\right)^\dagger \\ &= \frac{1}{2}\left(D^\dagger C^\dagger + C^\dagger D^\dagger\right) \\ &= \frac{1}{2}\left(DC+CD\right) \\ &= \frac{1}{2}\{C,D\},\end{aligned} \tag{2.94}$$

$$\begin{aligned}\left(\frac{1}{2}\left[C,D\right]i\right)^\dagger &= -\frac{i}{2}\left(CD-DC\right)^\dagger \\ &= -\frac{i}{2}\left(D^\dagger C^\dagger - C^\dagger D^\dagger\right) \\ &= -\frac{i}{2}\left(DC-CD\right) \\ &= \frac{1}{2}\left[C,D\right]i\end{aligned} \tag{2.95}$$

So for the absolute squared value of the expectation of product of two operators we have

$$\begin{aligned}\langle CD\rangle^2 &= \left|\left\langle \frac{1}{2}\{C,D\} + \frac{1}{2i}\left[C,D\right]i\right\rangle\right|^2 \\ &= \left|\frac{1}{2}\left\langle\{C,D\}\right\rangle + \frac{1}{2i}\left\langle\left[C,D\right]i\right\rangle\right|^2.\end{aligned} \tag{2.96}$$

Now, these expectation values are real, given the fact that these operators are Hermitian. Suppose we write $a = \langle\{C,D\}\rangle/2$, and $b = \left\langle\left[C,D\right]i\right\rangle/2$, then we have

$$\begin{aligned}\left|\frac{1}{2}\left\langle\{C,D\}\right\rangle + \frac{1}{2i}\left\langle\left[C,D\right]i\right\rangle\right|^2 &= |a-bi|^2 \\ &= (a-bi)(a+bi) \\ &= a^2+b^2\end{aligned} \tag{2.97}$$

So we have for the squared expectation value of the operator product CD

$$\begin{aligned}
\langle CD\rangle^2 &= \frac{1}{4}\left\langle\{C,D\}\right\rangle^2 + \frac{1}{4}\left\langle[C,D]\,i\right\rangle^2 \\
&= \frac{1}{4}\left|\left\langle\{C,D\}\right\rangle\right|^2 + \frac{1}{4}\left|\left\langle[C,D]\,i\right\rangle\right|^2 \\
&= \frac{1}{4}\left|\left\langle\{C,D\}\right\rangle\right|^2 + \frac{1}{4}\left|\left\langle[C,D]\right\rangle\right|^2 \\
&\ge \frac{1}{4}\left|\left\langle[C,D]\right\rangle\right|^2.
\end{aligned} \tag{2.98}$$

With $C = \Delta A$, and $D = \Delta B$, this almost completes the first part of the problem. The remaining thing to note is that $[\Delta A, \Delta B] = [A, B]$. This last is straight forward to show

$$\begin{aligned}
[\Delta A, \Delta B] &= [A - \langle A\rangle, B - \langle B\rangle] \\
&= (A - \langle A\rangle)(B - \langle B\rangle) - (B - \langle B\rangle)(A - \langle A\rangle) \\
&= \left(AB - \langle A\rangle B - \langle B\rangle A + \langle A\rangle\langle B\rangle\right) - \left(BA - \langle B\rangle A - \langle A\rangle B + \langle B\rangle\langle A\rangle\right) \\
&= AB - BA \\
&= [A, B]\,.
\end{aligned} \tag{2.99}$$

Putting the pieces together we have

$$\langle \Delta A \Delta B\rangle^2 \ge \frac{1}{4}\left|\left\langle[A,B]\right\rangle\right|^2. \tag{2.100}$$

With expectation value implied by the absolute squared, this reproduces relation eq. (2.89) as desired.

For the remaining part of the problem, with $|\alpha\rangle = \Delta A\,|\psi\rangle$, and $|\beta\rangle = \Delta B\,|\psi\rangle$, and noting that $(\Delta A)^\dagger = \Delta A$ for Hermitian operator A (or B too in this case), the Schwartz inequality

$$\langle\alpha|\alpha\rangle\,\langle\beta|\beta\rangle \ge |\langle\beta|\alpha\rangle|^2, \tag{2.101}$$

takes the following form

$$\langle\psi|\,(\Delta A)^\dagger \Delta A\,|\psi\rangle\,\langle\psi|\,(\Delta B)^\dagger B\,|\psi\rangle \ge \left|\langle\psi|\,(\Delta B)^\dagger A\,|\psi\rangle\right|^2. \tag{2.102}$$

These are expectation values, and allow us to use eq. (2.100) to show

$$\begin{aligned}
\left\langle(\Delta A)^2\right\rangle\left\langle(\Delta B)^2\right\rangle &\ge |\langle\Delta B \Delta A\rangle|^2 \\
&= \frac{1}{4}\left|\left\langle[B,A]\right\rangle\right|^2.
\end{aligned} \tag{2.103}$$

For $A = X$, and $B = P$, this is

$$\left\langle (\Delta X)^2 \right\rangle \left\langle (\Delta P)^2 \right\rangle \geq \frac{\hbar^2}{4} \tag{2.104}$$

Hmm. This does not look like it is quite the result that I expected? We have $\left\langle (\Delta X)^2 \right\rangle \left\langle (\Delta P)^2 \right\rangle$ instead of $\langle \Delta X \rangle^2 \langle \Delta P \rangle^2$?

Let us step back slightly. Without introducing the Schwartz inequality the result eq. (2.100) of the commutator manipulation, and $[X, P] = i\hbar$ gives us

$$\langle \Delta X \Delta P \rangle^2 \geq \frac{\hbar^2}{4}, \tag{2.105}$$

and taking roots we have

$$|\langle \Delta X \Delta P \rangle| \geq \frac{\hbar}{2}. \tag{2.106}$$

Is this really what we were intended to show?

Attempting to answer this myself, I refer to [9], where I find he uses a loose notation for this too, and writes in his equation 3.36

$$(\Delta C)^2 = \left\langle (C - \langle C \rangle)^2 \right\rangle = \left\langle C^2 \right\rangle - \langle C \rangle^2 \tag{2.107}$$

This usage seems consistent with that, so I think that it is a reasonable assumption that uncertainty relation $\Delta x \Delta p \geq \hbar/2$ is really shorthand notation for the more cumbersome relation involving roots of the expectations of mean-square deviation operators

$$\sqrt{\langle (X - \langle X \rangle)^2 \rangle} \sqrt{\langle (P - \langle P \rangle)^2 \rangle} \geq \frac{\hbar}{2}. \tag{2.108}$$

This is in fact what was proved arriving at eq. (2.104).

Ah ha! Found it. Referring to equation 2.93 in the text, I see that a lower case notation $\Delta x = \sqrt{(\Delta X)^2}$, was introduced. This explains what seemed like ambiguous notation ... it was just tricky notation, perfectly well explained, but done in passing in the text in a somewhat hidden seeming way.

Exercise 2.3 Hermitian radial differential operator (*[3] pr 2.5*)

Show that the operator

$$R = -i\hbar\frac{\partial}{\partial r}, \tag{2.109}$$

is not Hermitian, and find the constant a so that

$$T = -i\hbar\left(\frac{\partial}{\partial r} + \frac{a}{r}\right), \tag{2.110}$$

is Hermitian.

Answer for Exercise 2.3

For the first part of the problem we can show that

$$\left(\left\langle\hat{\psi}\middle| R \middle|\hat{\phi}\right\rangle\right)^* \neq \left\langle\hat{\phi}\middle| R \middle|\hat{\psi}\right\rangle. \tag{2.111}$$

For the RHS we have

$$\left\langle\hat{\phi}\middle| R \middle|\hat{\psi}\right\rangle = -i\hbar\iiint drd\theta d\phi r^2 \sin\theta\hat{\phi}^*\frac{\partial\hat{\psi}}{\partial r} \tag{2.112}$$

and for the LHS we have

$$\begin{aligned}\left(\left\langle\hat{\psi}\middle| R \middle|\hat{\phi}\right\rangle\right)^* &= i\hbar\iiint drd\theta d\phi r^2 \sin\theta\hat{\psi}\frac{\partial\hat{\phi}^*}{\partial r}\\ &= -i\hbar\iiint drd\theta d\phi \sin\theta\left(2r\hat{\psi} + r^2\frac{\partial r}{\partial\hat{\psi}}\right)\hat{\phi}^*\end{aligned} \tag{2.113}$$

So, unless $r\hat{\psi} = 0$, the operator R is not Hermitian.
Moving on to finding the constant a such that T is Hermitian we calculate

$$\begin{aligned}\left(\left\langle\hat{\psi}\middle| T \middle|\hat{\phi}\right\rangle\right)^* &= i\hbar\iiint drd\theta d\phi r^2 \sin\theta\hat{\psi}\left(\frac{\partial}{\partial r} + \frac{a}{r}\right)\hat{\phi}^*\\ &= i\hbar\iiint drd\theta d\phi \sin\theta\hat{\psi}\left(r^2\frac{\partial}{\partial r} + ar\right)\hat{\phi}^*\\ &= -i\hbar\iiint drd\theta d\phi \sin\theta\left(r^2\frac{\partial\hat{\psi}}{\partial r} + 2r\hat{\psi} - ar\hat{\psi}\right)\hat{\phi}^*\end{aligned} \tag{2.114}$$

and

$$\left\langle \hat{\boldsymbol{\phi}} \right| T \left| \hat{\boldsymbol{\psi}} \right\rangle = -i\hbar \iiint drd\theta d\phi r^2 \sin\theta \hat{\boldsymbol{\phi}}^* \left(r^2 \frac{\partial \hat{\boldsymbol{\psi}}}{\partial r} + ar\hat{\boldsymbol{\psi}} \right) \tag{2.115}$$

So, for T to be Hermitian, we require

$$2r - ar = ar. \tag{2.116}$$

So $a = 1$, and our Hermitian operator is

$$T = -i\hbar \left(\frac{\partial}{\partial r} + \frac{1}{r} \right). \tag{2.117}$$

Exercise 2.4 Radial directional derivative operator ([3] pr 2.6)

Show that

$$D = \mathbf{p} \cdot \hat{\mathbf{r}} + \hat{\mathbf{r}} \cdot \mathbf{p}, \tag{2.118}$$

is Hermitian. Expand this operator in spherical coordinates. Compare result to problem 5.

Answer for Exercise 2.4

Tackling the spherical coordinates expression of of the operator D, we have

$$\begin{aligned}
\frac{1}{-i\hbar} D\Psi &= \left(\boldsymbol{\nabla} \cdot \hat{\mathbf{r}} + \hat{\mathbf{r}} \cdot \boldsymbol{\nabla} \right) \Psi \\
&= \left(\boldsymbol{\nabla} \cdot \hat{\mathbf{r}} \right) \Psi + \left(\boldsymbol{\nabla} \Psi \right) \cdot \hat{\mathbf{r}} + \hat{\mathbf{r}} \cdot \left(\boldsymbol{\nabla} \Psi \right) \\
&= \left(\boldsymbol{\nabla} \cdot \hat{\mathbf{r}} \right) \Psi + 2\hat{\mathbf{r}} \cdot \left(\boldsymbol{\nabla} \Psi \right).
\end{aligned} \tag{2.119}$$

Here braces have been used to denote the extend of the operation of the gradient. In spherical polar coordinates, our gradient is

$$\boldsymbol{\nabla} \equiv \hat{\mathbf{r}} \frac{\partial}{\partial r} + \hat{\boldsymbol{\theta}} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\boldsymbol{\phi}} \frac{1}{r \sin\theta} \frac{\partial}{\partial \phi}. \tag{2.120}$$

This gets us most of the way there, and we have

$$\frac{1}{-i\hbar} D\Psi = 2\frac{\partial \Psi}{\partial r} + \left(\hat{\mathbf{r}} \cdot \frac{\partial \hat{\mathbf{r}}}{\partial r} + \frac{1}{r} \hat{\boldsymbol{\theta}} \cdot \frac{\partial \hat{\mathbf{r}}}{\partial \theta} + \frac{1}{r \sin\theta} \hat{\boldsymbol{\phi}} \cdot \frac{\partial \hat{\mathbf{r}}}{\partial \phi} \right) \Psi. \tag{2.121}$$

Since $\partial \hat{\mathbf{r}}/\partial r = 0$, we are left with evaluating $\hat{\boldsymbol{\theta}} \cdot \partial \hat{\mathbf{r}}/\partial \theta$, and $\hat{\boldsymbol{\phi}} \cdot \partial \hat{\mathbf{r}}/\partial \phi$. To do so I chose to employ the (Geometric Algebra) exponential form of the spherical unit vectors [6]

$$\begin{aligned}
I &= \mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3 \\
\hat{\boldsymbol{\phi}} &= \mathbf{e}_2 \exp(I \mathbf{e}_3 \phi) \\
\hat{\mathbf{r}} &= \mathbf{e}_3 \exp(I \hat{\boldsymbol{\phi}} \theta) \\
\hat{\boldsymbol{\theta}} &= \mathbf{e}_1 \mathbf{e}_2 \hat{\boldsymbol{\phi}} \exp(I \hat{\boldsymbol{\phi}} \theta).
\end{aligned} \tag{2.122}$$

The partials of interest are then

$$\frac{\partial \hat{\mathbf{r}}}{\partial \theta} = \mathbf{e}_3 I \hat{\boldsymbol{\phi}} \exp(I \hat{\boldsymbol{\phi}} \theta) = \hat{\boldsymbol{\theta}}, \tag{2.123}$$

and

$$\begin{aligned}
\frac{\partial \hat{\mathbf{r}}}{\partial \phi} &= \frac{\partial}{\partial \phi} \mathbf{e}_3 \left(\cos\theta + I \hat{\boldsymbol{\phi}} \sin\theta \right) \\
&= \mathbf{e}_1 \mathbf{e}_2 \sin\theta \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \phi} \\
&= \mathbf{e}_1 \mathbf{e}_2 \sin\theta \mathbf{e}_2 \mathbf{e}_1 \mathbf{e}_2 \exp(I \mathbf{e}_3 \phi) \\
&= \sin\theta \hat{\boldsymbol{\phi}}.
\end{aligned} \tag{2.124}$$

Only after computing these, did I find exactly these results for the partials of interest, in mathworld's Spherical Coordinates page, which confirms these calculations. Note that a different angle convention is used there, so one has to exchange ϕ, and θ and the corresponding unit vector labels.

Substitution back into our expression for the operator we have

$$D = -2i\hbar \left(\frac{\partial}{\partial r} + \frac{1}{r} \right), \tag{2.125}$$

an operator that is exactly twice the operator of problem 5, already shown to be Hermitian. Since the constant numerical scaling of a Hermitian operator leaves it Hermitian, this shows that D is Hermitian as expected.

$\hat{\boldsymbol{\theta}}$ directional momentum operator Let us try this for the other unit vector directions too. We also want

$$\left(\boldsymbol{\nabla} \cdot \hat{\boldsymbol{\theta}} + \hat{\boldsymbol{\theta}} \cdot \boldsymbol{\nabla} \right) \Psi = 2 \hat{\boldsymbol{\theta}} \cdot (\boldsymbol{\nabla} \Psi) + \left(\boldsymbol{\nabla} \cdot \hat{\boldsymbol{\theta}} \right) \Psi. \tag{2.126}$$

The work consists of evaluating

$$\boldsymbol{\nabla} \cdot \hat{\boldsymbol{\theta}} = \hat{\mathbf{r}} \cdot \frac{\partial \hat{\boldsymbol{\theta}}}{\partial r} + \frac{1}{r} \hat{\boldsymbol{\theta}} \cdot \frac{\partial \hat{\boldsymbol{\theta}}}{\partial \theta} + \frac{1}{r \sin\theta} \hat{\boldsymbol{\phi}} \cdot \frac{\partial \hat{\boldsymbol{\theta}}}{\partial \phi}. \tag{2.127}$$

This time we need the $\partial\hat{\boldsymbol{\theta}}/\partial\theta$, $\partial\hat{\boldsymbol{\theta}}/\partial\phi$ partials, which are

$$\begin{aligned}
\frac{\partial \hat{\boldsymbol{\theta}}}{\partial \theta} &= \mathbf{e}_1 \mathbf{e}_2 \hat{\boldsymbol{\phi}} I \hat{\boldsymbol{\phi}} \exp(I\hat{\boldsymbol{\phi}}\theta) \\
&= -\mathbf{e}_3 \exp(I\hat{\boldsymbol{\phi}}\theta) \\
&= -\hat{\mathbf{r}}.
\end{aligned} \tag{2.128}$$

This has no $\hat{\boldsymbol{\theta}}$ component, so does not contribute to $\boldsymbol{\nabla} \cdot \hat{\boldsymbol{\theta}}$. Noting that

$$\frac{\partial \hat{\boldsymbol{\phi}}}{\partial \phi} = -\mathbf{e}_1 \exp(I\mathbf{e}_3\phi) = \mathbf{e}_2 \mathbf{e}_1 \hat{\boldsymbol{\phi}}, \tag{2.129}$$

the ϕ partial is

$$\begin{aligned}
\frac{\partial \hat{\boldsymbol{\theta}}}{\partial \phi} &= \mathbf{e}_1 \mathbf{e}_2 \left(\frac{\partial \hat{\boldsymbol{\phi}}}{\partial \phi} \exp(I\hat{\boldsymbol{\phi}}\theta) + \hat{\boldsymbol{\phi}} I \sin\theta \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \phi} \right) \\
&= \hat{\boldsymbol{\phi}} \left(\exp(I\hat{\boldsymbol{\phi}}\theta) + I \sin\theta \mathbf{e}_2 \mathbf{e}_1 \hat{\boldsymbol{\phi}} \right),
\end{aligned} \tag{2.130}$$

with $\hat{\boldsymbol{\phi}}$ component

$$\begin{aligned}
\hat{\boldsymbol{\phi}} \cdot \frac{\partial \hat{\boldsymbol{\theta}}}{\partial \phi} &= \left\langle \exp(I\hat{\boldsymbol{\phi}}\theta) + I \sin\theta \mathbf{e}_2 \mathbf{e}_1 \hat{\boldsymbol{\phi}} \right\rangle \\
&= \cos\theta + \mathbf{e}_3 \cdot \hat{\boldsymbol{\phi}} \sin\theta \\
&= \cos\theta.
\end{aligned} \tag{2.131}$$

Assembling the results, and labeling this operator Θ we have

$$\begin{aligned}
\Theta &\equiv \frac{1}{2} \left(\mathbf{p} \cdot \hat{\boldsymbol{\theta}} + \hat{\boldsymbol{\theta}} \cdot \mathbf{p} \right) \\
&= -i\hbar \frac{1}{r} \left(\frac{\partial}{\partial \theta} + \frac{1}{2} \cot\theta \right).
\end{aligned} \tag{2.132}$$

It would be reasonable to expect this operator to also be Hermitian, and checking this explicitly by comparing $\langle \Phi | \Theta | \Psi \rangle^*$ and $\langle \Psi | \Theta | \Phi \rangle$, shows that this is in fact the case.

$\hat{\boldsymbol{\phi}}$ directional momentum operator Let us try this for the other unit vector directions too. We also want

$$\left(\boldsymbol{\nabla} \cdot \hat{\boldsymbol{\phi}} + \hat{\boldsymbol{\phi}} \cdot \boldsymbol{\nabla}\right) \Psi = 2\hat{\boldsymbol{\phi}} \cdot (\boldsymbol{\nabla}\Psi) + \left(\boldsymbol{\nabla} \cdot \hat{\boldsymbol{\phi}}\right) \Psi. \tag{2.133}$$

The work consists of evaluating

$$\boldsymbol{\nabla} \cdot \hat{\boldsymbol{\phi}} = \hat{\mathbf{r}} \cdot \frac{\partial \hat{\boldsymbol{\phi}}}{\partial r} + \frac{1}{r} \hat{\boldsymbol{\theta}} \cdot \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \theta} + \frac{1}{r \sin\theta} \hat{\boldsymbol{\phi}} \cdot \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \phi}. \tag{2.134}$$

This time we need the $\partial \hat{\boldsymbol{\phi}}/\partial \theta$, $\partial \hat{\boldsymbol{\phi}}/\partial \phi = \mathbf{e}_2 \mathbf{e}_1 \hat{\boldsymbol{\phi}}$ partials. The θ partial is

$$\begin{aligned} \frac{\partial \hat{\boldsymbol{\phi}}}{\partial \theta} &= \frac{\partial}{\partial \theta} \mathbf{e}_2 \exp(I \mathbf{e}_3 \phi) \\ &= 0. \end{aligned} \tag{2.135}$$

We conclude that $\boldsymbol{\nabla} \cdot \hat{\boldsymbol{\phi}} = 0$, and expect that we have one more Hermitian operator

$$\begin{aligned} \Phi &\equiv \frac{1}{2} \left(\mathbf{p} \cdot \hat{\boldsymbol{\phi}} + \hat{\boldsymbol{\phi}} \cdot \mathbf{p}\right) \\ &= -i \hbar \frac{1}{r \sin\theta} \frac{\partial}{\partial \phi}. \end{aligned} \tag{2.136}$$

It is simple to confirm that this is Hermitian since the integration by parts does not involve any of the volume element. In fact, any operator $-i\hbar f(r,\theta)\partial/\partial\phi$ would also be Hermitian, including the simplest case $-i\hbar\partial/\partial\phi$. Have to dig out my Bohm text again, since I seem to recall that one used in the spherical Harmonics chapter.

A note on the Hermitian test and Dirac notation I have been a bit loose with my notation. I have stated that my demonstrations of the Hermitian nature have been done by showing

$$\langle \phi | A | \psi \rangle^* - \langle \psi | A | \phi \rangle = 0. \tag{2.137}$$

However, what I have actually done is show that

$$\left(\int d^3 \mathbf{x} \phi^*(\mathbf{x}) A(\mathbf{x}) \psi(\mathbf{x}) \right)^* - \int d^3 \mathbf{x} \psi^*(\mathbf{x}) A(\mathbf{x}) \phi(\mathbf{x}) = 0. \tag{2.138}$$

To justify this note that

$$\begin{aligned}
\langle\phi| A |\psi\rangle^* &= \left(\iint d^3\mathbf{r} d^3\mathbf{s} \langle\phi|\mathbf{r}\rangle \langle\mathbf{r}| A |\mathbf{s}\rangle \langle\mathbf{s}|\psi\rangle\right)^* \\
&= \iint d^3\mathbf{r} d^3\mathbf{s} \phi(\mathbf{r})\delta^3(\mathbf{r}-\mathbf{s})A^*(\mathbf{s})\psi(\mathbf{s}) \\
&= \int d^3\mathbf{r}\phi(\mathbf{r})A^*(\mathbf{r})\psi(\mathbf{r}),
\end{aligned} \tag{2.139}$$

and

$$\begin{aligned}
\langle\phi| A |\psi\rangle^* &= \iint d^3\mathbf{r} d^3\mathbf{s} \langle\psi|\mathbf{r}\rangle \langle\mathbf{r}| A |\mathbf{s}\rangle \langle\mathbf{s}|\phi\rangle \\
&= \iint d^3\mathbf{r} d^3\mathbf{s} \langle\mathbf{r}| \psi(\mathbf{r})\delta^3(\mathbf{r}-\mathbf{s})A(\mathbf{s})\phi(\mathbf{s}) \\
&= \int d^3\mathbf{r}\psi(\mathbf{r})A(\mathbf{r})\phi(\mathbf{r}).
\end{aligned} \tag{2.140}$$

Working backwards one sees that the comparison of the wave function integrals in explicit inner product notation is sufficient to demonstrate the Hermitian property.

Exercise 2.5 Some commutators (*[3] pr 2.7*)

For D in problem 6, obtain

- i) $[D, x_i]$
- ii) $[D, p_i]$
- iii) $[D, L_i]$, where $L_i = \mathbf{e}_i \cdot (\mathbf{r} \times \mathbf{p})$.
- iv) Show that $e^{i\alpha D/\hbar} x_i e^{-i\alpha D/\hbar} = e^\alpha x_i$

Answer for Exercise 2.5

Expansion of $[D, x_i]$ While expressing the operator as $D = -2i\hbar(1/r)(1+\partial_r)$ has less complexity than the $D = \mathbf{p}\cdot\hat{\mathbf{r}} + \hat{\mathbf{r}}\cdot\mathbf{p}$, since no operation on $\hat{\mathbf{r}}$ is required, this does not look particularly convenient for use with Cartesian coordinates. Slightly better perhaps is

$$D = -2i\hbar\frac{1}{r}(\mathbf{r}\cdot\boldsymbol{\nabla} + 1) \tag{2.141}$$

$$
\begin{aligned}
[D, x_i]\Psi &= D x_i \Psi - x_i D \Psi \\
&= -2i\hbar \frac{1}{r} \left(\mathbf{r} \cdot \boldsymbol{\nabla} + 1 \right) x_i \Psi + 2i\hbar x_i \frac{1}{r} \left(\mathbf{r} \cdot \boldsymbol{\nabla} + 1 \right) \Psi \\
&= -2i\hbar \frac{1}{r} \mathbf{r} \cdot \boldsymbol{\nabla} x_i \Psi + 2i\hbar x_i \frac{1}{r} \mathbf{r} \cdot \boldsymbol{\nabla} \Psi \\
&= -2i\hbar \frac{1}{r} \mathbf{r} \cdot (\boldsymbol{\nabla} x_i) \Psi - 2i\hbar x_i \frac{1}{r} \mathbf{r} \cdot \boldsymbol{\nabla} \Psi + 2i\hbar x_i \frac{1}{r} \mathbf{r} \cdot \boldsymbol{\nabla} \Psi \\
&= -2i\hbar \frac{1}{r} \mathbf{r} \cdot \mathbf{e}_i \Psi.
\end{aligned}
\tag{2.142}
$$

So this first commutator is:

$$
[D, x_i] = -2i\hbar \frac{x_i}{r}. \tag{2.143}
$$

Alternate expansion of $[D, x_i]$ Let us try this instead completely in coordinate notation to verify. I will use implicit summation for repeated indices, and write $\partial_k = \partial/\partial x_k$. A few intermediate results will be required

$$
\begin{aligned}
\partial_k \frac{1}{r} &= \partial_k (x_m x_m)^{-1/2} \\
&= -\frac{1}{2} 2 x_k (x_m x_m)^{-3/2}
\end{aligned}
\tag{2.144}
$$

Or

$$
\partial_k \frac{1}{r} = -\frac{x_k}{r^3} \tag{2.145}
$$

$$
\partial_k \frac{x_i}{r} = \frac{\delta_{ik}}{r} - \frac{x_i}{r^3} \tag{2.146}
$$

$$
\partial_k \frac{x_k}{r} = \frac{3}{r} - \frac{x_k}{r^3} \tag{2.147}
$$

The action of the momentum operators on the coordinates is

$$
\begin{aligned}
p_k x_i \Psi &= -i\hbar \partial_k x_i \Psi \\
&= -i\hbar \left(\delta_{ik} + x_i \partial_k \right) \Psi \\
&= -i\hbar \delta_{ik} + x_i p_k
\end{aligned}
\tag{2.148}
$$

$$\begin{aligned} p_k x_k \Psi &= -i\hbar \partial_k x_k \Psi \\ &= -i\hbar \left(3 + x_k \partial_k\right) \Psi \end{aligned} \tag{2.149}$$

Or

$$\begin{aligned} p_k x_i &= -i\hbar \delta_{ik} + x_i p_k \\ p_k x_k &= -3i\hbar + x_k p_k \end{aligned} \tag{2.150}$$

And finally

$$\begin{aligned} p_k \frac{1}{r} \Psi &= (p_k \frac{1}{r}) \Psi + \frac{1}{r} p_k \Psi \\ &= -i\hbar \left(-\frac{x_k}{r^3}\right) \Psi + \frac{1}{r} p_k \Psi \end{aligned} \tag{2.151}$$

So

$$p_k \frac{1}{r} = i\hbar \frac{x_k}{r^3} + \frac{1}{r} p_k \tag{2.152}$$

We can use these to rewrite D

$$\begin{aligned} D &= p_k \frac{x_k}{r} + \frac{x_k}{r} p_k \\ &= p_k x_k \frac{1}{r} + \frac{x_k}{r} p_k \\ &= \left(-3i\hbar + x_k p_k\right) \frac{1}{r} + \frac{x_k}{r} p_k \\ &= -\frac{3i\hbar}{r} + x_k \left(i\hbar \frac{x_k}{r^3} + \frac{1}{r} p_k \right) + \frac{x_k}{r} p_k \end{aligned} \tag{2.153}$$

$$D = \frac{2}{r}(-i\hbar + x_k p_k) \tag{2.154}$$

This leaves us in the position to compute the commutator

$$\begin{aligned} \left[D, x_i\right] &= \frac{2}{r}(-i\hbar + x_k p_k) x_i - \frac{2x_i}{r}(-i\hbar + x_k p_k) \\ &= \frac{2}{r} x_k(-i\hbar \delta_{ik} + x_i p_k) - \frac{2x_i}{r} x_k p_k \\ &= -\frac{2i\hbar x_i}{r} \end{aligned} \tag{2.155}$$

So, unless I am doing something fundamentally wrong, the same way in both methods, this appears to be the desired result. I question my answer since utilizing this for the later computation of $e^{i\alpha D/\hbar} x_i e^{-i\alpha D/\hbar}$ did not yield the expected answer.

$\{D, p_i\}$

$$\begin{aligned}
[D, p_i] &= -\frac{2i\hbar}{r}(1 + x_k p_k)p_i + 2i\hbar p_i \frac{1}{r}(1 + x_k p_k) \\
&= -\frac{2i\hbar}{r}\left(p_i + x_k p_k p_i - \left(i\hbar\frac{x_i}{r^2} + p_i\right)(1 + x_k p_k)\right) \\
&= -\frac{2i\hbar}{r}\left(x_k p_k p_i - i\hbar\frac{x_i}{r^2} - i\hbar\frac{x_i x_k}{r^2} p_k - \left(-i\hbar\delta_{ki} + x_k p_i\right) p_k\right) \\
&= -\frac{2i\hbar}{r}\left(-i\hbar\frac{x_i}{r^2} - i\hbar\frac{x_i x_k}{r^2} p_k + i\hbar p_i\right) \\
&= -\frac{i\hbar}{r}\left(\frac{x_i}{r} D + 2i\hbar p_i\right) \qquad \square
\end{aligned} \tag{2.156}$$

If there is some significance to this expansion, other than to get a feel for operator manipulation, it escapes me.

$\{D, L_i\}$ To expand $[D, L_i]$, it will be sufficient to consider any specific index $i \in \{1, 2, 3\}$ and then utilize cyclic permutation of the indices in the result to generalize. Let us pick $i = 1$, for which we have

$$L_1 = x_2 p_3 - x_3 p_2 \tag{2.157}$$

It appears we will want to know

$$\begin{aligned}
p_m D &= -2i\hbar p_m \frac{1}{r}(1 + x_k p_k) \\
&= -2i\hbar\left(i\hbar\frac{x_m}{r^3} + \frac{1}{r}p_m\right)(1 + x_k p_k) \\
&= -2i\hbar\left(i\hbar\frac{x_m}{r^3} + \frac{1}{r}p_m + i\hbar\frac{x_m x_k}{r^3} p_k + \frac{1}{r}p_m x_k p_k\right) \\
&= -\frac{2i\hbar}{r}\left(i\hbar\frac{x_m}{r^2} + p_m + i\hbar\frac{x_m x_k}{r^2} p_k - i\hbar p_m + x_k p_m p_k\right)
\end{aligned} \tag{2.158}$$

and we also want

$$
\begin{aligned}
Dx_m &= -\frac{2i\hbar}{r}(1 + x_k p_k)x_m \\
&= -\frac{2i\hbar}{r}(x_m + x_k(-i\hbar\delta_{km} + x_m p_k)) \\
&= -\frac{2i\hbar}{r}(x_m - i\hbar x_m + x_m x_k p_k)
\end{aligned}
\tag{2.159}
$$

This also happens to be $Dx_m = x_m D + \frac{2(i\hbar)^2 x_m}{r}$, but does that help at all? Assembling these we have

$$
\begin{aligned}
\left[D, L_1\right] &= Dx_2 p_3 - Dx_3 p_2 - x_2 p_3 D + x_3 p_2 D \\
&= -\frac{2i\hbar}{r}(x_2 - i\hbar x_2 + x_2 x_k p_k)p_3 + \frac{2i\hbar}{r}(x_3 - i\hbar x_3 + x_3 x_k p_k)p_2 \\
&+ \frac{2i\hbar x_2}{r}\left(i\hbar\frac{x_3}{r^2} + p_3 + i\hbar\frac{x_3 x_k}{r^2}p_k - i\hbar p_3 + x_k p_3 p_k\right) \\
&- \frac{2i\hbar x_3}{r}\left(i\hbar\frac{x_2}{r^2} + p_2 + i\hbar\frac{x_2 x_k}{r^2}p_k - i\hbar p_2 + x_k p_2 p_k\right)
\end{aligned}
\tag{2.160}
$$

With a bit of brute force it is simple enough to verify that all these terms mystically cancel out, leaving us zero

$$
\left[D, L_1\right] = 0
\tag{2.161}
$$

There surely must be an easier way to demonstrate this. Likely utilizing the commutator relationships derived earlier.

$e^{i\alpha D/\hbar} x_i e^{-i\alpha D/\hbar}$ We will need to evaluate $D^k x_i$. We have the first power from our commutator relation

$$
Dx_i = x_i\left(D - \frac{2i\hbar}{r}\right)
\tag{2.162}
$$

A successive application of this operator therefore yields

$$
\begin{aligned}
D^2 x_i &= Dx_i\left(D - \frac{2i\hbar}{r}\right) \\
&= x_i\left(D - \frac{2i\hbar}{r}\right)^2
\end{aligned}
\tag{2.163}
$$

So we have

$$D^k x_i = x_i \left(D - \frac{2i\hbar}{r} \right)^k \tag{2.164}$$

This now preps us to expand the first product in the desired exponential sandwich

$$\begin{aligned} e^{i\alpha D/\hbar} x_i &= x_i + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{iD}{\hbar} \right)^k x_i \\ &= x_i + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{i}{\hbar} \right)^k D^k x_i \\ &= x_i + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{i}{\hbar} \right)^k x_i \\ &= x_i e^{\frac{i\alpha}{\hbar}\left(D - \frac{2i\hbar}{r} \right)} \\ &= x_i e^{2\alpha/r} e^{i\alpha D/\hbar}. \end{aligned} \tag{2.165}$$

The exponential sandwich then produces

$$e^{i\alpha D/\hbar} x_i e^{-i\alpha D/\hbar} = e^{2\alpha/r} x_i \tag{2.166}$$

Note that this is not the value we are supposed to get. Either my value for Dx_i is off by a factor of $2/r$ or the problem in the text contains a typo.

Exercise 2.6 Reduction of some commutators using the fundamental commutator relation ([3] pr 2.

Using the fundamental commutation relation

$$[p, x] = -i\hbar, \tag{2.167}$$

which we can also write as

$$px = xp - i\hbar, \tag{2.168}$$

expand $\left[x, p^2\right]$, $\left[x^2, p\right]$, and $\left[x^2, p^2\right]$.

Answer for Exercise 2.6

The first is

$$\begin{aligned}
\left[x, p^2\right] &= xp^2 - p^2 x \\
&= xp^2 - p(px) \\
&= xp^2 - p(xp - i\hbar) \\
&= xp^2 - (xp - i\hbar)p + i\hbar p \\
&= 2i\hbar p
\end{aligned} \tag{2.169}$$

The second is

$$\begin{aligned}
\left[x^2, p\right] &= x^2 p - px^2 \\
&= x^2 p - (xp - i\hbar)x \\
&= x^2 p - x(xp - i\hbar) + i\hbar x \\
&= 2i\hbar x
\end{aligned} \tag{2.170}$$

Note that it is helpful for the last reduction of this problem to observe that we can write this as

$$px^2 = x^2 p - 2i\hbar x \tag{2.171}$$

Finally for this last we have

$$\begin{aligned}
\left[x^2, p^2\right] &= x^2 p^2 - p^2 x^2 \\
&= x^2 p^2 - p(x^2 p - 2i\hbar x) \\
&= x^2 p^2 - (x^2 p - 2i\hbar x)p + 2i\hbar(xp - i\hbar) \\
&= 4i\hbar xp - 2(i\hbar)^2
\end{aligned} \tag{2.172}$$

That is about as reduced as this can be made, but it is not very tidy looking. From this point we can simplify it a bit by factoring

$$\begin{aligned}
\left[x^2, p^2\right] &= 4i\hbar xp - 2(i\hbar)^2 \\
&= 2i\hbar(2xp - i\hbar) \\
&= 2i\hbar(xp + px) \\
&= 2i\hbar\{x, p\}
\end{aligned} \tag{2.173}$$

Exercise 2.7 Finite displacement operator (*[3] pr 2.9*)

FIXME: describe.

Answer for Exercise 2.7

Part I For

$$F(d) = e^{-ipd/\hbar}, \tag{2.174}$$

the first part of this problem is to show that

$$\left[x, F(d)\right] = xF(d) - F(d)x = dF(d) \tag{2.175}$$

We need to evaluate

$$e^{-ipd/\hbar}x = \sum_{k=0}^{\infty} \frac{1}{k!}\left(\frac{-ipd}{\hbar}\right)^k x. \tag{2.176}$$

To do so requires a reduction of $p^k x$. For $k = 2$ we have

$$\begin{aligned} p^2 x &= p(xp - i\hbar) \\ &= (xp - i\hbar)p - i\hbar p \\ &= xp^2 - 2i\hbar p. \end{aligned} \tag{2.177}$$

For the cube we get $p^3 x = xp^3 - 3i\hbar p^2$, supplying confirmation of an induction hypothesis $p^k x = xp^k - ki\hbar p^{k-1}$, which can be verified

$$\begin{aligned} p^{k+1} x &= p(xp^k - ki\hbar p^{k-1}) \\ &= (xp - i\hbar)p^k - ki\hbar p^k \\ &= xp^{k+1} - (k+1)i\hbar p^k \qquad \square \end{aligned} \tag{2.178}$$

For our exponential we then have

$$\begin{aligned} e^{-ipd/\hbar}x &= x + \sum_{k=1}^{\infty} \frac{1}{k!}\left(\frac{-id}{\hbar}\right)^k (xp^k - ki\hbar p^{k-1}) \\ &= xe^{-ipd/\hbar} + \sum_{k=1}^{\infty} \frac{1}{(k-1)!}\left(\frac{-ipd}{\hbar}\right)^{k-1} (-id/\hbar)(-i\hbar) \\ &= (x - d)e^{-ipd/\hbar}. \end{aligned} \tag{2.179}$$

Put back into our commutator we have

$$\left[x, e^{-ipd/\hbar}\right] = de^{-ipd/\hbar}, \tag{2.180}$$

completing the proof.

Part II For state $|\alpha\rangle$ with $|\alpha_d\rangle = F(d)\,|\alpha\rangle$, show that the expectation values satisfy

$$\langle X\rangle_d = \langle X\rangle + d \tag{2.181}$$

$$\begin{aligned}
\langle X\rangle_d &= \langle\alpha_d|\,X\,|\alpha_d\rangle \\
&= \iint dx'dx''\,\langle\alpha_d|x'\rangle\left\langle x'\middle|\,X\,\middle|x''\right\rangle\langle x''|\alpha_d\rangle \\
&= \iint dx'dx''\alpha_d^* x'\delta(x'-x'')x'\alpha_d(x'') \\
&= \int dx'\alpha_d^*(x')x'\alpha_d(x')
\end{aligned} \tag{2.182}$$

But

$$\begin{aligned}
\alpha_d(x') &= \exp\left(-\frac{id}{\hbar}(-i\hbar)\frac{\partial}{\partial x'}\right)\alpha(x') \\
&= e^{-d\frac{\partial}{\partial x'}}\alpha(x') \\
&= \alpha(x'-d),
\end{aligned} \tag{2.183}$$

so our position expectation is

$$\langle X\rangle_d = \int dx'\alpha^*(x'-d)x'\alpha(x'-d). \tag{2.184}$$

A change of variables $x = x' - d$ gives us

$$\begin{aligned}
\langle X\rangle_d &= \int dx\alpha^*(x)(x+d)\alpha(x) \\
\langle X\rangle + d + d &\int dx\alpha^* x\alpha(x) \qquad \square
\end{aligned} \tag{2.185}$$

Exercise 2.8 **Hamiltonian position commutator and double commutator** (*[3] pr 2.10*)

For

$$H = \frac{1}{2m}p^2 + V(x) \tag{2.186}$$

calculate $[H, x]$, and $[[H, x], x]$.

Answer for Exercise 2.8

These are

$$\begin{aligned}
[H, x] &= \frac{1}{2m} p^2 x + V(x)x - \frac{1}{2m} x p^2 - x V(x) \\
&= \frac{1}{2m} p(xp - i\hbar) - \frac{1}{2m} x p^2 \\
&= \frac{1}{2m} \left((xp - i\hbar)p - i\hbar p\right) - \frac{1}{2m} x p^2 \\
&= -\frac{i\hbar p}{m}
\end{aligned} \tag{2.187}$$

and

$$\begin{aligned}
[[H, x], x] &= -\frac{i\hbar}{m} [p, x] \\
&= \frac{(-i\hbar)^2}{m} \\
&= -\frac{\hbar^2}{m}
\end{aligned} \tag{2.188}$$

We also have to show that

$$\sum_k (E_k - E_n) |\langle k| x |n\rangle|^2 = \frac{\hbar^2}{2m} \tag{2.189}$$

Expanding the absolute value in terms of conjugates we have

$$\begin{aligned}
\sum_k (E_k - E_n) |\langle k| x |n\rangle|^2 &= \sum_k (E_k - E_n) \langle k| x |n\rangle \langle n| x |k\rangle \\
&= \sum_k \langle k| x |n\rangle \langle n| x E_k |k\rangle - \langle k| x E_n |n\rangle \langle n| x |k\rangle \\
&= \sum_k \langle n| xH |k\rangle \langle k| x |n\rangle - \langle n| x |k\rangle \langle k| xH |n\rangle \\
&= \langle n| xHx |n\rangle - \langle n| xxH |n\rangle \\
&= \langle n| x [H, x] |n\rangle \\
&= -\frac{i\hbar}{m} \langle n| xp |n\rangle
\end{aligned} \tag{2.190}$$

It is not obvious where to go from here. Taking the clue from the problem that the result involves the double commutator, we have

$$\begin{aligned}
-\frac{\hbar^2}{m} &= \langle n| \left[\left[H, x\right], x\right] |n\rangle \\
&= \langle n| Hx^2 - 2xHx + x^2 H |n\rangle \\
&= 2E_n \langle n| x^2 |n\rangle - 2 \langle n| xHx |n\rangle \\
&= 2E_n \langle n| x^2 |n\rangle - 2 \langle n| (-\left[H, x\right] + Hx)x |n\rangle \\
&= 2 \langle n| \left[H, x\right] x |n\rangle \\
&= -\frac{2i\hbar}{m} \langle n| px |n\rangle \\
&= -\frac{2i\hbar}{m} \langle n| xp - i\hbar |n\rangle \\
&= -\frac{2i\hbar}{m} \langle n| xp |n\rangle + \frac{2(i\hbar)^2}{m}
\end{aligned} \tag{2.191}$$

So, somewhat flukily by working backwards, with a last rearrangement, we now have

$$\begin{aligned}
-\frac{i\hbar}{m} \langle n| xp |n\rangle &= \frac{\hbar^2}{m} - \frac{\hbar^2}{2m} \\
&= \frac{\hbar^2}{2m}
\end{aligned} \tag{2.192}$$

Substitution above gives the desired result. This is extremely ugly, and does not follow any sort of logical progression. Is there a good way to sequence this proof?

Exercise 2.9 Another double commutator. (*[3] pr 2.11*)

FIXME: describe.

Answer for Exercise 2.9

Attempt 1. Incomplete

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) \tag{2.193}$$

use $\left[\left[H, e^{i\mathbf{k}\cdot\mathbf{r}}\right], e^{-i\mathbf{k}\cdot\mathbf{r}}\right]$ to obtain

$$\sum_n (E_n - E_s) \left|\langle n| e^{i\mathbf{k}\cdot\mathbf{r}} |s\rangle\right|^2 \tag{2.194}$$

First evaluate the commutators. The first is

$$\left[H, e^{i\mathbf{k}\cdot\mathbf{r}}\right] = \frac{1}{2m}\left[\mathbf{p}^2, e^{i\mathbf{k}\cdot\mathbf{r}}\right] \tag{2.195}$$

The Laplacian applied to this exponential is

$$\begin{aligned}
\boldsymbol{\nabla}^2 e^{i\mathbf{k}\cdot\mathbf{r}}\Psi &= \partial_m\partial_m e^{ik_n x_n}\Psi \\
&= \partial_m(ik_m e^{i\mathbf{k}\cdot\mathbf{r}}\Psi + e^{i\mathbf{k}\cdot\mathbf{r}}\partial_m\Psi) \\
&= -\mathbf{k}^2 e^{i\mathbf{k}\cdot\mathbf{r}}\Psi + ie^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{k}\cdot\boldsymbol{\nabla}\Psi + ie^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{k}\cdot\boldsymbol{\nabla}\Psi + e^{i\mathbf{k}\cdot\mathbf{r}}\boldsymbol{\nabla}^2\Psi
\end{aligned} \tag{2.196}$$

Factoring out the exponentials this is

$$\boldsymbol{\nabla}^2 e^{i\mathbf{k}\cdot\mathbf{r}} = e^{i\mathbf{k}\cdot\mathbf{r}}\left(-\mathbf{k}^2 + 2i\mathbf{k}\cdot\boldsymbol{\nabla} + \boldsymbol{\nabla}^2\right), \tag{2.197}$$

and in terms of **p**, we have

$$\mathbf{p}^2 e^{i\mathbf{k}\cdot\mathbf{r}} = e^{i\mathbf{k}\cdot\mathbf{r}}\left((\hbar\mathbf{k})^2 + 2(\hbar\mathbf{k})\cdot\mathbf{p} + \mathbf{p}^2\right) = e^{i\mathbf{k}\cdot\mathbf{r}}(\hbar\mathbf{k} + \mathbf{p})^2 \tag{2.198}$$

So, finally, our first commutator is

$$\left[H, e^{i\mathbf{k}\cdot\mathbf{r}}\right] = \frac{1}{2m}e^{i\mathbf{k}\cdot\mathbf{r}}\left((\hbar\mathbf{k})^2 + 2(\hbar\mathbf{k})\cdot\mathbf{p}\right) \tag{2.199}$$

The double commutator is then

$$\left[\left[H, e^{i\mathbf{k}\cdot\mathbf{r}}\right], e^{-i\mathbf{k}\cdot\mathbf{r}}\right] = e^{i\mathbf{k}\cdot\mathbf{r}}\frac{\hbar\mathbf{k}}{m}\cdot\left(\mathbf{p}e^{-i\mathbf{k}\cdot\mathbf{r}} - e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{p}\right) \tag{2.200}$$

To simplify this we want

$$\begin{aligned}
\mathbf{k}\cdot\boldsymbol{\nabla}e^{-i\mathbf{k}\cdot\mathbf{r}}\Psi &= k_n\partial_n e^{-ik_m x_m}\Psi \\
&= e^{-i\mathbf{k}\cdot\mathbf{r}}\left(k_n(-ik_n)\Psi + k_n\partial_n\Psi\right) \\
&= e^{-i\mathbf{k}\cdot\mathbf{r}}\left(-i\mathbf{k}^2 + \mathbf{k}\cdot\boldsymbol{\nabla}\right)\Psi
\end{aligned} \tag{2.201}$$

The double commutator is then left with just

$$\left[\left[H, e^{i\mathbf{k}\cdot\mathbf{r}}\right], e^{-i\mathbf{k}\cdot\mathbf{r}}\right] = -\frac{1}{m}(\hbar\mathbf{k})^2 \tag{2.202}$$

Now, returning to the energy expression

$$
\begin{aligned}
\sum_n (E_n - E_s) \left| \langle n | e^{i\mathbf{k}\cdot\mathbf{r}} | s \rangle \right|^2 &= \sum_n (E_n - E_s) \langle s | e^{-i\mathbf{k}\cdot\mathbf{r}} | n \rangle \langle n | e^{i\mathbf{k}\cdot\mathbf{r}} | s \rangle \\
&= \sum_n \langle s | e^{-i\mathbf{k}\cdot\mathbf{r}} H | n \rangle \langle n | e^{i\mathbf{k}\cdot\mathbf{r}} | s \rangle - \langle s | e^{-i\mathbf{k}\cdot\mathbf{r}} | n \rangle \langle n | e^{i\mathbf{k}\cdot\mathbf{r}} H | s \rangle \\
&= \langle s | e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}} | s \rangle - \langle s | e^{-i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} H | s \rangle \\
&= \langle s | e^{-i\mathbf{k}\cdot\mathbf{r}} \left[H, e^{i\mathbf{k}\cdot\mathbf{r}} \right] | s \rangle \\
&= \frac{1}{2m} \langle s | e^{-i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} \left((\hbar\mathbf{k})^2 + 2(\hbar\mathbf{k}) \cdot \mathbf{p} \right) | s \rangle \\
&= \frac{1}{2m} \langle s | (\hbar\mathbf{k})^2 + 2(\hbar\mathbf{k}) \cdot \mathbf{p} | s \rangle \\
&= \frac{(\hbar\mathbf{k})^2}{2m} + \frac{1}{m} \langle s | (\hbar\mathbf{k}) \cdot \mathbf{p} | s \rangle
\end{aligned}
\tag{2.203}
$$

I can not figure out what to do with the $\hbar\mathbf{k} \cdot \mathbf{p}$ expectation, and keep going around in circles.

I figure there is some trick related to the double commutator, so expanding the expectation of that seems appropriate

$$
\begin{aligned}
-\frac{1}{m} (\hbar\mathbf{k})^2 &= \langle s | \left[\left[H, e^{i\mathbf{k}\cdot\mathbf{r}} \right], e^{-i\mathbf{k}\cdot\mathbf{r}} \right] | s \rangle \\
&= \langle s | \left[H, e^{i\mathbf{k}\cdot\mathbf{r}} \right] e^{-i\mathbf{k}\cdot\mathbf{r}} - e^{-i\mathbf{k}\cdot\mathbf{r}} \left[H, e^{i\mathbf{k}\cdot\mathbf{r}} \right] | s \rangle \\
&= \frac{1}{2m} \langle s | e^{i\mathbf{k}\cdot\mathbf{r}} ((\hbar\mathbf{k})^2 + 2\,\hbar\mathbf{k} \cdot \mathbf{p}) e^{-i\mathbf{k}\cdot\mathbf{r}} - e^{-i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} ((\hbar\mathbf{k})^2 + 2\,\hbar\mathbf{k} \cdot \mathbf{p}) | s \rangle \\
&= \frac{1}{m} \langle s | e^{i\mathbf{k}\cdot\mathbf{r}} (\hbar\mathbf{k} \cdot \mathbf{p}) e^{-i\mathbf{k}\cdot\mathbf{r}} - \hbar\mathbf{k} \cdot \mathbf{p} | s \rangle
\end{aligned}
\tag{2.204}
$$

Attempt 2 I was going in circles above. With the help of betel on physicsforums, I got pointed in the right direction. Here is a rework of this problem from scratch, also benefiting from hindsight.

Our starting point is the same, with the evaluation of the first commutator

$$
\left[H, e^{i\mathbf{k}\cdot\mathbf{r}} \right] = \frac{1}{2m} \left[\mathbf{p}^2, e^{i\mathbf{k}\cdot\mathbf{r}} \right].
\tag{2.205}
$$

To continue we need to know how the momentum operator acts on an exponential of this form

$$
\begin{aligned}
\mathbf{p} e^{\pm i\mathbf{k}\cdot\mathbf{r}} \Psi &= -i\hbar \mathbf{e}_m \partial_m e^{\pm i k_n x_n} \Psi \\
&= e^{\pm i\mathbf{k}\cdot\mathbf{r}} \left(-i\hbar (\pm i \mathbf{e}_m k_m) \Psi - i\hbar \mathbf{e}_m \partial_m \Psi \right).
\end{aligned}
\tag{2.206}
$$

This gives us the helpful relationship

$$\mathbf{p}e^{\pm i\mathbf{k}\cdot\mathbf{r}} = e^{\pm i\mathbf{k}\cdot\mathbf{r}}(\mathbf{p} \pm \hbar\mathbf{k}). \tag{2.207}$$

Squared application of the momentum operator on the positive exponential found in the first commutator eq. (2.205), gives us

$$\mathbf{p}^2 e^{i\mathbf{k}\cdot\mathbf{r}} = e^{i\mathbf{k}\cdot\mathbf{r}}(\hbar\mathbf{k} + \mathbf{p})^2 = e^{i\mathbf{k}\cdot\mathbf{r}}((\hbar\mathbf{k})^2 + 2\hbar\mathbf{k}\cdot\mathbf{p} + \mathbf{p}^2), \tag{2.208}$$

with which we can evaluate this first commutator.

$$\left[H, e^{i\mathbf{k}\cdot\mathbf{r}}\right] = \frac{1}{2m} e^{i\mathbf{k}\cdot\mathbf{r}}((\hbar\mathbf{k})^2 + 2\hbar\mathbf{k}\cdot\mathbf{p}). \tag{2.209}$$

For the double commutator we have

$$\begin{aligned} 2m\left[\left[H, e^{i\mathbf{k}\cdot\mathbf{r}}\right], e^{-i\mathbf{k}\cdot\mathbf{r}}\right] &= e^{i\mathbf{k}\cdot\mathbf{r}}((\hbar\mathbf{k})^2 + 2\hbar\mathbf{k}\cdot\mathbf{p})e^{-i\mathbf{k}\cdot\mathbf{r}} - ((\hbar\mathbf{k})^2 + 2\hbar\mathbf{k}\cdot\mathbf{p}) \\ &= e^{i\mathbf{k}\cdot\mathbf{r}} 2(\hbar\mathbf{k}\cdot\mathbf{p})e^{-i\mathbf{k}\cdot\mathbf{r}} - 2\hbar\mathbf{k}\cdot\mathbf{p} \\ &= 2\hbar\mathbf{k}\cdot(\mathbf{p} - \hbar\mathbf{k}) - 2\hbar\mathbf{k}\cdot\mathbf{p}, \end{aligned} \tag{2.210}$$

so for the double commutator we have just a scalar

$$\left[\left[H, e^{i\mathbf{k}\cdot\mathbf{r}}\right], e^{-i\mathbf{k}\cdot\mathbf{r}}\right] = -\frac{(\hbar\mathbf{k})^2}{m}. \tag{2.211}$$

Now consider the expectation of this double commutator, expanded with some unintuitive steps that have been motivated by working backwards

$$\begin{aligned} \langle s| \left[\left[H, e^{i\mathbf{k}\cdot\mathbf{r}}\right], e^{-i\mathbf{k}\cdot\mathbf{r}}\right] |s\rangle &= \langle s| 2H - e^{i\mathbf{k}\cdot\mathbf{r}} H e^{-i\mathbf{k}\cdot\mathbf{r}} - e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}} |s\rangle \\ &= \langle s| 2e^{-i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} H - 2e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}} |s\rangle \\ &= 2\sum_n \langle s| e^{-i\mathbf{k}\cdot\mathbf{r}} |n\rangle \langle n| e^{i\mathbf{k}\cdot\mathbf{r}} H |s\rangle - \langle s| e^{-i\mathbf{k}\cdot\mathbf{r}} H |n\rangle \langle n| e^{i\mathbf{k}\cdot\mathbf{r}} |s\rangle \\ &= 2\sum_n E_s \langle s| e^{-i\mathbf{k}\cdot\mathbf{r}} |n\rangle \langle n| e^{i\mathbf{k}\cdot\mathbf{r}} |s\rangle - E_n \langle s| e^{-i\mathbf{k}\cdot\mathbf{r}} |n\rangle \langle n| e^{i\mathbf{k}\cdot\mathbf{r}} |s\rangle \\ &= 2\sum_n (E_s - E_n) \left|\langle n| e^{i\mathbf{k}\cdot\mathbf{r}} |s\rangle\right|^2 \end{aligned} \tag{2.212}$$

By eq. (2.211), we have completed the problem

$$\sum_n (E_n - E_s) \left| \langle n | e^{i\mathbf{k}\cdot\mathbf{r}} | s \rangle \right|^2 = \frac{(\hbar \mathbf{k})^2}{2m}. \tag{2.213}$$

There is one subtlety above that is worth explicit mention before moving on, in particular, I did not find it intuitive that the following was true

$$\langle s | e^{i\mathbf{k}\cdot\mathbf{r}} H e^{-i\mathbf{k}\cdot\mathbf{r}} + e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}} | s \rangle = \langle s | 2 e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}} | s \rangle . \tag{2.214}$$

However, observe that both of these exponential sandwich operators $e^{i\mathbf{k}\cdot\mathbf{r}} H e^{-i\mathbf{k}\cdot\mathbf{r}}$, and $e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}}$ are Hermitian, since we have for example

$$\begin{aligned}
(e^{i\mathbf{k}\cdot\mathbf{r}} H e^{-i\mathbf{k}\cdot\mathbf{r}})^\dagger &= (e^{-i\mathbf{k}\cdot\mathbf{r}})^\dagger H^\dagger (e^{i\mathbf{k}\cdot\mathbf{r}})^\dagger \\
&= e^{i\mathbf{k}\cdot\mathbf{r}} H e^{-i\mathbf{k}\cdot\mathbf{r}}
\end{aligned} \tag{2.215}$$

Also observe that these operators are both complex conjugates of each other, and with $\mathbf{k}\cdot\mathbf{r} = \alpha$ for short, can be written

$$\begin{aligned}
e^{i\alpha} H e^{-i\alpha} &= \cos\alpha H \cos\alpha + \sin\alpha H \sin\alpha + i \sin\alpha H \cos\alpha - i \cos\alpha H \sin\alpha \\
e^{-i\alpha} H e^{i\alpha} &= \cos\alpha H \cos\alpha + \sin\alpha H \sin\alpha - i \sin\alpha H \cos\alpha + i \cos\alpha H \sin\alpha
\end{aligned} \tag{2.216}$$

Because H is real valued, and the expectation value of a Hermitian operator is real valued, none of the imaginary terms can contribute to the expectation values, and in the summation of eq. (2.214) we can thus pick and double either of the exponential sandwich terms, as desired.

Exercise 2.10 ps II

A particle of mass m is free to move along the x-direction such that $V(X) = 0$. Express the time evolution operator $U(t, t_0)$ defined by Eq. (2.166) using the momentum eigenstates $|p\rangle$ with delta-function normalization. Find $\langle x| U(t, t_0) |x'\rangle$, where $|x\rangle$ and $|x'\rangle$ are position eigenstates. What is the physical meaning of this expression?

Answer for Exercise 2.10

Momentum matrix element We can expand the time evolution operator in series

$$\begin{aligned}
U(t, t_0) &= e^{-iH(t-t_0)/\hbar} \\
&= e^{-iP^2(t-t_0)/2m\hbar} \\
&= 1 + \sum_{k=1}^{\infty} \frac{1}{k!} \left(-i \frac{P^2(t-t_0)}{2m\hbar} \right)^k .
\end{aligned} \tag{2.217}$$

We can now evaluate the momentum matrix element $\langle p| U(t,t_0) |p'\rangle$, which will essentially require the value of $\langle p| P^{2k} |p'\rangle$. That is

$$\begin{aligned}\langle p| P^{2k} \left|p'\right\rangle &= \langle p| P^{2k-1} P \left|p'\right\rangle \\ &= \langle p| P^{2k-1} \left|p'\right\rangle p' \\ &= \cdots \\ &= \left\langle p|p'\right\rangle (p')^{2k}.\end{aligned} \tag{2.218}$$

The momentum matrix element is therefore reduced to

$$\langle p| U(t,t_0) \left|p'\right\rangle = \left\langle p|p'\right\rangle \exp\left(-i\frac{p^2(t-t_0)}{2m\hbar}\right) = \delta(p-p') \exp\left(-i\frac{p^2(t-t_0)}{2m\hbar}\right) \tag{2.219}$$

Position matrix element For the position matrix element we have a similar sum

$$\langle x| U(t,t_0) \left|x'\right\rangle = \left\langle x|x'\right\rangle + \sum_{k=1}^{\infty} \frac{1}{k!} \langle x| \left(-i\frac{P^2(t-t_0)}{2m\hbar}\right)^k \left|x'\right\rangle, \tag{2.220}$$

and require $\langle x| P^{2k} |x'\rangle$ to continue. That is

$$\begin{aligned}\langle x| P^{2k} \left|x'\right\rangle &= \int dx'' \langle x| P^{2k-1} \left|x''\right\rangle \left\langle x''\right| P \left|x'\right\rangle \\ &= \int dx'' \langle x| P^{2k-1} \left|x''\right\rangle \delta(x''-x')(-i\hbar)\frac{d}{dx'} \\ &= \langle x| P^{2k-1} \left|x'\right\rangle (-i\hbar)\frac{d}{dx'} \\ &= \cdots \\ &= \left\langle x|x'\right\rangle \left((-i\hbar)\frac{d}{dx'}\right)^{2k}\end{aligned} \tag{2.221}$$

Our position matrix element is therefore the differential operator

$$\langle x| U(t,t_0) \left|x'\right\rangle = \left\langle x|x'\right\rangle \exp\left(\frac{i(t-t_0)\hbar}{2m}\frac{d^2}{dx'^2}\right) = \delta(x-x') \exp\left(\frac{i(t-t_0)\hbar}{2m}\frac{d^2}{dx'^2}\right) \tag{2.222}$$

Physical interpretation of the position matrix element operator Finally, we need to determine the physical meaning of such a matrix element operator.

With the delta function that this matrix element operator includes it really only takes on a meaning with a convolution integral. The simplest such integral would be

$$\begin{aligned}\int dx' \left\langle x\right| U \left|x'\right\rangle \left\langle x' | \phi_0 \right\rangle &= \left\langle x\right| U \left|\phi_0\right\rangle \\ &= \left\langle x | \phi(t)\right\rangle \\ &= \phi(x,t),\end{aligned} \tag{2.223}$$

or

$$\phi(x,t) = \int dx' \left\langle x\right| U \left|x'\right\rangle \phi(x',0) \tag{2.224}$$

The LHS has a physical meaning, and in the absolute square

$$\int_{x_0}^{x_0+\Delta x} |\phi(x,t)|^2 dx, \tag{2.225}$$

provides the probability that the particle will be found in the region $[x_0, x_0 + \Delta x]$.

If we ignore the absolute square requirement and think of the (presumed normalized) wave function $\phi(x,t)$ more loosely as representing a probability directly, then we can in turn give a meaning to the matrix element $\left\langle x\right| U \left|x'\right\rangle$ for the time evolution operator. This provides an operator valued weighting function that provides us with the probability that a particle initially at position x' will be at position x at time t. This probability is indirect since we need to absolute square and sum over a finite interval to obtain the probability of finding the particle in that interval.

Observe that the integral on the RHS of eq. (2.225) is a summation over all x', so we can think of this as adding the probabilities that the particle was at each point to arrive at the total probability for finding it at the new location x. The time evolution operator matrix element provides the weighting in this conditional probability.

In eq. (2.222) we found that the time evolution operators matrix element is differential operator in the position representation. In the general case this means that this probability weighting is not just numeric since the operation of the matrix element initial time wave function can produce wave functions for additional states. In some special cases, we may find that this weighting is strictly numeric, and one such example would be the Gaussian wave packet $\phi(x',0) = e^{-ax'^2}$. Application of the differential operations would then produce polynomial weighted multiples of the original Gaussian. In this special case we would be able to write

$$\phi(x,t) = \int dx' \left\langle x\right| U \left|x'\right\rangle \phi(x',0) = \int dx' K(x,x',t)\phi(x',0) \tag{2.226}$$

Where $K(x, x', t)$ is a polynomial valued function (and is in fact another exponential), and now just provides a numerical weighting for the conditional probability for the particle to move from x' to x in time t. In [9], this $K(x, x', t)$ is called the Propagator function. It is perhaps justifiable to also call our similar operator valued matrix element a Propagator.

Exercise 2.11 ps III.

A particle of mass m is free to move along the x-direction such that $V(X) = 0$. The state of the system is represented by the wavefunction Eq. (4.74)

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{ikx} e^{-i\omega t} f(k) \tag{2.227}$$

with $f(k)$ given by Eq. (4.59).

$$f(k) = N e^{-\alpha k^2} \tag{2.228}$$

Note that I have inserted a $1/\sqrt{2\pi}$ factor above that is not in the text, because otherwise $\psi(x,t)$ will not be unit normalized (assuming $f(k)$ is normalized in wavenumber space).

a. What is the group velocity associated with this state?
b. What is the probability for measuring the particle at position $x = x_0 > 0$ at time $t = t_0 > 0$?
c. What is the probability per unit length for measuring the particle at position $x = x_0 > 0$ at time $t = t_0 > 0$?
d. Explain the physical meaning of the above results.

Answer for Exercise 2.11

Part a. Group velocity To calculate the group velocity we need to know the dependence of ω on k.

Let us step back and consider the time evolution action on $\psi(x, 0)$. For the free particle case we have

$$H = \frac{\mathbf{p}^2}{2m} = -\frac{\hbar^2}{2m}\partial_{xx}. \tag{2.229}$$

Writing $N' = N/\sqrt{2\pi}$ we have

$$\begin{aligned}
-\frac{it}{\hbar} H\psi(x,0) &= \frac{it\hbar}{2m} N' \int_{-\infty}^{\infty} dk (ik)^2 e^{ikx-\alpha k^2} \\
&= N' \int_{-\infty}^{\infty} dk \frac{-it\hbar k^2}{2m} e^{ikx-\alpha k^2}
\end{aligned} \tag{2.230}$$

Each successive application of $-iHt/\hbar$ will introduce another power of $-it\hbar k^2/2m$, so once we sum all the terms of the exponential series $U(t) = e^{-iHt/\hbar}$ we have

$$\psi(x,t) = N' \int_{-\infty}^{\infty} dk \exp\left(\frac{-it\hbar k^2}{2m} + ikx - \alpha k^2\right). \tag{2.231}$$

Comparing with eq. (2.227) we find

$$\omega(k) = \frac{\hbar k^2}{2m}. \tag{2.232}$$

This completes this section of the problem since we are now able to calculate the group velocity

$$v_g = \frac{\partial \omega(k)}{\partial k} = \frac{\hbar k}{m}. \tag{2.233}$$

Part b. Measurement probability In order to evaluate the probability, it looks desirable to evaluate the wave function integral eq. (2.231). Writing $2\beta = i/(\alpha + it\hbar/2m)$, the exponent of that integral is

$$\begin{aligned} -k^2\left(\alpha + \frac{it\hbar}{2m}\right) + ikx &= -\left(\alpha + \frac{it\hbar}{2m}\right)\left(k^2 - \frac{ikx}{\alpha + \frac{it\hbar}{2m}}\right) \\ &= -\frac{i}{2\beta}\left((k - x\beta)^2 - x^2\beta^2\right) \end{aligned} \tag{2.234}$$

The x^2 portion of the exponential

$$\frac{ix^2\beta^2}{2\beta} = \frac{ix^2\beta}{2} = -\frac{x^2}{4(\alpha + it\hbar/2m)} \tag{2.235}$$

then comes out of the integral. We can also make a change of variables $q = k - x\beta$ to evaluate the remainder of the Gaussian and are left with

$$\psi(x,t) = N' \sqrt{\frac{\pi}{\alpha + it\hbar/2m}} \exp\left(-\frac{x^2}{4(\alpha + it\hbar/2m)}\right). \tag{2.236}$$

Observe that from eq. (2.228) we can compute $N = (2\alpha/\pi)^{1/4}$, which could be substituted back into eq. (2.236) if desired.

Our probability density is

$$\begin{aligned}
|\psi(x,t)|^2 &= \frac{1}{2\pi} N^2 \left| \frac{\pi}{\alpha + it\hbar/2m} \right| \exp\left(-\frac{x^2}{4} \left(\frac{1}{(\alpha + it\hbar/2m)} + \frac{1}{(\alpha - it\hbar/2m)} \right) \right) \\
&= \frac{1}{2\pi} \sqrt{\frac{2\alpha}{\pi}} \frac{\pi}{\sqrt{\alpha^2 + (t\hbar/2m)^2}} \exp\left(-\frac{x^2}{4} \frac{1}{\alpha^2 + (t\hbar/2m)^2} \left(\alpha - it\hbar/2m + \alpha + it\hbar/2m\right) \right) \\
&=
\end{aligned} \tag{2.237}$$

With a final regrouping of terms, this is

$$|\psi(x,t)|^2 = \sqrt{\frac{\alpha}{2\pi(\alpha^2 + (t\hbar/2m)^2})} \exp\left(-\frac{x^2}{2} \frac{\alpha}{\alpha^2 + (t\hbar/2m)^2} \right). \tag{2.238}$$

As a sanity check we observe that this integrates to unity for all t as desired. The probability that we find the particle at position $x > x_0$ is then

$$P_{x>x_0}(t) = \sqrt{\frac{\alpha}{2\pi(\alpha^2 + (t\hbar/2m)^2})} \int_{x=x_0}^{\infty} dx \exp\left(-\frac{x^2}{2} \frac{\alpha}{\alpha^2 + (t\hbar/2m)^2} \right) \tag{2.239}$$

The only simplification we can make is to rewrite this in terms of the complementary error function

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt. \tag{2.240}$$

Writing

$$\beta(t) = \frac{\alpha}{\alpha^2 + (t\hbar/2m)^2}, \tag{2.241}$$

we have

$$P_{x>x_0}(t_0) = \frac{1}{2} \operatorname{erfc}\left(\sqrt{\beta(t_0)/2} x_0 \right) \tag{2.242}$$

Sanity checking this result, we note that since $\operatorname{erfc}(0) = 1$ the probability for finding the particle in the $x > 0$ range is $1/2$ as expected.

Part c. Probability density for positive position and time This unit length probability is thus

$$P_{x>x_0+1/2}(t_0) - P_{x>x_0-1/2}(t_0) = \frac{1}{2}\operatorname{erfc}\left(\sqrt{\frac{\beta(t_0)}{2}}\left(x_0 + \frac{1}{2}\right)\right) - \frac{1}{2}\operatorname{erfc}\left(\sqrt{\frac{\beta(t_0)}{2}}\left(x_0 - \frac{1}{2}\right)\right) \tag{2.243}$$

Part d. Physical meaning To get an idea what the group velocity means, observe that we can write our wavefunction eq. (2.227) as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk e^{ik(x-v_g t)} f(k) \tag{2.244}$$

We see that the phase coefficient of the Gaussian $f(k)$ "moves" at the rate of the group velocity v_g. Also recall that in the text it is noted that the time dependent term eq. (2.241) can be expressed in terms of position and momentum uncertainties $(\Delta x)^2$, and $(\Delta p)^2 = \hbar^2(\Delta k)^2$. That is

$$\frac{1}{\beta(t)} = (\Delta x)^2 + \frac{(\Delta p)^2}{m^2}t^2 \equiv (\Delta x(t))^2 \tag{2.245}$$

This makes it evident that the probability density flattens and spreads over time with the rate equal to the uncertainty of the group velocity $\Delta p/m = \Delta v_g$ (since $v_g = \hbar k/m$). It is interesting that something as simple as this phase change results in a physically measurable phenomena. We see that a direct result of this linear with time phase change, we are less able to find the particle localized around it is original time $x = 0$ position as more time elapses.

Grading comments I lost one mark on the group velocity response. Instead of eq. (2.233) he wanted

$$v_g = \left.\frac{\partial\omega(k)}{\partial k}\right|_{k=k_0} = \frac{\hbar k_0}{m} = 0 \tag{2.246}$$

since $f(k)$ peaks at $k = 0$.

I will have to go back and think about that a bit, because I am unsure of the last bits of the reasoning there.

I also lost 0.5 and 0.25 (twice) because I did not explicitly state that the probability that the particle is at x_0, a specific single point, is zero. I thought that was obvious and did not have to be stated, but it appears expressing this explicitly is what he was looking for.

Curiously, one thing that I did not loose marks on was, the wrong answer for the probability per unit length. What he was actually asking for was the following

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{x_0-\epsilon/2}^{x_0+\epsilon/2} |\Psi(x_0, t_0)|^2 dx = |\Psi(x_0, t_0)|^2 \tag{2.247}$$

That is a whole lot more sensible seeming quantity to calculate than what I did, but I do not think that I can be faulted too much since the phrase was never used in the text nor in the lectures.

3 DYNAMICAL EQUATIONS

3.1 LECTURE NOTES: REVIEW

For

$$|\phi\rangle = \int dk f(k) |k\rangle \tag{3.1}$$

How do we find $|\phi(t)\rangle$, the time evolved state? Here we have the option of choosing which of the pictures (Schrödinger, Heisenberg, interaction) we deal with. Since the Heisenberg picture deals with time evolved operators, and the interaction picture with evolving Hamiltonians, neither of these is required to answer this question. Consider the Schrödinger picture which gives

$$|\phi(t)\rangle = \int dk f(k) |k\rangle e^{-iE_k t/\hbar} \tag{3.2}$$

where E_k is the eigenvalue of the Hamiltonian operator H.

3.2 PROBLEMS

Exercise 3.1 Virial Theorem ([3] *pr 3.1*)

With the assumption that $\langle \mathbf{r} \cdot \mathbf{p} \rangle$ is independent of time, and

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) = T + V \tag{3.3}$$

show that

$$2 \langle T \rangle = \langle \mathbf{r} \cdot \boldsymbol{\nabla} V \rangle . \tag{3.4}$$

Answer for Exercise 3.1

I floundered with this a bit, but found the required hint in physicsforums. We can start with the Hamiltonian time derivative relation

$$i\hbar \frac{dA_H}{dt} = [A_H, H] \tag{3.5}$$

So, with the assumption that $\langle \mathbf{r} \cdot \mathbf{p} \rangle$ is independent of time, and the use of a stationary state $|\psi\rangle$ for the expectation calculation we have

$$\begin{aligned}
0 &= \frac{d}{dt} \langle \mathbf{r} \cdot \mathbf{p} \rangle \\
&= \frac{d}{dt} \langle \psi | \, \mathbf{r} \cdot \mathbf{p} \, | \psi \rangle \\
&= \langle \psi | \, \frac{d}{dt} (\mathbf{r} \cdot \mathbf{p}) \, | \psi \rangle \\
&= \frac{1}{i\hbar} \left\langle [\mathbf{r} \cdot \mathbf{p}, H] \right\rangle \\
&= -\left\langle \left[\mathbf{r} \cdot \boldsymbol{\nabla}, \frac{\mathbf{p}^2}{2m} \right] \right\rangle - \left\langle [\mathbf{r} \cdot \boldsymbol{\nabla}, V(\mathbf{r})] \right\rangle .
\end{aligned} \tag{3.6}$$

The exercise now becomes one of evaluating the remaining commutators. For the Laplacian commutator we have

$$\begin{aligned}
\left[\mathbf{r} \cdot \boldsymbol{\nabla}, \boldsymbol{\nabla}^2 \right] \psi &= x_m \partial_m \partial_n \partial_n \psi - \partial_n \partial_n x_m \partial_m \psi \\
&= x_m \partial_m \partial_n \partial_n \psi - \partial_n \partial_n \psi - \partial_n x_m \partial_n \partial_m \psi \\
&= x_m \partial_m \partial_n \partial_n \psi - \partial_n \partial_n \psi - \partial_n \partial_n \psi - x_m \partial_n \partial_n \partial_m \psi \\
&= -2 \boldsymbol{\nabla}^2 \psi
\end{aligned} \tag{3.7}$$

For the potential commutator we have

$$\begin{aligned}
[\mathbf{r} \cdot \boldsymbol{\nabla}, V(\mathbf{r})] \, \psi &= x_m \partial_m V \psi - V x_m \partial_m \psi \\
&= x_m (\partial_m V) \psi x_m V \partial_m \psi - V x_m \partial_m \psi \\
&= \left(\mathbf{r} \cdot (\boldsymbol{\nabla} V) \right) \psi
\end{aligned} \tag{3.8}$$

Putting all the $\hbar$ factors back in, we get

$$2 \left\langle \frac{\mathbf{p}^2}{2m} \right\rangle = \langle \mathbf{r} \cdot (\boldsymbol{\nabla} V) \rangle , \tag{3.9}$$

which is the desired result.

Followup: why assume $\langle \mathbf{r} \cdot \mathbf{p} \rangle$ is independent of time?

Exercise 3.2 Application of virial theorem ([3] pr 3.2)

Calculate $\langle T \rangle$ with $V = \lambda \ln(r/a)$.

Answer for Exercise 3.2

$$
\begin{aligned}
\mathbf{r} \cdot \boldsymbol{\nabla} V &= r\hat{\mathbf{r}} \cdot \hat{\mathbf{r}} \lambda \frac{\partial \ln(r/a)}{\partial r} \\
&= \lambda r \frac{1}{a} \frac{a}{r} \\
&= \lambda \\
\implies & \\
\langle T \rangle &= \lambda/2
\end{aligned}
\tag{3.10}
$$

Exercise 3.3 Heisenberg Position operator representation ([3] pr 3.3)

Answer for Exercise 3.3

Part I Express x as an operator x_H for $H = \mathbf{p}^2/2m$.

With

$$
\langle \psi | x | \psi \rangle = \langle \psi_0 | U^\dagger x U | \psi_0 \rangle
\tag{3.11}
$$

We want to expand

$$
\begin{aligned}
x_H &= U^\dagger x U \\
&= e^{iHt/\hbar} x e^{-iHt/\hbar} \\
&= \sum_{k,l=0}^{\infty} \frac{1}{k!} \frac{1}{l!} \left(\frac{iHt}{\hbar} \right)^k x \left(\frac{-iHt}{\hbar} \right)^l .
\end{aligned}
\tag{3.12}
$$

We to evaluate $H^k x H^l$ to proceed. Using $p^n x = -i\hbar n p^{n-1} + x p^n$, we have

$$\begin{aligned}
H^k x &= \frac{1}{(2m)^k} p^2 k x \\
&= \frac{1}{(2m)^k} \left(-i\hbar (2k) p^{2k-1} + x p^2 k \right) \\
&= x H^k + \frac{1}{2m} (-i\hbar)(2k) p p^{2(k-1)} / (2m)^{k-1} \\
&= x H^k - \frac{i\hbar k}{m} p H^{k-1}.
\end{aligned} \tag{3.13}$$

This gives us

$$\begin{aligned}
x_H &= x - \frac{i\hbar p}{m} \sum_{k,l=0}^{\infty} \frac{k}{k!} \frac{1}{l!} \left(\frac{it}{\hbar} \right)^k H^{k-1+l} \left(\frac{-it}{\hbar} \right)^l \\
&= x - \frac{i\hbar p i t}{m\hbar}
\end{aligned} \tag{3.14}$$

Or

$$x_H = x + \frac{pt}{m} \tag{3.15}$$

Part II Express x as an operator x_H for $H = \mathbf{p}^2/2m + V$ with $V = \lambda x^m$.

In retrospect, for the first part of this problem, it would have been better to use the series expansion for this exponential sandwich

Or, in explicit form

$$e^A B e^{-A} = B + \frac{1}{1!} [A, B] + \frac{1}{2!} [A, [A, B]] + \cdots \tag{3.16}$$

Doing so, we would find for the first commutator

$$\frac{it}{2m\hbar} \left[\mathbf{p}^2, x \right] = \frac{tp}{m}, \tag{3.17}$$

so that the series has only the first two terms, and we would obtain the same result. That seems like a logical approach to try here too. For the first commutator, we get the same tp/m result since $[V, x] = 0$.

Employing

$$x^n p = i\hbar n x^{n-1} + p x^n, \tag{3.18}$$

I find

$$
\begin{aligned}
\left(\frac{it}{\hbar}\right)^2 [H, [H, x]] &= \frac{i\lambda t^2}{\hbar m} [x^n, p] \\
&= -\frac{nt^2\lambda}{m} x^{n-1} \\
&= -\frac{nt^2 V}{mx}
\end{aligned}
\tag{3.19}
$$

The triple commutator gets no prettier, and I get

$$
\begin{aligned}
\left(\frac{it}{\hbar}\right)^3 [H, [H, [H, x]]] &= \frac{it}{\hbar}\left[\frac{\mathbf{p}^2}{2m} + \lambda x^n, -\frac{nt^2 V}{mx}\right] \\
&= -\frac{it}{\hbar}\frac{nt^2}{m}\frac{\lambda}{2m}\left[\mathbf{p}^2, x^{n-1}\right] \\
&= \cdots \\
&= \frac{n(n-1)t^3 V}{2m^2 x^3}(i\hbar n + 2px).
\end{aligned}
\tag{3.20}
$$

Putting all the pieces together this gives

$$
x_H = e^{iHt/\hbar} x e^{-iHt/\hbar} = x + \frac{tp}{m} - \frac{nt^2 V}{2mx} + \frac{n(n-1)t^3 V}{12m^2 x^3}(i\hbar n + 2px) + \cdots \tag{3.21}
$$

If there is a closed form for this it is not obvious to me. Would a fixed lower degree potential function shed any more light on this. How about the Harmonic oscillator Hamiltonian

$$
H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2 \tag{3.22}
$$

... this one works out nicely since there is an even-odd alternation.
Get

$$
x_H = x\cos(\omega^2 t^2/2) + \frac{pt}{m}\frac{\sin(\omega^2 t^2/2)}{\omega^2 t^2/2} \tag{3.23}
$$

I had not expect such a tidy result for an arbitrary $V(x) = \lambda x^n$ potential.

Exercise 3.4 Feynman-Hellman relation ([3] *pr 3.4*)

Answer for Exercise 3.4

For continuously parameterized eigenstate, eigenvalue and Hamiltonian $|\psi(\lambda)\rangle$, $E(\lambda)$ and $H(\lambda)$ respectively, we can relate the derivatives

$$\begin{aligned}\frac{\partial}{\partial\lambda}(H|\psi\rangle) &= \frac{\partial}{\partial\lambda}(E|\psi\rangle) \\ &\Longrightarrow \\ \frac{\partial H}{\partial\lambda}|\psi\rangle + H\frac{\partial|\psi\rangle}{\partial\lambda} &= \frac{\partial E}{\partial\lambda}|\psi\rangle + E\frac{\partial|\psi\rangle}{\partial\lambda}\end{aligned} \tag{3.24}$$

Left multiplication by $\langle\psi|$ gives

$$\begin{aligned}\langle\psi|\frac{\partial H}{\partial\lambda}|\psi\rangle + \langle\psi|H\frac{\partial|\psi\rangle}{\partial\lambda} &= \langle\psi|\frac{\partial E}{\partial\lambda}|\psi\rangle + E\langle\psi|\frac{\partial|\psi\rangle}{\partial\lambda} \\ &\Longrightarrow \\ \langle\psi|\frac{\partial H}{\partial\lambda}|\psi\rangle + (\langle\psi|E)\frac{\partial|\psi\rangle}{\partial\lambda} &= \langle\psi|\frac{\partial E}{\partial\lambda}|\psi\rangle + E\langle\psi|\frac{\partial|\psi\rangle}{\partial\lambda} \\ &\Longrightarrow \\ \langle\psi|\frac{\partial H}{\partial\lambda}|\psi\rangle &= \frac{\partial E}{\partial\lambda}\langle\psi|\psi\rangle,\end{aligned} \tag{3.25}$$

which provides the desired identity

$$\frac{\partial E}{\partial\lambda} = \langle\psi(\lambda)|\frac{\partial H}{\partial\lambda}|\psi(\lambda)\rangle \tag{3.26}$$

Exercise 3.5 *([3] pr 3.5)*

With eigenstates $|\phi_1\rangle$ and $|\phi_2\rangle$, of H with eigenvalues E_1 and E_2, respectively, and

$$\begin{aligned}|\chi_1\rangle &= \frac{1}{\sqrt{2}}(|\phi_1\rangle + |\phi_2\rangle) \\ |\chi_2\rangle &= \frac{1}{\sqrt{2}}(|\phi_1\rangle - |\phi_2\rangle)\end{aligned} \tag{3.27}$$

and $|\psi(0)\rangle = |\chi_1\rangle$, determine $|\psi(t)\rangle$ in terms of $|\phi_1\rangle$ and $|\phi_2\rangle$.

Answer for Exercise 3.5

$$
\begin{aligned}
|\psi(t)\rangle &= e^{-iHt/\hbar} |\psi(0)\rangle \\
&= e^{-iHt/\hbar} |\chi_1\rangle \\
&= \frac{1}{\sqrt{2}} e^{-iHt/\hbar} (|\phi_1\rangle - |\phi_2\rangle) \\
&= \frac{1}{\sqrt{2}} (e^{-iE_1 t/\hbar} |\phi_1\rangle - e^{-iE_2 t/\hbar} |\phi_2\rangle) \qquad \square
\end{aligned}
\tag{3.28}
$$

Exercise 3.6 ([3] pr 3.6)

Consider a Coulomb like potential $-\lambda/r$ with angular momentum $l = 0$. If the eigenfunction is

$$
u(r) = u_0 e^{-\beta r}
\tag{3.29}
$$

determine u_0, β, and the energy eigenvalue E in terms of λ, and m.

Answer for Exercise 3.6

We can start with the normalization constant u_0 by integrating

$$
\begin{aligned}
1 &= u_0^2 \int_0^\infty dr e^{-\beta r} e^{-\beta r} \\
&= u_0^2 \left. \frac{e^{-2\beta r}}{-2\beta} \right|_{0^\infty} \\
&= u_0^2 \frac{1}{2\beta}
\end{aligned}
\tag{3.30}
$$

$$
u_0 = \sqrt{2\beta}
\tag{3.31}
$$

To go further, we need the Hamiltonian. Note that we can write the Laplacian with the angular momentum operator factored out using

$$
\boldsymbol{\nabla}^2 = \frac{1}{\mathbf{x}^2} \left((\mathbf{x} \cdot \boldsymbol{\nabla})^2 + \mathbf{x} \cdot \boldsymbol{\nabla} + (\mathbf{x} \times \boldsymbol{\nabla})^2 \right)
\tag{3.32}
$$

With zero for the angular momentum operator $\mathbf{x} \times \boldsymbol{\nabla}$, and switching to spherical coordinates, we have

$$\begin{aligned}
\boldsymbol{\nabla}^2 &= \frac{1}{r}\partial_r + \frac{1}{r}\partial_r r \partial_r \\
&= \frac{1}{r}\partial_r + \frac{1}{r}\partial_r + \frac{1}{r} r \partial_{rr} \\
&= \frac{2}{r}\partial_r + \partial_{rr}
\end{aligned} \tag{3.33}$$

We can now write the Hamiltonian for the zero angular momentum case

$$H = -\frac{\hbar^2}{2m}\left(\frac{2}{r}\partial_r + \partial_{rr}\right) - \frac{\lambda}{r} \tag{3.34}$$

With application of this Hamiltonian to the eigenfunction we have

$$\begin{aligned}
E u_0 e^{-\beta r} &= \left(-\frac{\hbar^2}{2m}\left(\frac{2}{r}\partial_r + \partial_{rr}\right) - \frac{\lambda}{r}\right) u_0 e^{-\beta r} \\
&= \left(-\frac{\hbar^2}{2m}\left(\frac{2}{r}(-\beta) + \beta^2\right) - \frac{\lambda}{r}\right) u_0 e^{-\beta r}.
\end{aligned} \tag{3.35}$$

In particular for $r = \infty$ we have

$$-\frac{\hbar^2 \beta^2}{2m} = E \tag{3.36}$$

$$\begin{aligned}
&-\frac{\hbar^2 \beta^2}{2m} = \left(-\frac{\hbar^2}{2m}\left(\frac{2}{r}(-\beta) + \beta^2\right) - \frac{\lambda}{r}\right) \\
&\Longrightarrow \\
&\frac{\hbar^2}{2m}\frac{2}{r}\beta = \frac{\lambda}{r}
\end{aligned} \tag{3.37}$$

Collecting all the results we have

$$\begin{aligned}
\beta &= \frac{\lambda m}{\hbar^2} \\
E &= -\frac{\lambda^2 m}{2\,\hbar^2} \\
u_0 &= \frac{\sqrt{2\lambda m}}{\hbar}
\end{aligned} \tag{3.38}$$

Exercise 3.7 ([3] pr 3.7)

A particle in a uniform field $\mathbf{E}_0$. Show that the expectation value of the position operator $\langle \mathbf{r} \rangle$ satisfies

$$m \frac{d^2 \langle \mathbf{r} \rangle}{dt^2} = e\mathbf{E}_0. \tag{3.39}$$

Answer for Exercise 3.7

This follows from Ehrenfest's theorem once we formulate the force $e\mathbf{E}_0 = -\boldsymbol{\nabla}\phi$, in terms of a potential ϕ. That potential is

$$\phi = -e\mathbf{E}_0 \cdot (x, y, z) \tag{3.40}$$

The Hamiltonian is therefore

$$H = \frac{\mathbf{p}^2}{2m} - e\mathbf{E}_0 \cdot (x, y, z). \tag{3.41}$$

Ehrenfest's theorem gives us

$$\begin{aligned} \frac{d}{dt} \langle x_k \rangle &= \frac{1}{m} \langle p_k \rangle \\ \frac{d}{dt} \langle p_k \rangle &= -\left\langle \frac{\partial V}{\partial x_k} \right\rangle, \end{aligned} \tag{3.42}$$

or

$$\frac{d^2}{dt^2} \langle x_k \rangle = -\frac{1}{m} \left\langle \frac{\partial V}{\partial x_k} \right\rangle. \tag{3.43}$$

$$\frac{\partial V}{\partial x_k} = -e(\mathbf{E}_0)_k \tag{3.44}$$

Putting all the last bits together, and summing over the directions $\mathbf{e}_k$ we have

$$m \frac{d^2}{dt^2} \mathbf{e}_k \langle x_k \rangle = \mathbf{e}_k \langle e(\mathbf{E}_0)_k \rangle = e\mathbf{E}_0 \qquad \square \tag{3.45}$$

Exercise 3.8 ([3] pr 3.8)

For Hamiltonian eigenstates $|E_n\rangle$, $C = AB$, $A = [B, H]$, obtain the matrix element $\langle E_m| C |E_n\rangle$ in terms of the matrix element of A.

Answer for Exercise 3.8

I was able to get most of what was asked for here, with a small exception. I started with the matrix element for A, which is

$$\langle E_m | A | E_n \rangle = \langle E_m | BH - HB | E_n \rangle = (E_n - E_m) \langle E_m | B | E_n \rangle \tag{3.46}$$

Next, computing the matrix element for C we have

$$\begin{aligned}
\langle E_m | C | E_n \rangle &= \langle E_m | BHB - HB^2 | E_n \rangle \\
&= \sum_a \langle E_m | BH | E_a \rangle \langle E_a | B | E_n \rangle - E_m \langle E_m | B | E_a \rangle \langle E_a | B | E_n \rangle \\
&= \sum_a E_a \langle E_m | B | E_a \rangle \langle E_a | B | E_n \rangle - E_m \langle E_m | B | E_a \rangle \langle E_a | B | E_n \rangle \\
&= \sum_a (E_a - E_m) \langle E_m | B | E_a \rangle \langle E_a | B | E_n \rangle \\
&= \sum_a \langle E_m | A | E_a \rangle \langle E_a | B | E_n \rangle \\
&= \langle E_m | A | E_n \rangle \langle E_n | B | E_n \rangle + \sum_{a \neq n} \langle E_m | A | E_a \rangle \langle E_a | B | E_n \rangle \\
&= \langle E_m | A | E_n \rangle \langle E_n | B | E_n \rangle + \sum_{a \neq n} \langle E_m | A | E_a \rangle \frac{\langle E_a | A | E_n \rangle}{E_n - E_a}
\end{aligned} \tag{3.47}$$

Except for the $\langle E_n | B | E_n \rangle$ part of this expression, the problem as stated is complete. The relationship eq. (3.46) is no help for with $n = m$, so I see no choice but to leave that small part of the expansion in terms of B.

Exercise 3.9 ([3] pr 3.9)

Operator A has eigenstates $|a_i\rangle$, with a unitary change of basis operation $U |a_i\rangle = |b_i\rangle$. Determine in terms of U, and A the operator B and its eigenvalues for which $|b_i\rangle$ are eigenstates.

Answer for Exercise 3.9

Consider for motivation the matrix element of A in terms of $|b_i\rangle$. We will also let $A |a_i\rangle = \alpha_i |a_i\rangle$. We then have

$$\langle a_i | A \left| a_j \right\rangle = \langle b_i | U A U^\dagger \left| b_j \right\rangle \tag{3.48}$$

We also have

$$\begin{aligned}
\langle a_i | A \left| a_j \right\rangle &= a_j \langle a_i | \left| a_j \right\rangle \\
&= a_j \delta_{ij}
\end{aligned} \tag{3.49}$$

So it appears that the operator $UAU^\dagger$ has the orthonormality relation required. In terms of action on the basis $\{|b_i\rangle\}$, let us see how it behaves. We have

$$\begin{aligned} UAU^\dagger |b_i\rangle &= UA|a_i\rangle \\ &= U\alpha_i |a_i\rangle \\ &= \alpha_i |b_i\rangle \end{aligned} \tag{3.50}$$

So we see that the operators A and $B = UAU^\dagger$ have common eigenvalues.

Exercise 3.10 *([3] pr 3.10)*

With $H|n\rangle = E_n|n\rangle$, $A = [H, F]$ and $\langle 0| F|0\rangle = 0$, show that

$$\sum_{n\neq 0} \frac{\langle 0| A|n\rangle \langle n| A|0\rangle}{E_n - E_0} = \langle 0| AF|0\rangle \tag{3.51}$$

Answer for Exercise 3.10

$$\begin{aligned} \langle 0| AF|0\rangle &= \langle 0| HFF - FHF|0\rangle \\ &= \sum_n E_0 \langle 0| F|n\rangle \langle n| F|0\rangle - E_n \langle 0| F|n\rangle \langle n| F|0\rangle \\ &= \sum_n (E_0 - E_n) \langle 0| F|n\rangle \langle n| F|0\rangle \\ &= \sum_{n\neq 0} (E_0 - E_n) \langle 0| F|n\rangle \langle n| F|0\rangle \end{aligned} \tag{3.52}$$

We also have

$$\begin{aligned} \langle 0| A|n\rangle \langle n| A|0\rangle &= \langle 0| HF - FH|n\rangle \langle n| A|0\rangle \\ &= (E_0 - E_n) \langle 0| F|n\rangle \langle n| HF - FH|0\rangle \\ &= -(E_0 - E_n)^2 \langle 0| F|n\rangle \langle n| F|0\rangle \end{aligned} \tag{3.53}$$

Or, for $n \neq 0$,

$$\langle 0| F|n\rangle \langle n| F|0\rangle = -\frac{\langle 0| A|n\rangle \langle n| A|0\rangle}{(E_0 - E_n)^2}. \tag{3.54}$$

This gives

$$
\begin{aligned}
\langle 0| AF |0\rangle &= -\sum_{n\neq 0}(E_0 - E_n)\frac{\langle 0| A |n\rangle \langle n| A |0\rangle}{(E_0 - E_n)^2} \\
&= \sum_{n\neq 0}\frac{\langle 0| A |n\rangle \langle n| A |0\rangle}{E_n - E_0} \qquad \square
\end{aligned}
\tag{3.55}
$$

Exercise 3.11 Commutator of angular momentum with Hamiltonian ([3] pr 3.11)

Show that $[\mathbf{L}, H] = 0$, where $H = \mathbf{p}^2/2m + V(r)$.

Answer for Exercise 3.11

This follows by considering $\left[\mathbf{L}, \mathbf{p}^2\right]$, and $[\mathbf{L}, V(r)]$. Let

$$
L_{jk} = x_j p_k - x_k p_j,
\tag{3.56}
$$

so that

$$
\mathbf{L} = \mathbf{e}_i \epsilon_{ijk} L_{jk}.
\tag{3.57}
$$

We now need to consider the commutators of the operators L_{jk} with $\mathbf{p}^2$ and $V(r)$. Let us start with p^2. In particular

$$
\begin{aligned}
\mathbf{p}^2 x_m p_n &= p_k p_k x_m p_n \\
&= p_k (p_k x_m) p_n \\
&= p_k (-i\hbar\delta_{km} + x_m p_k) p_n \\
&= -i\hbar p_m p_n + (p_k x_m) p_k p_n \\
&= -i\hbar p_m p_n + (-i\hbar\delta_{km} + x_m p_k) p_k p_n \\
&= -2i\hbar p_m p_n + x_m p_n \mathbf{p}^2.
\end{aligned}
\tag{3.58}
$$

So our commutator with $\mathbf{p}^2$ is

$$
\left[L_{jk}, \mathbf{p}^2\right] = (x_j p_k - x_j p_k)\mathbf{p}^2 - (-2i\hbar p_j p_k + x_j p_k \mathbf{p}^2 + 2i\hbar p_k p_j - x_k p_j \mathbf{p}^2).
\tag{3.59}
$$

Since $p_j p_k = p_k p_j$, all terms cancel out, and the problem is reduced to showing that

$$
[\mathbf{L}, H] = [\mathbf{L}, V(r)] = 0.
\tag{3.60}
$$

Now assume that $V(r)$ has a series representation

$$V(r) = \sum_j a_j r^j = \sum_j a_j (x_k x_k)^{j/2} \tag{3.61}$$

We would like to consider the action of $x_m p_n$ on this function

$$\begin{aligned} x_m p_n V(r)\Psi &= -i\hbar x_m \sum_j a_j \partial_n (x_k x_k)^{j/2} \Psi \\ &= -i\hbar x_m \sum_j a_j (j x_n (x_k x_k)^{j/2-1} + r^j \partial_n \Psi) \\ &= -\frac{i\hbar x_m x_n}{r^2} \sum_j a_j j r^j + x_m V(r) p_n \Psi \end{aligned} \tag{3.62}$$

$$\begin{aligned} L_{mn} V(r) &= (x_m p_n - x_n p_m) V(r) \\ &= -\frac{i\hbar x_m x_n}{r^2} \sum_j a_j j r^j + \frac{i\hbar x_n x_m}{r^2} \sum_j a_j j r^j + V(r)(x_m p_n - x_n p_m) \\ &= V(r) L_{mn} \end{aligned} \tag{3.63}$$

Thus $[L_{mn}, V(r)] = 0$ as expected, implying $[\mathbf{L}, H] = 0$.

Exercise 3.12 Two level quantum system (2008 PHY355H1F final 2.)

Consider a two-level quantum system, with basis states $\{|a\rangle, |b\rangle\}$. Suppose that the Hamiltonian for this system is given by

$$H = \frac{\hbar\Delta}{2}(|b\rangle\langle b| - |a\rangle\langle a|) + i\frac{\hbar\Omega}{2}(|a\rangle\langle b| - |b\rangle\langle a|) \tag{3.64}$$

where Δ and Ω are real positive constants.

Find the energy eigenvalues and the normalized energy eigenvectors (expressed in terms of the $\{|a\rangle, |b\rangle\}$ basis).

Write the time evolution operator $U(t) = e^{-iHt/\hbar}$ using these eigenvectors.

Answer for Exercise 9.3

The eigenvalue part of this problem is probably easier to do in matrix form. Let

$$\begin{aligned} |a\rangle &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ |b\rangle &= \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \end{aligned} \tag{3.65}$$

Our Hamiltonian is then

$$H = \frac{\hbar}{2}\begin{bmatrix} -\Delta & i\Omega \\ -i\Omega & \Delta \end{bmatrix}. \tag{3.66}$$

Computing $\det H - \lambda I = 0$, we get

$$\lambda = \pm\frac{\hbar}{2}\sqrt{\Delta^2 + \Omega^2}. \tag{3.67}$$

Let $\delta = \sqrt{\Delta^2 + \Omega^2}$. Our normalized eigenvectors are found to be

$$|\pm\rangle = \frac{1}{\sqrt{2\delta(\delta \pm \Delta)}}\begin{bmatrix} i\Omega \\ \Delta \pm \delta \end{bmatrix}. \tag{3.68}$$

In terms of $|a\rangle$ and $|b\rangle$, we then have

$$|\pm\rangle = \frac{1}{\sqrt{2\delta(\delta \pm \Delta)}}\left(i\Omega\,|a\rangle + (\Delta \pm \delta)\,|b\rangle\right). \tag{3.69}$$

Note that our Hamiltonian has a simple form in this basis. That is

$$H = \frac{\delta\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|) \tag{3.70}$$

Observe that once we do the diagonalization, we have a Hamiltonian that appears to have the form of a scaled projector for an open Stern-Gerlach apparatus.

Observe that the diagonalized Hamiltonian operator makes the time evolution operator's form also simple, which is, by inspection

$$U(t) = e^{-it\frac{\delta}{2}}\,|+\rangle\langle+| + e^{it\frac{\delta}{2}}\,|-\rangle\langle-|\,. \tag{3.71}$$

Since we are asked for this in terms of $|a\rangle$, and $|b\rangle$, the projectors $|\pm\rangle\langle\pm|$ are required. These are

$$|\pm\rangle\langle\pm| = \frac{1}{2\delta(\delta \pm \Delta)}\left(i\Omega\,|a\rangle + (\Delta \pm \delta)\,|b\rangle\right)\left(-i\Omega\,\langle a| + (\Delta \pm \delta)\,\langle b|\right) \tag{3.72}$$

$$|\pm\rangle\langle\pm| = \frac{1}{2\delta(\delta \pm \Delta)}\left(\Omega^2\,|a\rangle\langle a| + (\delta \pm \delta)^2\,|b\rangle\langle b| + i\Omega(\Delta \pm \delta)(|a\rangle\langle b| - |b\rangle\langle a|)\right) \tag{3.73}$$

Substitution into eq. (3.71) and a fair amount of algebra leads to

$$U(t) = \cos(\delta t/2)\big(|a\rangle\langle a| + |b\rangle\langle b|\big) + i\frac{\Omega}{\delta}\sin(\delta t/2)\big(|a\rangle\langle a| - |b\rangle\langle b| - i(|a\rangle\langle b| - |b\rangle\langle a|)\big). \tag{3.74}$$

Note that while a big cumbersome, we can also verify that we can recover the original Hamiltonian from eq. (3.70) and eq. (3.73).

Q: (b) Suppose that the initial state of the system at time $t = 0$ is $|\phi(0)\rangle = |b\rangle$. Find an expression for the state at some later time $t > 0$, $|\phi(t)\rangle$.

A: Most of the work is already done. Computation of $|\phi(t)\rangle = U(t)|\phi(0)\rangle$ follows from eq. (3.74)

$$|\phi(t)\rangle = \cos(\delta t/2)|b\rangle - i\frac{\Omega}{\delta}\sin(\delta t/2)\big(|b\rangle + i|a\rangle\big). \tag{3.75}$$

Q: (c) Suppose that an observable, specified by the operator $X = |a\rangle\langle b| + |b\rangle\langle a|$, is measured for this system. What is the probability that, at time t, the result 1 is obtained? Plot this probability as a function of time, showing the maximum and minimum values of the function, and the corresponding values of t.

A: The language of questions like these attempt to bring some physics into the mathematics. The phrase "the result 1 is obtained", is really a statement that the operator X, after measurement is found to have the eigenstate with numeric value 1.

We can calculate the eigenvectors for this operator easily enough and find them to be ± 1. For the positive eigenvalue we can also compute the eigenstate to be

$$|X+\rangle = \frac{1}{\sqrt{2}}\big(|a\rangle + |b\rangle\big). \tag{3.76}$$

The question of what the probability for this measurement is then really a question asking for the computation of the amplitude

$$\left|\frac{1}{\sqrt{2}}\langle (a+b)|\phi(t)\rangle\right|^2 \tag{3.77}$$

From eq. (3.75) we find this probability to be

$$\begin{aligned}\left|\frac{1}{\sqrt{2}}\langle (a+b)|\phi(t)\rangle\right|^2 &= \frac{1}{2}\left(\left(\cos(\delta t/2) + \frac{\Omega}{\delta}\sin(\delta t/2)\right)^2 + \frac{\Omega^2\sin^2(\delta t/2)}{\delta^2}\right) \\ &= \frac{1}{4}\left(1 + 3\frac{\Omega^2}{\delta^2} + \frac{\Delta^2}{\delta^2}\cos(\delta t) + 2\frac{\Omega}{\delta}\sin(\delta t)\right)\end{aligned} \tag{3.78}$$

We have a simple superposition of two sinusoids out of phase, periodic with period $2\pi/\delta$. I had attempted a rough sketch of this on paper, but will not bother scanning it here or describing it further.

Q: (d) Suppose an experimenter has control over the values of the parameters Δ and Ω. Explain how she might prepare the state $(|a\rangle + |b\rangle)/\sqrt{2}$.

A: For this part of the question I was not sure what approach to take. I thought perhaps this linear combination of states could be made to equal one of the energy eigenstates, and if one could prepare the system in that state, then for certain values of δ and Δ one would then have this desired state.

To get there I note that we can express the states $|a\rangle$, and $|b\rangle$ in terms of the eigenstates by inverting

$$\begin{bmatrix}|+\rangle \\ |-\rangle\end{bmatrix} = \frac{1}{\sqrt{2\delta}}\begin{bmatrix}\frac{i\Omega}{\sqrt{\delta+\Delta}} & \sqrt{\delta+\Delta} \\ \frac{i\Omega}{\sqrt{\delta-\Delta}} & -\sqrt{\delta-\Delta}\end{bmatrix}\begin{bmatrix}|a\rangle \\ |b\rangle\end{bmatrix}. \tag{3.79}$$

Skipping all the algebra one finds

$$\begin{bmatrix}|a\rangle \\ |b\rangle\end{bmatrix} = \begin{bmatrix}-i\sqrt{\delta-\Delta} & -i\sqrt{\delta+\Delta} \\ \frac{\Omega}{\sqrt{\delta-\Delta}} & -\frac{\Omega}{\sqrt{\delta+\Delta}}\end{bmatrix}\begin{bmatrix}|+\rangle \\ |-\rangle\end{bmatrix}. \tag{3.80}$$

Unfortunately, this does not seem helpful. I find

$$\frac{1}{\sqrt{2}}(|a\rangle + |b\rangle) = \frac{|+\rangle}{\sqrt{\delta-\Delta}}(\Omega - i(\delta-\Delta)) - \frac{|-\rangle}{\sqrt{\delta+\Delta}}(\Omega + i(\delta+\Delta)) \tag{3.81}$$

There is no obvious way to pick Ω and Δ to leave just $|+\rangle$ or $|-\rangle$. When I did this on paper originally I got a different answer for this sum, but looking at it now, I can not see how I managed to get that answer (it had no factors of i in the result as the one above does).

A physical system for this Hamiltonian I wondered what physical system such a Hamiltonian would correspond to, and noted that this bore some similarity to the up vs. down states of the Ammonia atom as discussed in [4]. In that text the Hamiltonian is reasoned to have the form

$$H = E_0(|b\rangle\langle b| + |a\rangle\langle a|) - A(|a\rangle\langle b| + |b\rangle\langle a|). \tag{3.82}$$

In Feynman's treatment, the Hamiltonian is just specified by giving values to H_{ij}, but the expression can easily seen to be equivalent. While these do not look equivalent on the surface, they both have the same diagonalization, which allows us to give a physical interpretation to this sort of problem (one which is recurrant in the old QMI exams).

4

FREE PARTICLES

4.1 ANTISYMMETRIC TENSOR SUMMATION IDENTITY

$$\sum_i \epsilon_{ijk}\epsilon_{iab} = \delta_{ja}\delta_{kb} - \delta_{jb}\delta_{ka} \tag{4.1}$$

This is obviously the coordinate equivalent of the dot product of two bivectors

$$(\mathbf{e}_j \wedge \mathbf{e}_k) \cdot (\mathbf{e}_a \wedge \mathbf{e}_b) = ((\mathbf{e}_j \wedge \mathbf{e}_k) \cdot \mathbf{e}_a) \cdot \mathbf{e}_b) = \delta_{ka}\delta_{jb} - \delta_{ja}\delta_{kb} \tag{4.2}$$

We can prove eq. (4.1) by expanding the LHS of eq. (4.2) in coordinates

$$\begin{aligned}
(\mathbf{e}_j \wedge \mathbf{e}_k) \cdot (\mathbf{e}_a \wedge \mathbf{e}_b) &= \sum_{ie} \left\langle \epsilon_{ijk}\mathbf{e}_j\mathbf{e}_k\epsilon_{eab}\mathbf{e}_a\mathbf{e}_b \right\rangle \\
&= \sum_{ie} \epsilon_{ijk}\epsilon_{eab}\left\langle (\mathbf{e}_i\mathbf{e}_i)\mathbf{e}_j\mathbf{e}_k(\mathbf{e}_e\mathbf{e}_e)\mathbf{e}_a\mathbf{e}_b \right\rangle \\
&= \sum_{ie} \epsilon_{ijk}\epsilon_{eab}\left\langle \mathbf{e}_i\mathbf{e}_e I^2 \right\rangle \\
&= -\sum_{ie} \epsilon_{ijk}\epsilon_{eab}\delta_{ie} \\
&= -\sum_{i} \epsilon_{ijk}\epsilon_{iab} \qquad \square
\end{aligned} \tag{4.3}$$

4.2 QUESTION ON RAISING AND LOWERING ARGUMENTS

How equation (4.240) was arrived at is not clear. In (4.239) he writes

$$\int_0^{2\pi}\int_0^{\pi} d\theta d\phi (L_- Y_{lm})^\dagger L_- Y_{lm} \sin\theta \tag{4.4}$$

Should not that Hermitian conjugation be just complex conjugation? if so one would have

$$\int_0^{2\pi}\int_0^{\pi} d\theta d\phi L_-^* Y_{lm}^* L_- Y_{lm} \sin\theta \tag{4.5}$$

How does he end up with the L_- and the Y_{lm}^* interchanged. What justifies this commutation? A much clearer discussion of this can be found in The operators $L_\pm$, where Dirac notation is used for the normalization discussion.

Vatche's explanation Asked Vatche about this and had it explained nicely. He also used the braket notation, and wrote

$$\langle \theta, \phi | l, m \rangle \equiv Y_{lm}(\theta, \phi) \tag{4.6}$$

and introduces the identity

$$I = \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi \, |\theta, \phi\rangle \langle \theta, \phi| \tag{4.7}$$

Now, if we want to normalize the state $L_- |l, m\rangle$ we write

$$\begin{aligned}
&\langle l, m | L_-^\dagger L_- |l, m\rangle \\
&\quad = \langle l, m | L_-^\dagger L_- |l, m\rangle \\
&\quad = \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi \int_0^\pi d\theta' \sin\theta' \int_0^{2\pi} d\phi' \, \langle l, m|\theta, \phi\rangle \langle \theta, \phi| L_+ L_- \left|\theta', \phi'\right\rangle \langle \theta', \phi' | l, m\rangle \\
&\quad = \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi \int_0^\pi d\theta' \sin\theta' \int_0^{2\pi} d\phi' Y_{lm}^*(\theta, \phi) \langle \theta, \phi| L_+ L_- \left|\theta', \phi'\right\rangle Y_{lm}(\theta', \phi')
\end{aligned} \tag{4.8}$$

Now he points out that the matrix element has both the differential operator portion, as well as a delta function portion, so we would have

$$\langle \theta, \phi| L_+ L_- \left|\theta', \phi'\right\rangle = \frac{1}{\sin\theta} \delta(\theta - \theta')\delta(\phi - \phi') L_+(\theta, \phi) L_-(\theta, \phi) \tag{4.9}$$

where the raising and lowering operators are now in their differential form

$$L_+(\theta, \phi) L_-(\theta, \phi) = \hbar e^{i\theta} \left(\partial_\theta + i \cot\theta \partial_\phi\right) \hbar e^{-i\theta} \left(-\partial_\theta + i \cot\theta \partial_\phi\right) \tag{4.10}$$

This now gives us

$$\begin{aligned}
\langle l, m | L_-^\dagger L_- |l, m\rangle &= \int_0^\pi d\theta \int_0^{2\pi} d\phi \int_0^\pi d\theta' \sin\theta' \int_0^{2\pi} d\phi' Y_{lm}^*(\theta, \phi) L_+(\theta, \phi) L_-(\theta, \phi) Y_{lm}(\theta', \phi') \delta(\theta \\
&\qquad - \theta')\delta(\phi - \phi') \\
&= \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi Y_{lm}^*(\theta, \phi) L_+(\theta, \phi) L_-(\theta, \phi) Y_{lm}(\theta, \phi)
\end{aligned} \tag{4.11}$$

This now fills in the reasoning (and notational) gap that the text has between (4.239) and (4.240). It is now clear that in 4.239 (where Hermitian conjugation seemed out of place), that it should just have been regular complex number conjugation. In the context of the normalization integral, Hermitian conjugation plays no role. Here the $L_{-}Y_{lm}$ used in the text are just functions.

4.3 ANOTHER QUESTION ON RAISING AND LOWERING ARGUMENTS

The reasoning leading to (4.238) is not clear to me. I fail to see how the L_{-} commutation with $\mathbf{L}^2$ implies this?

4.4 LECTURE NOTES: REVIEW

For three dimensions with $V(x, y, z) = 0$

$$\begin{aligned} H &= \frac{1}{2m}\mathbf{p}^2 \\ \mathbf{p} &= \sum_i p_i \mathbf{e}_i \end{aligned} \tag{4.12}$$

In the position representation, where

$$p_i = -i\hbar \frac{d}{dx_i} \tag{4.13}$$

the Schrödinger equation is

$$\begin{aligned} Hu(x, y, z) &= Eu(x, y, z) \\ H &= -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 \\ &= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \end{aligned} \tag{4.14}$$

Separation of variables assumes it is possible to let

$$u(x, y, z) = X(x)Y(y)Z(z) \tag{4.15}$$

(these capital letters are functions, not operators).

$$-\frac{\hbar^2}{2m}\left(YZ\frac{\partial^2 X}{\partial x^2} + XZ\frac{\partial^2 Y}{\partial y^2} + YZ\frac{\partial^2 Z}{\partial z^2}\right) = EXYZ \tag{4.16}$$

Dividing as usual by XYZ we have

$$-\frac{\hbar^2}{2m}\left(\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right) = E \tag{4.17}$$

The curious thing is that we have these three derivatives, which is supposed to be related to an Energy, which is independent of any x, y, z, so it must be that each of these is separately constant. We can separate these into three individual equations

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} &= E_1 \\ -\frac{\hbar^2}{2m}\frac{1}{Y}\frac{\partial^2 Y}{\partial x^2} &= E_2 \\ -\frac{\hbar^2}{2m}\frac{1}{Z}\frac{\partial^2 Z}{\partial x^2} &= E_3 \end{aligned} \tag{4.18}$$

or

$$\begin{aligned} \frac{\partial^2 X}{\partial x^2} &= \left(-\frac{2mE_1}{\hbar^2}\right)X \\ \frac{\partial^2 Y}{\partial x^2} &= \left(-\frac{2mE_2}{\hbar^2}\right)Y \\ \frac{\partial^2 Z}{\partial x^2} &= \left(-\frac{2mE_3}{\hbar^2}\right)Z \end{aligned} \tag{4.19}$$

We have then

$$X(x) = C_1 e^{ikx} \tag{4.20}$$

with

$$\begin{aligned} E_1 &= \frac{\hbar^2 k_1^2}{2m} = \frac{p_1^2}{2m} \\ E_2 &= \frac{\hbar^2 k_2^2}{2m} = \frac{p_2^2}{2m} \\ E_3 &= \frac{\hbar^2 k_3^2}{2m} = \frac{p_3^2}{2m} \end{aligned} \tag{4.21}$$

We are free to use any sort of normalization procedure we wish (periodic boundary conditions, infinite Dirac, ...)

4.5 PROBLEMS

Exercise 4.1 ([3] pr 4.1)

Write down the free particle Schrödinger equation for two dimensions in (i) Cartesian and (ii) polar coordinates. Obtain the corresponding wavefunction.

Answer for Exercise 4.1

Cartesian case For the Cartesian coordinates case we have

$$H = -\frac{\hbar^2}{2m}(\partial_{xx} + \partial_{yy}) = i\hbar\partial_t \tag{4.22}$$

Application of separation of variables with $\Psi = XYT$ gives

$$-\frac{\hbar^2}{2m}\left(\frac{X''}{X} + \frac{Y''}{Y}\right) = i\hbar\frac{T'}{T} = E. \tag{4.23}$$

Immediately, we have the time dependence

$$T \propto e^{-iEt/\hbar}, \tag{4.24}$$

with the PDE reduced to

$$\frac{X''}{X} + \frac{Y''}{Y} = -\frac{2mE}{\hbar^2}. \tag{4.25}$$

Introducing separate independent constants

$$\begin{aligned}\frac{X''}{X} &= a^2 \\ \frac{Y''}{Y} &= b^2\end{aligned} \tag{4.26}$$

provides the pre-normalized wave function and the constraints on the constants

$$\begin{aligned}\Psi &= Ce^{ax}e^{by}e^{-iEt/\hbar} \\ a^2 + b^2 &= -\frac{2mE}{\hbar^2}.\end{aligned} \tag{4.27}$$

Rectangular normalization We are now ready to apply normalization constraints. One possibility is a rectangular periodicity requirement.

$$
\begin{aligned}
e^{ax} &= e^{a(x+\lambda_x)} \\
e^{ay} &= e^{a(y+\lambda_y)},
\end{aligned}
\tag{4.28}
$$

or

$$
\begin{aligned}
a\lambda_x &= 2\pi i m \\
a\lambda_y &= 2\pi i n.
\end{aligned}
\tag{4.29}
$$

This provides a more explicit form for the energy expression

$$
E_{mn} = \frac{1}{2m} 4\pi^2 \hbar^2 \left(\frac{m^2}{{\lambda_x}^2} + \frac{n^2}{{\lambda_y}^2} \right).
\tag{4.30}
$$

We can also add in the area normalization using

$$
\langle \psi | \phi \rangle = \int_{x=0}^{\lambda_x} dx \int_{y=0}^{\lambda_x} dy \psi^*(x, y) \phi(x, y).
\tag{4.31}
$$

Our eigenfunctions are now completely specified

$$
u_{mn}(x, y, t) = \frac{1}{\sqrt{\lambda_x \lambda_y}} e^{2\pi i x/\lambda_x} e^{2\pi i y/\lambda_y} e^{-iEt/\hbar}.
\tag{4.32}
$$

The interesting thing about this solution is that we can make arbitrary linear combinations

$$
f(x, y) = a_{mn} u_{mn}
\tag{4.33}
$$

and then “solve” for a_{mn}, for an arbitrary $f(x, y)$ by taking inner products

$$
a_{mn} = \langle u_m n | f \rangle = \int_{x=0}^{\lambda_x} dx \int_{y=0}^{\lambda_x} dy f(x, y) u_m n^*(x, y).
\tag{4.34}
$$

This gives the appearance that any function $f(x, y)$ is a solution, but the equality of eq. (4.33) only applies for functions in the span of this function vector space. The procedure works for arbitrary square integrable functions $f(x, y)$, but the equality really means that the RHS will be the periodic extension of $f(x, y)$.

Infinite space normalization An alternate normalization is possible by using the Fourier transform normalization, in which we substitute

$$\begin{aligned}\frac{2\pi m}{\lambda_x} &= k_x \\ \frac{2\pi n}{\lambda_y} &= k_y\end{aligned} \tag{4.35}$$

Our inner product is now

$$\langle\psi|\phi\rangle = \int_{-\infty}^{\infty} dx \int_{\infty}^{\infty} dy \psi^*(x, y)\phi(x, y). \tag{4.36}$$

And the corresponding normalized wavefunction and associated energy constant E are

$$\begin{aligned}u_{\mathbf{k}}(x, y, t) &= \frac{1}{2\pi} e^{ik_x x} e^{ik_y y} e^{-iEt/\hbar} = \frac{1}{2\pi} e^{i\mathbf{k}\cdot\mathbf{x}} e^{-iEt/\hbar} \\ E &= \frac{\hbar^2\mathbf{k}^2}{2m}\end{aligned} \tag{4.37}$$

Now via this Fourier inner product we are able to construct a solution from any square integrable function. Again, this will not be an exact equality since the Fourier transform has the effect of averaging across discontinuities.

Polar case In polar coordinates our gradient is

$$\boldsymbol{\nabla} = \hat{\mathbf{r}}\partial_r + \frac{\hat{\boldsymbol{\theta}}}{r}\partial_\theta. \tag{4.38}$$

with

$$\begin{aligned}\hat{\mathbf{r}} &= \mathbf{e}_1 e^{\mathbf{e}_1\mathbf{e}_2\theta} \\ \hat{\boldsymbol{\theta}} &= \mathbf{e}_2 e^{\mathbf{e}_1\mathbf{e}_2\theta}.\end{aligned} \tag{4.39}$$

Squaring the gradient for the Laplacian we will need the partials, which are

$$\begin{aligned}\partial_r\hat{\mathbf{r}} &= 0 \\ \partial_r\hat{\boldsymbol{\theta}} &= 0 \\ \partial_\theta\hat{\mathbf{r}} &= \hat{\boldsymbol{\theta}} \\ \partial_\theta\hat{\boldsymbol{\theta}} &= -\hat{\mathbf{r}}.\end{aligned} \tag{4.40}$$

The Laplacian is therefore

$$\begin{aligned}\boldsymbol{\nabla}^2 &= (\hat{\mathbf{r}}\partial_r + \frac{\hat{\boldsymbol{\theta}}}{r}\partial_\theta) \cdot (\hat{\mathbf{r}}\partial_r + \frac{\hat{\boldsymbol{\theta}}}{r}\partial_\theta) \\ &= \partial_{rr} + \frac{\hat{\boldsymbol{\theta}}}{r} \cdot \partial_\theta \hat{\mathbf{r}}\partial_r \frac{\hat{\boldsymbol{\theta}}}{r} \cdot \partial_\theta \frac{\hat{\boldsymbol{\theta}}}{r}\partial_\theta \\ &= \partial_{rr} + \frac{\hat{\boldsymbol{\theta}}}{r} \cdot (\partial_\theta \hat{\mathbf{r}})\partial_r + \frac{\hat{\boldsymbol{\theta}}}{r} \cdot \frac{\hat{\boldsymbol{\theta}}}{r}\partial_{\theta\theta} + \frac{\hat{\boldsymbol{\theta}}}{r} \cdot (\partial_\theta \hat{\boldsymbol{\theta}})\frac{1}{r}\partial_\theta.\end{aligned} \tag{4.41}$$

Evaluating the derivatives we have

$$\boldsymbol{\nabla}^2 = \partial_{rr} + \frac{1}{r}\partial_r + \frac{1}{r^2}\partial_{\theta\theta}, \tag{4.42}$$

and are now prepared to move on to the solution of the Hamiltonian $H = -(\hbar^2/2m)\boldsymbol{\nabla}^2$. With separation of variables again using $\Psi = R(r)\Theta(\theta)T(t)$ we have

$$-\frac{\hbar^2}{2m}\left(\frac{R''}{R} + \frac{R'}{rR} + \frac{1}{r^2}\frac{\Theta''}{\Theta}\right) = i\hbar\frac{T'}{T} = E. \tag{4.43}$$

Rearranging to separate the Θ term we have

$$\frac{r^2R''}{R} + \frac{rR'}{R} + \frac{2mE}{\hbar^2}r^2E = -\frac{\Theta''}{\Theta} = \lambda^2. \tag{4.44}$$

The angular solutions are given by

$$\Theta = \frac{1}{\sqrt{2\pi}}e^{i\lambda\theta} \tag{4.45}$$

Where the normalization is given by

$$\langle\psi|\phi\rangle = \int_0^{2\pi} d\theta\psi^*(\theta)\phi(\theta). \tag{4.46}$$

And the radial by the solution of the PDE

$$r^2R'' + rR' + \left(\frac{2mE}{\hbar^2}r^2E - \lambda^2\right)R = 0 \tag{4.47}$$

Exercise 4.2 ([3] pr 4.2)

Use the orthogonality property of $P_l(\cos\theta)$

$$\int_{-1}^{1} dx P_l(x) P_{l'}(x) = \frac{2}{2l+1}\delta_{ll'}, \tag{4.48}$$

confirm that at least the first two terms of (4.171)

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta) \tag{4.49}$$

are correct.

Answer for Exercise 4.2

Taking the inner product using the integral of eq. (4.48) we have

$$\int_{-1}^{1} dx e^{ikrx} P_l'(x) = 2 i^l j_l(kr) \tag{4.50}$$

To confirm the first two terms we need

$$\begin{aligned}
P_0(x) &= 1 \\
P_1(x) &= x \\
j_0(\rho) &= \frac{\sin\rho}{\rho} \\
j_1(\rho) &= \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}.
\end{aligned} \tag{4.51}$$

On the LHS for $l' = 0$ we have

$$\int_{-1}^{1} dx e^{ikrx} = 2\frac{\sin kr}{kr} \tag{4.52}$$

On the LHS for $l' = 1$ note that

$$\begin{aligned}
\int dx x e^{ikrx} &= \int dx x \frac{d}{dx}\frac{e^{ikrx}}{ikr} \\
&= x\frac{e^{ikrx}}{ikr} - \frac{e^{ikrx}}{(ikr)^2}.
\end{aligned} \tag{4.53}$$

So, integration in $[-1, 1]$ gives us

$$\int_{-1}^{1} dx e^{ikrx} = -2i \frac{\cos kr}{kr} + 2i \frac{1}{(kr)^2} \sin kr. \tag{4.54}$$

Now compare to the RHS for $l' = 0$, which is

$$2 j_0(kr) = 2 \frac{\sin kr}{kr}, \tag{4.55}$$

which matches eq. (4.52). For $l' = 1$ we have

$$2i j_1(kr) = 2i \frac{1}{kr} \left(\frac{\sin kr}{kr} - \cos kr \right), \tag{4.56}$$

which in turn matches eq. (4.54), completing the exercise.

Exercise 4.3 ([3] pr 4.3)

Obtain the commutation relations $[L_i, L_j]$ by calculating the vector $\mathbf{L} \times \mathbf{L}$ using the definition $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ directly instead of introducing a differential operator.

Answer for Exercise 4.3

Expressing the product $\mathbf{L} \times \mathbf{L}$ in determinant form sheds some light on this question. That is

$$\begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ L_1 & L_2 & L_3 \\ L_1 & L_2 & L_3 \end{vmatrix} = \mathbf{e}_1 \left[L_2, L_3 \right] + \mathbf{e}_2 \left[L_3, L_1 \right] + \mathbf{e}_3 \left[L_1, L_2 \right] = \mathbf{e}_i \epsilon_{ijk} \left[L_j, L_k \right] \tag{4.57}$$

We see that evaluating this cross product in turn requires evaluation of the set of commutators. We can do that with the canonical commutator relationships directly using $L_i = \epsilon_{ijk} r_j p_k$ like so

$$\begin{aligned}
\left[L_i, L_j \right] &= \epsilon_{imn} r_m p_n \epsilon_{jab} r_a p_b - \epsilon_{jab} r_a p_b \epsilon_{imn} r_m p_n \\
&= \epsilon_{imn} \epsilon_{jab} r_m (p_n r_a) p_b - \epsilon_{jab} \epsilon_{imn} r_a (p_b r_m) p_n \\
&= \epsilon_{imn} \epsilon_{jab} r_m (r_a p_n - i \hbar \delta_{an}) p_b - \epsilon_{jab} \epsilon_{imn} r_a (r_m p_b - i \hbar \delta m b) p_n \\
&= \epsilon_{imn} \epsilon_{jab} (r_m r_a p_n p_b - r_a r_m p_b p_n) - i \hbar (\epsilon_{imn} \epsilon_{jnb} r_m p_b - \epsilon_{jam} \epsilon_{imn} r_a p_n).
\end{aligned} \tag{4.58}$$

The first two terms cancel, and we can employ (4.179) to eliminate the antisymmetric tensors from the last two terms

$$
\begin{aligned}
[L_i, L_j] &= i\hbar(\epsilon_{nim}\epsilon_{njb} r_m p_b - \epsilon_{mja}\epsilon_{min} r_a p_n) \\
&= i\hbar((\delta_{ij}\delta_{mb} - \delta_{ib}\delta_{mj}) r_m p_b - (\delta_{ji}\delta_{an} - \delta_{jn}\delta_{ai}) r_a p_n) \\
&= i\hbar(\delta_{ij}\delta_{mb} r_m p_b - \delta_{ji}\delta_{an} r_a p_n - \delta_{ib}\delta_{mj} r_m p_b + \delta_{jn}\delta_{ai} r_a p_n) \\
&= i\hbar(\delta_{ij} r_m p_m - \delta_{ji} r_a p_a - r_j p_i + r_i p_j)
\end{aligned}
\tag{4.59}
$$

For $k \neq i, j$, this is $i\hbar(\mathbf{r} \times \mathbf{p})_k$, so we can write

$$
\mathbf{L} \times \mathbf{L} = i\hbar \mathbf{e}_k \epsilon_{kij}(r_i p_j - r_j p_i) = i\hbar \mathbf{L} = i\hbar \mathbf{e}_k L_k = i\hbar \mathbf{L}.
\tag{4.60}
$$

In [9], the commutator relationships are summarized this way, instead of using the antisymmetric tensor (4.224)

$$
[L_i, L_j] = i\hbar \epsilon_{ijk} L_k
\tag{4.61}
$$

as here in Desai. Both say the same thing.

Exercise 4.4 *([3] pr 4.5)*

A free particle is moving along a path of radius R. Express the Hamiltonian in terms of the derivatives involving the polar angle of the particle and write down the Schrödinger equation. Determine the wavefunction and the energy eigenvalues of the particle.

Answer for Exercise 4.4

In classical mechanics our Lagrangian for this system is

$$
\mathcal{L} = \frac{1}{2} m R^2 \dot{\theta}^2,
\tag{4.62}
$$

with the canonical momentum

$$
p_\theta = \frac{\partial \mathcal{L}}{\partial \dot{\theta}} = m R^2 \dot{\theta}.
\tag{4.63}
$$

Thus the classical Hamiltonian is

$$
H = \frac{1}{2mR^2} {p_\theta}^2.
\tag{4.64}
$$

By analogy the QM Hamiltonian operator will therefore be

$$H = -\frac{\hbar^2}{2mR^2}\partial_{\theta\theta}. \tag{4.65}$$

For $\Psi = \Theta(\theta)T(t)$, separation of variables gives us

$$-\frac{\hbar^2}{2mR^2}\frac{\Theta''}{\Theta} = i\hbar\frac{T'}{T} = E, \tag{4.66}$$

from which we have

$$\begin{aligned} T &\propto e^{-iEt/\hbar} \\ \Theta &\propto e^{\pm i\sqrt{2mE}R\theta/\hbar}. \end{aligned} \tag{4.67}$$

Requiring single valued Θ, equal at any multiples of 2π, we have

$$e^{\pm i\sqrt{2mE}R(\theta+2\pi)/\hbar} = e^{\pm i\sqrt{2mE}R\theta/\hbar}, \tag{4.68}$$

or

$$\pm\sqrt{2mE}\frac{R}{\hbar}2\pi = 2\pi n, \tag{4.69}$$

Suffixing the energy values with this index we have

$$E_n = \frac{n^2\hbar^2}{2mR^2}. \tag{4.70}$$

Allowing both positive and negative integer values for n we have

$$\Psi = \frac{1}{\sqrt{2\pi}}e^{in\theta}e^{-iE_nt/\hbar}, \tag{4.71}$$

where the normalization was a result of the use of a $[0, 2\pi]$ inner product over the angles

$$\langle\psi|\phi\rangle \equiv \int_0^{2\pi}\psi^*(\theta)\phi(\theta)d\theta. \tag{4.72}$$

Exercise 4.5 ([3] pr 4.6)

Determine $[L_i, r]$ and $[L_i, \mathbf{r}]$.

Answer for Exercise 4.5

Since L_i contain only θ and ϕ partials, $\left[L_i, r\right] = 0$. For the position vector, however, we have an angular dependence, and are left to evaluate $\left[L_i, \mathbf{r}\right] = r\left[L_i, \hat{\mathbf{r}}\right]$. We will need the partials for $\hat{\mathbf{r}}$. We have

$$\begin{aligned}
\hat{\mathbf{r}} &= \mathbf{e}_3 e^{I\hat{\boldsymbol{\phi}}\theta} \\
\hat{\boldsymbol{\phi}} &= \mathbf{e}_2 e^{\mathbf{e}_1\mathbf{e}_2\phi} \\
I &= \mathbf{e}_1\mathbf{e}_2\mathbf{e}_3
\end{aligned} \tag{4.73}$$

Evaluating the partials we have

$$\partial_\theta \hat{\mathbf{r}} = \hat{\mathbf{r}} I \hat{\boldsymbol{\phi}} \tag{4.74}$$

With

$$\begin{aligned}
\hat{\boldsymbol{\theta}} &= \tilde{R}\mathbf{e}_1 R \\
\hat{\boldsymbol{\phi}} &= \tilde{R}\mathbf{e}_2 R \\
\hat{\mathbf{r}} &= \tilde{R}\mathbf{e}_3 R
\end{aligned} \tag{4.75}$$

where $\tilde{R}R = 1$, and $\hat{\boldsymbol{\theta}}\hat{\boldsymbol{\phi}}\hat{\mathbf{r}} = \mathbf{e}_1\mathbf{e}_2\mathbf{e}_3$, we have

$$\partial_\theta \hat{\mathbf{r}} = \tilde{R}\mathbf{e}_3\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3\mathbf{e}_2 R = \tilde{R}\mathbf{e}_1 R = \hat{\boldsymbol{\theta}} \tag{4.76}$$

For the ϕ partial we have

$$\begin{aligned}
\partial_\phi \hat{\mathbf{r}} &= \mathbf{e}_3 \sin\theta I \hat{\boldsymbol{\phi}} \mathbf{e}_1\mathbf{e}_2 \\
&= \sin\theta \hat{\boldsymbol{\phi}}
\end{aligned} \tag{4.77}$$

We are now prepared to evaluate the commutators. Starting with the easiest we have

$$\begin{aligned}
\left[L_z, \hat{\mathbf{r}}\right]\Psi &= -i\hbar(\partial_\phi \hat{\mathbf{r}}\Psi - \hat{\mathbf{r}}\partial_\phi \Psi) \\
&= -i\hbar(\partial_\phi \hat{\mathbf{r}})\Psi
\end{aligned} \tag{4.78}$$

So we have

$$\left[L_z, \hat{\mathbf{r}}\right] = -i\hbar \sin\theta \hat{\boldsymbol{\phi}} \tag{4.79}$$

Observe that by virtue of chain rule, only the action of the partials on $\hat{\mathbf{r}}$ itself contributes, and all the partials applied to Ψ cancel out due to the commutator differences. That simplifies the remaining commutator evaluations. For reference the polar form of L_x, and L_y are

$$\begin{aligned}
L_x &= -i\hbar(-S_\phi \partial_\theta - C_\phi \cot\theta \partial_\phi) \\
L_y &= -i\hbar(C_\phi \partial_\theta - S_\phi \cot\theta \partial_\phi),
\end{aligned} \tag{4.80}$$

where the sines and cosines are written with S, and C respectively for short. We therefore have

$$\begin{aligned}
[L_x, \hat{\mathbf{r}}] &= -i\hbar(-S_\phi(\partial_\theta \hat{\mathbf{r}}) - C_\phi \cot\theta(\partial_\phi \hat{\mathbf{r}})) \\
&= -i\hbar(-S_\phi \hat{\boldsymbol{\theta}} - C_\phi \cot\theta S_\theta \hat{\boldsymbol{\phi}}) \\
&= -i\hbar(-S_\phi \hat{\boldsymbol{\theta}} - C_\phi C_\theta \hat{\boldsymbol{\phi}})
\end{aligned} \tag{4.81}$$

and

$$\begin{aligned}
[L_y, \hat{\mathbf{r}}] &= -i\hbar(C_\phi(\partial_\theta \hat{\mathbf{r}}) - S_\phi \cot\theta(\partial_\phi \hat{\mathbf{r}})) \\
&= -i\hbar(C_\phi \hat{\boldsymbol{\theta}} - S_\phi C_\theta \hat{\boldsymbol{\phi}}).
\end{aligned} \tag{4.82}$$

Adding back in the factor of r, and summarizing we have

$$\begin{aligned}
[L_i, r] &= 0 \\
[L_x, \mathbf{r}] &= -i\hbar r(-\sin\phi \hat{\boldsymbol{\theta}} - \cos\phi\cos\theta \hat{\boldsymbol{\phi}}) \\
[L_y, \mathbf{r}] &= -i\hbar r(\cos\phi \hat{\boldsymbol{\theta}} - \sin\phi\cos\theta \hat{\boldsymbol{\phi}}) \\
[L_z, \mathbf{r}] &= -i\hbar r \sin\theta \hat{\boldsymbol{\phi}}
\end{aligned} \tag{4.83}$$

5 SPIN 1/2

5.1 LECTURE NOTES: REVIEW

HOMEWORK: go through the steps to understand how to formulate $\boldsymbol{\nabla}^2$ in spherical polar coordinates. This is a lot of work, but is good practice and background for dealing with the Hydrogen atom, something with spherical symmetry that is most naturally analyzed in the spherical polar coordinates.

In spherical coordinates (We will not go through this here, but it is good practice) with

$$\begin{aligned} x &= r \sin\theta \cos\phi \\ y &= r \sin\theta \sin\phi \\ z &= r \cos\theta \end{aligned} \tag{5.1}$$

we have with $u = u(r, \theta, \phi)$

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r}\partial_{rr}(ru) + \frac{1}{r^2 \sin\theta}\partial_\theta(\sin\theta\partial_\theta u) + \frac{1}{r^2 \sin^2\theta}\partial_{\phi\phi} u\right) = Eu \tag{5.2}$$

We see the start of a separation of variables attack with $u = R(r)Y(\theta, \phi)$. We end up with

$$-\frac{\hbar^2}{2m}\left(\frac{r}{R}(rR')' + \frac{1}{Y \sin\theta}\partial_\theta(\sin\theta\partial_\theta Y) + \frac{1}{Y \sin^2\theta}\partial_{\phi\phi} Y\right) \tag{5.3}$$

$$r(rR')' + \left(\frac{2mE}{\hbar^2}r^2 - \lambda\right)R = 0 \tag{5.4}$$

$$\frac{1}{Y \sin\theta}\partial_\theta(\sin\theta\partial_\theta Y) + \frac{1}{Y \sin^2\theta}\partial_{\phi\phi} Y = -\lambda \tag{5.5}$$

Application of separation of variables again, with $Y = P(\theta)Q(\phi)$ gives us

$$\frac{1}{P \sin\theta}\partial_\theta(\sin\theta\partial_\theta P) + \frac{1}{Q \sin^2\theta}\partial_{\phi\phi} Q = -\lambda \tag{5.6}$$

$$\frac{\sin\theta}{P}\partial_\theta(\sin\theta\partial_\theta P) + \lambda\sin^2\theta + \frac{1}{Q}\partial_{\phi\phi}Q = 0 \tag{5.7}$$

$$\frac{\sin\theta}{P}\partial_\theta(\sin\theta\partial_\theta P) + \lambda\sin^2\theta - \mu = 0\frac{1}{Q}\partial_{\phi\phi}Q = -\mu \tag{5.8}$$

or

$$\frac{1}{P\sin\theta}\partial_\theta(\sin\theta\partial_\theta P) + \lambda - \frac{\mu}{\sin^2\theta} = 0 \tag{5.9}$$

$$\partial_{\phi\phi}Q = -\mu Q \tag{5.10}$$

The equation for P can be solved using the Legendre function $P_l^m(\cos\theta)$ where $\lambda = l(l+1)$ and l is an integer

Replacing μ with m^2, where m is an integer

$$\frac{d^2Q}{d\phi^2} = -m^2 Q \tag{5.11}$$

Imposing a periodic boundary condition $Q(\phi) = Q(\phi + 2\pi)$, where $(m = 0, \pm 1, \pm 2, \cdots)$ we have

$$Q = \frac{1}{\sqrt{2\pi}}e^{im\phi} \tag{5.12}$$

There is the overall solution $r(r,\theta,\phi) = R(r)Y(\theta,\phi)$ for a free particle. The functions $Y(\theta,\phi)$ are

$$Y_{lm}(\theta,\phi) = N\left(\frac{1}{\sqrt{2\pi}}e^{im\phi}\right)\overset{-l \leq m \leq l}{\boxed{P_l^m(\cos\theta)}} \tag{5.13}$$

where N is a normalization constant, and $m = 0, \pm 1, \pm 2, \cdots$. Y_{lm} is an eigenstate of the $\mathbf{L}^2$ operator and L_z (two for the price of one). There is no specific reason for the direction z, but it is the direction picked out of convention.

Angular momentum is given by

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \tag{5.14}$$

where

$$\mathbf{R} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} \tag{5.15}$$

and

$$\mathbf{p} = p_x\hat{\mathbf{x}} + p_y\hat{\mathbf{y}} + p_z\hat{\mathbf{z}} \tag{5.16}$$

The important thing to remember is that the aim of following all the math is to show that

$$\mathbf{L}^2 Y_{lm} = \hbar^2 l(l+1) Y_{lm} \tag{5.17}$$

and simultaneously

$$\mathbf{L}_z Y_{lm} = \hbar m Y_{lm} \tag{5.18}$$

Part of the solution involves working with $[L_z, L_+]$, and $[L_z, L_-]$, where

$$\begin{aligned} L_+ &= L_x + iL_y \\ L_- &= L_x - iL_y \end{aligned} \tag{5.19}$$

An exercise (not in the book) is to evaluate

$$[L_z, L_+] = L_z L_x + iL_z L_y - L_x L_z - iL_y L_z \tag{5.20}$$

where

$$\begin{aligned} [L_x, L_y] &= i\hbar L_z \\ [L_y, L_z] &= i\hbar L_x \\ [L_z, L_x] &= i\hbar L_y \end{aligned} \tag{5.21}$$

Substitution back in eq. (5.20) we have

$$\begin{aligned} [L_z, L_+] &= [L_z, L_x] + i\,[L_z, L_y] \\ &= i\hbar(L_y - iL_x) \\ &= \hbar(iL_y + L_x) \\ &= \hbar L_+ \end{aligned} \tag{5.22}$$

5.2 LECTURE: ORBITAL AND INTRINSIC MOMENTUM

Last time, we started thinking about angular momentum. This time, we will examine orbital and intrinsic angular momentum.

Orbital angular momentum in classical physics and quantum physics is expressed as

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}, \tag{5.23}$$

and

$$\mathbf{L} = \mathbf{R} \times \mathbf{P}, \tag{5.24}$$

where $\mathbf{R}$ and $\mathbf{P}$ are quantum mechanical operators corresponding to position and momentum

$$\begin{aligned} \mathbf{R} &= X\hat{\mathbf{x}} + Y\hat{\mathbf{y}} + Z\hat{\mathbf{z}} \\ \mathbf{P} &= P_x\hat{\mathbf{x}} + P_y\hat{\mathbf{y}} + P_z\hat{\mathbf{z}} \\ \mathbf{L} &= L_x\hat{\mathbf{x}} + L_y\hat{\mathbf{y}} + L_z\hat{\mathbf{z}} \end{aligned} \tag{5.25}$$

Example 5.1: Angular momentum commutators

Determine the commutators $[L_x, L_y]$, $[L_y, L_z]$, $[L_z, L_x]$ and

$$\begin{aligned} [L_x, L_y] &= (r_y p_z - r_z p_y)(r_z p_x - r_x p_z) - (r_z p_x - r_x p_z)(r_y p_z - r_z p_y) \\ &= r_y p_z(r_z p_x - r_x p_z) - r_z p_y(r_z p_x - r_x p_z) - r_z p_x(r_y p_z - r_z p_y) + r_x p_z(r_y p_z - r_z p_y) \\ &= r_y p_z r_z p_x - r_y p_z r_x p_z - r_z p_y r_z p_x + r_z p_y r_x p_z - r_z p_x r_y p_z + r_z p_x r_z p_y + r_x p_z r_y p_z - r_x p_z r_z p_y \end{aligned} \tag{5.26}$$

With $p_i r_j = r_j p_i - i\hbar\delta_{ij}$, we have

$$\begin{aligned} \left[L_x, L_y\right] &= r_y r_z p_z p_x - r_y r_z p_x p_z - r_z r_y p_z p_x + r_z r_y p_x p_z - r_z r_x p_y p_z \\ &\quad + r_z r_x p_z p_y + r_x r_z p_y p_z - r_x r_z p_z p_y + -i\hbar\left(r_y p_x - r_x p_y\right) \end{aligned}$$

Since the $p_i p_j$ operators commute, all the first terms cancel, leaving just

$$[L_x, L_y] = i\hbar L_z \tag{5.27}$$

Example 5.2: L_z in spherical coordinates

The answer is

$$L_z \leftrightarrow -i\hbar \frac{\partial}{\partial \phi} \tag{5.28}$$

FIXME: Work through this.

Part of the task in this intro QM treatment is to carefully determine the eigenfunctions for these operators.

The spherical harmonics are given by $Y_{lm}(\theta, \phi)$ such that

$$Y_{lm}(\theta, \phi) \propto e^{im\phi} \tag{5.29}$$

$$\begin{aligned} L_z Y_{lm}(\theta, \phi) &= -i\hbar \frac{\partial}{\partial \phi} Y_{lm}(\theta, \phi) \\ &= -i\hbar \frac{\partial}{\partial \phi} \text{constants}(e^{im\phi}) \\ &= \hbar m \text{constants} e^{im\phi} \\ &= \hbar m Y_{lm}(\theta, \phi) \end{aligned} \tag{5.30}$$

The z-component is quantized since, m is an integer $m = 0, \pm 1, \pm 2, ...$ The total angular momentum

$$\mathbf{L}^2 = \mathbf{L} \cdot \mathbf{L} = L_x^2 + L_y^2 + L_z^2 \tag{5.31}$$

is also quantized (details in the book).

The eigenvalue properties here represent very important physical features. This is also important in the hydrogen atom problem. In the hydrogen atom problem, the particle is effectively free in the angular components, having only r dependence. This allows us to apply the work for the free particle to our subsequent potential bounded solution.

Note that for the above, we also have the alternate, abstract ket notation, method of writing the eigenvalue behavior.

$$L_z \left| lm \right\rangle = \hbar m \left| lm \right\rangle \tag{5.32}$$

Just like

$$X|x\rangle = x|x\rangle \\ P|p\rangle = p|p\rangle \tag{5.33}$$

For the total angular momentum our spherical harmonic eigenfunctions have the property

$$\mathbf{L}^2|lm\rangle = \hbar^2 l(l+1)|lm\rangle \tag{5.34}$$

with $l = 0, 1, 2, \cdots$.
Alternately in plain old non-abstract notation we can write this as

$$\mathbf{L}^2 Y_{lm}(\theta,\phi) = \hbar^2 l(l+1) Y_{lm}(\theta,\phi) \tag{5.35}$$

Now we can introduce the Raising and Lowering Operators, which are

$$L_+ = L_x + iL_y \\ L_- = L_x - iL_y, \tag{5.36}$$

respectively. These are abstract quantities, but also physically important since they relate quantum levels of the angular momentum. How do we show this?
Last time, we saw that

$$[L_z, L_+] = +\hbar L_+ \\ [L_z, L_-] = -\hbar L_- \tag{5.37}$$

Note that it is implied that we are operating on ket vectors

$$L_z(L_-|lm\rangle) \tag{5.38}$$

with

$$|lm\rangle \leftrightarrow Y_{lm}(\theta,\phi) \tag{5.39}$$

Question: What is $L_-|lm\rangle$?
Substitute

$$\begin{aligned} L_zL_- - L_-L_z &= -\hbar L_- \\ &\Longrightarrow \\ L_zL_- &= L_-L_z - \hbar L_- \end{aligned} \tag{5.40}$$

$$
\begin{aligned}
L_z \left(L_- \left| lm \right\rangle \right) &= L_- L_z \left| lm \right\rangle - \hbar L_- \left| lm \right\rangle \\
&= L_- m \hbar \left| lm \right\rangle - L_- \left| lm \right\rangle \\
&= \hbar \left(m L_- \left| lm \right\rangle - L_- \left| lm \right\rangle \right) \\
&= \hbar (m-1) \left(L_- \left| lm \right\rangle \right)
\end{aligned}
\tag{5.41}
$$

So $L_- \left| lm \right\rangle = \left| \psi \right\rangle$ is another spherical harmonic, and we have

$$
L_z \left| \psi \right\rangle = \hbar (m-1) \left| \psi \right\rangle
\tag{5.42}
$$

This lowering operator quantity causes a physical change in the state of the system, lowering the observable state (ie: the eigenvalue) by $\hbar$.

Now we want to normalize $\left| \psi \right\rangle = L_- \left| lm \right\rangle$, via $\left\langle \psi | \psi \right\rangle = 1$.

$$
\begin{aligned}
1 &= \left\langle \psi | \psi \right\rangle \\
&= \left\langle lm \right| L_-^\dagger L_- \left| \psi \right\rangle \\
&= \left\langle lm \right| L_+ L_- \left| \psi \right\rangle
\end{aligned}
\tag{5.43}
$$

We can use

$$
L_+ L_- = \mathbf{L}^2 - L_z^2 + \hbar L_z,
\tag{5.44}
$$

So, knowing (how exactly?) that

$$
L_- \left| lm \right\rangle = C \left| l, m-1 \right\rangle
\tag{5.45}
$$

we have from eq. (5.44)

$$
\begin{aligned}
\left| C \right|^2 &= \left\langle lm \right| (\mathbf{L}^2 - L_z^2 + \hbar L_z) \left| \psi \right\rangle \\
&= \overbrace{\boxed{\left\langle lm | lm \right\rangle}}^{=1} \left(\hbar^2 l(l+1) - (\hbar m)^2 + \hbar^2 m \right) \\
&= \hbar^2 \left(l(l+1) - m^2 + m \right).
\end{aligned}
\tag{5.46}
$$

we have

$$|C|^2 \overbrace{\boxed{\langle l, m-1 | l, m-1 \rangle}}^{1} = \hbar^2 \Big(l(l+1) - m^2 + m \Big). \tag{5.47}$$

and can normalize the functions $|\psi\rangle$ as

$$L_- |lm\rangle = \hbar \Big(l(l+1) - m^2 + m \Big)^{1/2} |l, m-1\rangle \tag{5.48}$$

Abstract notation side note:

$$\langle \theta, \phi | lm \rangle = Y_{lm}(\theta, \phi) \tag{5.49}$$

Generalizing orbital angular momentum To explain the results of the Stern-Gerlach experiment, assume that there is an intrinsic angular momentum $\mathbf{S}$ that has most of the same properties as $\mathbf{L}$. But $\mathbf{S}$ has no classical counterpart such as $\mathbf{r} \times \mathbf{p}$.

This experiment is the classic QM experiment because the silver atoms not only have the orbital angular momentum, but also have an additional observed intrinsic spin in the outermost electron. In turns out that if you combine relativity and QM, you can get out something that looks like the the $\mathbf{S}$ operator. That marriage produces the Dirac electron theory.

We assume the commutation relations

$$\begin{aligned} \left[S_x, S_y\right] &= i\hbar S_z \\ \left[S_y, S_z\right] &= i\hbar S_x \\ \left[S_z, S_x\right] &= i\hbar S_y \end{aligned} \tag{5.50}$$

Where we have the analogous eigenproperties

$$\begin{aligned} \mathbf{S}^2 |sm\rangle &= \hbar^2 s(s+1) |sm\rangle \\ S_z |sm\rangle &= \hbar m |sm\rangle \end{aligned} \tag{5.51}$$

with $s = 0, 1/2, 1, 3/2, \ldots$

Electrons and protons are examples of particles that have spin one half.

Note that there is no position representation of $|sm\rangle$. We cannot project these states.

This basic quantum mechanics end up applying to quantum computing and cryptography as well, when we apply the mathematics we are learning here to explain the Stern-Gerlach experiment to photon spin states.

(DRAWS Stern-Gerlach picture with spin up and down labeled $|z+\rangle$, and $|z-\rangle$ with the magnetic field oriented in along the z axis.)

Silver atoms have $s = 1/2$ and $m = \pm 1/2$, where m is the quantum number associated with the z-direction intrinsic angular momentum. The angular momentum that is being acted on in the Stern-Gerlach experiment is primarily due to the outermost electron.

$$\begin{aligned}
S_z |z+\rangle &= \frac{\hbar}{2} |z+\rangle \\
S_z |z-\rangle &= -\frac{\hbar}{2} |z-\rangle \\
\mathbf{S}^2 |z\pm\rangle &= \frac{1}{2}\left(\frac{1}{2} + 1\right) \hbar^2 |z\pm\rangle
\end{aligned} \tag{5.52}$$

where

$$\begin{aligned}
|z+\rangle &= \left|\frac{1}{2}\frac{1}{2}\right\rangle \\
|z-\rangle &= \left|\frac{1}{2} - \frac{1}{2}\right\rangle
\end{aligned} \tag{5.53}$$

What about S_x? We can leave the detector in the x, z plane, but rotate the magnet so that it lies in the x direction.

We have the correspondence

$$S_z \leftrightarrow \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{5.54}$$

but this is perhaps more properly viewed as the matrix representation of the less specific form

$$S_z = \frac{\hbar}{2} \left(|z+\rangle \langle z+| - |z-\rangle \langle z-| \right). \tag{5.55}$$

Where the translation to the form of eq. (5.54) is via the matrix elements

$$\begin{aligned}
&\langle z+| S_z |z+\rangle \\
&\langle z+| S_z |z-\rangle \\
&\langle z-| S_z |z+\rangle \\
&\langle z-| S_z |z-\rangle .
\end{aligned} \tag{5.56}$$

We can work out the same for S_x using S_+ and S_-, or equivalently for σ_x using σ_+ and σ_-, where

$$\begin{aligned} S_x &= \frac{\hbar}{2}\sigma_x \\ S_y &= \frac{\hbar}{2}\sigma_y \\ S_z &= \frac{\hbar}{2}\sigma_z \end{aligned} \tag{5.57}$$

The operators $\sigma_x, \sigma_y, \sigma_z$ are the Pauli operators, and avoid the pesky $\hbar/2$ factors. We find

$$\begin{aligned} \sigma_x &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \sigma_y &= \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \\ \sigma_z &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \end{aligned} \tag{5.58}$$

And from $|\sigma_x - \lambda I| = (-\lambda)^2 - 1$, we have eigenvalues $\lambda = \pm 1$ for the σ_x operator. The corresponding eigenkets in column matrix notation are found

$$\begin{aligned} &\begin{bmatrix} \mp 1 & 1 \\ 1 & \mp 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = 0 \\ &\implies \mp a_1 + a_2 = 0 \\ &\qquad \implies a_2 = \pm a_1 \end{aligned} \tag{5.59}$$

Or

$$|x\pm\rangle \propto \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = a_1 \begin{bmatrix} 1 \\ \pm 1 \end{bmatrix} \tag{5.60}$$

which can be normalized as

$$|x\pm\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm 1 \end{bmatrix} \tag{5.61}$$

We see that this is different from

$$|z+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{5.62}$$

We will still end up with two spots, but there has been a projection of spin in a different fashion? Does this mean the measurement will be different. There is still a lot more to learn before understanding exactly how to relate the spin operators to a real physical system.

5.3 PROBLEMS

Exercise 5.1 ([3] pr 5.1)

Obtain S_x, S_y, S_z for spin 1 in the representation in which S_z and S^2 are diagonal.

Answer for Exercise 5.1

For spin 1, we have

$$S^2 = 1(1+1)\hbar^2 \mathbf{1} \tag{5.63}$$

and are interested in the states $|1,-1\rangle, |1,0\rangle, and |1,1\rangle$. If, like angular momentum, we assume that we have for $m_s = -1, 0, 1$

$$S_z |1, m_s\rangle = m_s \hbar |1, m_s\rangle \tag{5.64}$$

and introduce a column matrix representations for the kets as follows

$$\begin{aligned}
|1,1\rangle &= \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \\
|1,0\rangle &= \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \\
|1,-1\rangle &= \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix},
\end{aligned} \tag{5.65}$$

then we have, by inspection

$$S_z = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \tag{5.66}$$

Note that, like the Pauli matrices, and unlike angular momentum, the spin states $|-1, m_s\rangle$, $|0, m_s\rangle$ have not been considered. Do those have any physical interpretation?

That question aside, we can proceed as in the text, utilizing the ladder operator commutators

$$S_\pm = S_x \pm i S_y, \tag{5.67}$$

to determine the values of S_x and S_y indirectly. We find

$$\begin{aligned} [S_+, S_-] &= 2\hbar S_z \\ [S_+, S_z] &= -\hbar S_+ \\ [S_-, S_z] &= \hbar S_-. \end{aligned} \tag{5.68}$$

Let

$$S_+ = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}. \tag{5.69}$$

Looking for equality between $[S_z, S_+] / \hbar = S_+$, we find

$$\begin{bmatrix} 0 & b & 2c \\ -d & 0 & f \\ -2g & -h & 0 \end{bmatrix} = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}, \tag{5.70}$$

so we must have

$$S_+ = \begin{bmatrix} 0 & b & 0 \\ 0 & 0 & f \\ 0 & 0 & 0 \end{bmatrix}. \tag{5.71}$$

Furthermore, from $[S_+, S_-] = 2\hbar S_z$, we find

$$\begin{bmatrix} |b|^2 & 0 & 0 \\ 0 & |f|^2 - |b|^2 & 0 \\ 0 & 0 & -|f|^2 \end{bmatrix} = 2\hbar^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \tag{5.72}$$

We must have $|b|^2 = |f|^2 = 2\hbar^2$. We could probably pick any $b = \sqrt{2}\hbar e^{i\phi}$, and $f = \sqrt{2}\hbar e^{i\theta}$, but assuming we have no reason for a non-zero phase we try

$$S_+ = \sqrt{2}\hbar \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}. \tag{5.73}$$

Putting all the pieces back together, with $S_x = (S_+ + S_-)/2$, and $S_y = (S_+ - S_-)/2i$, we finally have

$$\begin{aligned} S_x &= \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \\ S_y &= \frac{\hbar}{\sqrt{2}i} \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} \\ S_z &= \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \end{aligned} \tag{5.74}$$

A quick calculation verifies that we have $S_x^2 + S_y^2 + S_z^2 = 2\hbar\mathbf{1}$, as expected.

Exercise 5.2 ([3] pr 5.2)

Obtain eigensolution for operator $A = a\sigma_y + b\sigma_z$. Call the eigenstates $|1\rangle$ and $|2\rangle$, and determine the probabilities that they will correspond to $\sigma_x = +1$.

Answer for Exercise 5.2

The first part is straight forward, and we have

$$\begin{aligned} A &= a \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + b \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ &= \begin{bmatrix} b & -ia \\ ia & -b \end{bmatrix}. \end{aligned} \tag{5.75}$$

Taking $|A - \lambda I| = 0$ we get

$$\lambda = \pm\sqrt{a^2 + b^2}, \tag{5.76}$$

with eigenvectors proportional to

$$|\pm\rangle = \begin{bmatrix} ia \\ b \mp \sqrt{a^2 + b^2} \end{bmatrix} \tag{5.77}$$

The normalization constant is $1/\sqrt{2(a^2 + b^2) \mp 2b\sqrt{a^2 + b^2}}$. Now we can call these $|1\rangle$, and $|2\rangle$ but what does the last part of the question mean? What is meant by $\sigma_x = +1$?

Asking the prof about this, he says:

"I think it means that the result of a measurement of the x component of spin is +1. This corresponds to the eigenvalue of σ_x being +1. The spin operator S_x has eigenvalue $+\hbar/2$".

Aside: Question to consider later. Is is significant that $\langle 1|\sigma_x|1\rangle = \langle 2|\sigma_x|2\rangle = 0$?

So, how do we translate this into a mathematical statement?

First let us recall a couple of details. Recall that the x spin operator has the matrix representation

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{5.78}$$

This has eigenvalues ± 1, with eigenstates $(1, \pm 1)/\sqrt{2}$. At the point when the x component spin is observed to be +1, the state of the system was then

$$|x+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{5.79}$$

Let us look at the ways that this state can be formed as linear combinations of our states $|1\rangle$, and $|2\rangle$. That is

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \alpha |1\rangle + \beta |2\rangle, \tag{5.80}$$

or

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{\alpha}{\sqrt{(a^2 + b^2) - b\sqrt{a^2 + b^2}}} \begin{bmatrix} ia \\ b - \sqrt{a^2 + b^2} \end{bmatrix} + \frac{\beta}{\sqrt{(a^2 + b^2) + b\sqrt{a^2 + b^2}}} \begin{bmatrix} ia \\ b + \sqrt{a^2 + b^2} \end{bmatrix} \tag{5.81}$$

Letting $c = \sqrt{a^2 + b^2}$, this is

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{\alpha}{\sqrt{c^2 - bc}} \begin{bmatrix} ia \\ b - c \end{bmatrix} + \frac{\beta}{\sqrt{c^2 + bc}} \begin{bmatrix} ia \\ b + c \end{bmatrix}. \tag{5.82}$$

We can solve the α and β with Cramer's rule, yielding

$$\begin{aligned} \begin{vmatrix} 1 & ia \\ 1 & b - c \end{vmatrix} &= \frac{\beta}{\sqrt{c^2 + bc}} \begin{vmatrix} ia & ia \\ b + c & b - c \end{vmatrix} \\ \begin{vmatrix} 1 & ia \\ 1 & b + c \end{vmatrix} &= \frac{\alpha}{\sqrt{c^2 - bc}} \begin{vmatrix} ia & ia \\ b - c & b + c \end{vmatrix}, \end{aligned} \tag{5.83}$$

or

$$\begin{aligned} \alpha &= \frac{(b + c - ia)\sqrt{c^2 - bc}}{2iac} \\ \beta &= \frac{(b - c - ia)\sqrt{c^2 + bc}}{-2iac} \end{aligned} \tag{5.84}$$

It is $|\alpha|^2$ and $|\beta|^2$ that are probabilities, and after a bit of algebra we find that those are

$$|\alpha|^2 = |\beta|^2 = \frac{1}{2}, \tag{5.85}$$

so if the x spin of the system is measured as +1, we have a 50% chance that the measured eigenvalue for the operator A would be $\sqrt{a^2 + b^2}$ (ie: with state $|1\rangle$.

Is that what the question was asking? I think that I have actually got it backwards. I think that the question was asking for the probability of finding state $|x+\rangle$ (measuring a spin 1 value for σ_x) given the state $|1\rangle$ or $|2\rangle$.

So, suppose that we have

$$\begin{aligned} \mu_+ |x+\rangle + \nu_+ |x-\rangle &= |1\rangle \\ \mu_- |x+\rangle + \nu_- |x-\rangle &= |2\rangle, \end{aligned} \tag{5.86}$$

or (considering both cases simultaneously),

$$\begin{aligned} \mu_\pm \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \nu_\pm \begin{bmatrix} 1 \\ -1 \end{bmatrix} &= \frac{1}{\sqrt{c^2 \mp bc}} \begin{bmatrix} ia \\ b \mp c \end{bmatrix} \\ &\implies \\ \mu_\pm \begin{vmatrix} 1 & 1 \\ 1 & -1 \end{vmatrix} &= \frac{1}{\sqrt{c^2 \mp bc}} \begin{vmatrix} ia & 1 \\ b \mp c & -1 \end{vmatrix}, \end{aligned} \tag{5.87}$$

or

$$\mu_\pm = \frac{ia + b \mp c}{2\sqrt{c^2 \mp bc}}. \tag{5.88}$$

Unsurprisingly, this mirrors the previous scenario and we find that we have a probability $|\mu|^2 = 1/2$ of measuring a spin 1 value for σ_x when the state of the operator A has been measured as $\pm\sqrt{a^2 + b^2}$ (ie: in the states $|1\rangle$, or $|2\rangle$ respectively).

No measurement of the operator $A = a\sigma_y + b\sigma_z$ gives a biased prediction of the state of the state σ_x. Loosely, this seems to justify calling these operators orthogonal. This is consistent with the geometrical antisymmetric nature of the spin components where we have $\sigma_y\sigma_x = -\sigma_x\sigma_y$, just like two orthogonal vectors under the Clifford product.

Exercise 5.3 *([3] pr 5.3)*

Obtain the expectation values of S_x, S_y, S_z for the case of a spin 1/2 particle with the spin pointed in the direction of a vector with azimuthal angle β and polar angle α.

Answer for Exercise 5.3

Let us work with σ_k instead of S_k to eliminate the $\hbar/2$ factors. Before considering the expectation values in the arbitrary spin orientation, let us consider just the expectation values for σ_k. Introducing a matrix representation (assumed normalized) for a reference state

$$|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}, \tag{5.89}$$

we find

$$\begin{aligned}
\langle\psi|\,\sigma_x\,|\psi\rangle &= \begin{bmatrix} a^* & b^* \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = a^*b + b^*a \\
\langle\psi|\,\sigma_y\,|\psi\rangle &= \begin{bmatrix} a^* & b^* \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = -ia^*b + ib^*a \\
\langle\psi|\,\sigma_x\,|\psi\rangle &= \begin{bmatrix} a^* & b^* \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = a^*a - b^*b
\end{aligned} \tag{5.90}$$

Each of these expectation values are real as expected due to the Hermitian nature of σ_k. We also find that

$$\sum_{k=1}^{3} \langle\psi|\,\sigma_k\,|\psi\rangle^2 = (|a|^2 + |b|^2)^2 = 1 \tag{5.91}$$

So a vector formed with the expectation values as components is a unit vector. This does not seem too unexpected from the section on the projection operators in the text where it was stated that $\langle\chi|\boldsymbol{\sigma}|\chi\rangle = \mathbf{p}$, where $\mathbf{p}$ was a unit vector, and this seems similar. Let us now consider the arbitrarily oriented spin vector $\boldsymbol{\sigma}\cdot\mathbf{n}$, and look at its expectation value.

With $\mathbf{n}$ as the the rotated image of $\hat{\mathbf{z}}$ by an azimuthal angle β, and polar angle α, we have

$$\mathbf{n} = (\sin\alpha\cos\beta, \sin\alpha\sin\beta, \cos\alpha) \tag{5.92}$$

that is

$$\boldsymbol{\sigma}\cdot\mathbf{n} = \sin\alpha\cos\beta\sigma_x + \sin\alpha\sin\beta\sigma_y + \cos\alpha\sigma_z \tag{5.93}$$

The $k = x, y, y$ projections of this operator

$$\frac{1}{2}\operatorname{Tr}\sigma_k(\boldsymbol{\sigma}\cdot\mathbf{n})\sigma_k \tag{5.94}$$

are just the Pauli matrices scaled by the components of $\mathbf{n}$

$$\begin{aligned}
\frac{1}{2}\operatorname{Tr}\sigma_x(\boldsymbol{\sigma}\cdot\mathbf{n})\sigma_x &= \sin\alpha\cos\beta\sigma_x \\
\frac{1}{2}\operatorname{Tr}\sigma_y(\boldsymbol{\sigma}\cdot\mathbf{n})\sigma_y &= \sin\alpha\sin\beta\sigma_y \\
\frac{1}{2}\operatorname{Tr}\sigma_z(\boldsymbol{\sigma}\cdot\mathbf{n})\sigma_z &= \cos\alpha\sigma_z,
\end{aligned} \tag{5.95}$$

so our S_k expectation values are by inspection

$$\begin{aligned}
\langle\psi|S_x|\psi\rangle &= \frac{\hbar}{2}\sin\alpha\cos\beta(a^*b + b^*a) \\
\langle\psi|S_y|\psi\rangle &= \frac{\hbar}{2}\sin\alpha\sin\beta(-ia^*b + ib^*a) \\
\langle\psi|S_z|\psi\rangle &= \frac{\hbar}{2}\cos\alpha(a^*a - b^*b)
\end{aligned} \tag{5.96}$$

Is this correct? While $(\boldsymbol{\sigma}\cdot\mathbf{n})^2 = \mathbf{n}^2 = I$ is a unit norm operator, we find that the expectation values of the coordinates of $\boldsymbol{\sigma}\cdot\mathbf{n}$ cannot be viewed as the coordinates of a unit vector. Let us consider a specific case, with $\mathbf{n} = (0, 0, 1)$, where the spin is oriented in the x, y plane. That gives us

$$\boldsymbol{\sigma}\cdot\mathbf{n} = \sigma_z \tag{5.97}$$

so the expectation values of S_k are

$$
\begin{aligned}
\langle S_x \rangle &= 0 \\
\left\langle S_y \right\rangle &= 0 \\
\langle S_z \rangle &= \frac{\hbar}{2}(a^* a - b^* b)
\end{aligned}
\tag{5.98}
$$

Given this is seems reasonable that from eq. (5.96) we find

$$
\sum_k \langle \psi | S_k | \psi \rangle^2 \neq \hbar^2/4,
\tag{5.99}
$$

(since we do not have any reason to believe that in general $(a^* a - b^* b)^2 = 1$ is true).

The most general statement we can make about these expectation values (an average observed value for the measurement of the operator) is that

$$
|\langle S_k \rangle| \le \frac{\hbar}{2}
\tag{5.100}
$$

with equality for specific states and orientations only.

Exercise 5.4 *([3] pr 5.4)*

FIXME: describe.

Answer for Exercise 5.4

Take the azimuthal angle, $\beta = 0$, so that the spin is in the x-z plane at an angle α with respect to the z-axis, and the unit vector is $\mathbf{n} = (\sin\alpha, 0, \cos\alpha)$. Write

$$
|\chi_{n+}\rangle = |+\alpha\rangle
\tag{5.101}
$$

for this case. Show that the probability that it is in the spin-up state in the direction θ with respect to the z-axis is

$$
|\langle +\theta | +\alpha \rangle|^2 = \cos^2\left(\frac{\alpha - \theta}{2}\right)
\tag{5.102}
$$

Also obtain the expectation value of $\boldsymbol{\sigma} \cdot \mathbf{n}$ with respect to the state $|+\theta\rangle$.

Solution For this orientation we have

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \sin\alpha \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \cos\alpha \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} \cos\alpha & \sin\alpha \\ \sin\alpha & -\cos\alpha \end{bmatrix} \tag{5.103}$$

Confirmation that our eigenvalues are ± 1 is simple, and our eigenstates for the $+1$ eigenvalue is found to be

$$\lvert +\alpha \rangle \propto \begin{bmatrix} \sin\alpha \\ 1 - \cos\alpha \end{bmatrix} = \begin{bmatrix} \sin\alpha/2 \cos\alpha/2 \\ 2\sin^2\alpha/2 \end{bmatrix} \propto \begin{bmatrix} \cos\alpha/2 \\ \sin\alpha/2 \end{bmatrix} \tag{5.104}$$

This last has unit norm, so we can write

$$\lvert +\alpha \rangle = \begin{bmatrix} \cos\alpha/2 \\ \sin\alpha/2 \end{bmatrix} \tag{5.105}$$

If the state has been measured to be

$$\lvert \phi \rangle = 1 \lvert +\alpha \rangle + 0 \lvert -\alpha \rangle, \tag{5.106}$$

then the probability of a second measurement obtaining $\lvert +\theta \rangle$ is

$$\lvert \langle +\theta \vert \phi \rangle \rvert^2 = \lvert \langle +\theta \vert +\alpha \rangle \rvert^2. \tag{5.107}$$

Expanding just the inner product first we have

$$\begin{aligned} \langle +\theta \vert +\alpha \rangle &= \begin{bmatrix} C_{\theta/2} & S_{\theta/2} \end{bmatrix} \begin{bmatrix} C_{\alpha/2} \\ S_{\alpha/2} \end{bmatrix} \\ &= S_{\theta/2} S_{\alpha/2} + C_{\theta/2} C_{\alpha/2} \\ &= \cos\left(\frac{\theta - \alpha}{2}\right) \end{aligned} \tag{5.108}$$

So our probability of measuring spin up state $\lvert +\theta \rangle$ given the state was known to have been in spin up state $\lvert +\alpha \rangle$ is

$$\lvert \langle +\theta \vert +\alpha \rangle \rvert^2 = \cos^2\left(\frac{\theta - \alpha}{2}\right) \tag{5.109}$$

Finally, the expectation value for $\boldsymbol{\sigma} \cdot \mathbf{n}$ with respect to $|+\theta\rangle$ is

$$
\begin{aligned}
\begin{bmatrix} C_{\theta/2} & S_{\theta/2} \end{bmatrix} \begin{bmatrix} C_\alpha & S_\alpha \\ S_\alpha & -C_\alpha \end{bmatrix} \begin{bmatrix} C_{\theta/2} \\ S_{\theta/2} \end{bmatrix} &= \begin{bmatrix} C_{\theta/2} & S_{\theta/2} \end{bmatrix} \begin{bmatrix} C_\alpha C_{\theta/2} + S_\alpha S_{\theta/2} \\ S_\alpha C_{\theta/2} - C_\alpha S_{\theta/2} \end{bmatrix} \\
&= C_{\theta/2} C_\alpha C_{\theta/2} + C_{\theta/2} S_\alpha S_{\theta/2} + S_{\theta/2} S_\alpha C_{\theta/2} - S_{\theta/2} C_\alpha S_{\theta/2} \\
&= C_\alpha (C_{\theta/2}^2 - S_{\theta/2}^2) + 2 S_\alpha S_{\theta/2} C_{\theta/2} \\
&= C_\alpha C_\theta + S_\alpha S_\theta \\
&= \cos(\alpha - \theta)
\end{aligned}
\tag{5.110}
$$

Sanity checking this we observe that we have +1 as desired for the $\alpha = \theta$ case.

Exercise 5.5 ([3] pr 5.5)

Consider an arbitrary density matrix, ρ, for a spin 1/2 system. Express each matrix element in terms of the ensemble averages $[S_i]$ where $i = x, y, z$.

Answer for Exercise 5.5

Let us omit the spin direction temporarily and write for the density matrix

$$
\begin{aligned}
\rho &= w_+ |+\rangle \langle +| + w_- |-\rangle \langle -| \\
&= w_+ |+\rangle \langle +| + (1 - w_+) |-\rangle \langle -| \\
&= |-\rangle \langle -| + w_+ (|+\rangle \langle +| - |+\rangle \langle +|)
\end{aligned}
\tag{5.111}
$$

For the ensemble average (no sum over repeated indices) we have

$$
\begin{aligned}
[S] = \langle S \rangle_{av} &= w_+ \langle +| S |+\rangle + w_- \langle -| S |-\rangle \\
&= \frac{\hbar}{2}(w_+ - w_-) \\
&= \frac{\hbar}{2}(w_+ - (1 - w_+)) \\
&= \hbar w_+ - \frac{1}{2}
\end{aligned}
\tag{5.112}
$$

This gives us

$$
w_+ = \frac{1}{\hbar}[S] + \frac{1}{2}
\tag{5.113}
$$

and our density matrix becomes

$$
\begin{aligned}
\rho &= \frac{1}{2}(|+\rangle\langle+| + |-\rangle\langle-|) + \frac{1}{\hbar}[S](|+\rangle\langle+| - |+\rangle\langle+|) \\
&= \frac{1}{2}I + \frac{1}{\hbar}[S](|+\rangle\langle+| - |+\rangle\langle+|)
\end{aligned}
\tag{5.114}
$$

Utilizing

$$
\begin{aligned}
|x+\rangle &= \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} \\
|x-\rangle &= \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix} \\
|y+\rangle &= \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} \\
|y-\rangle &= \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-i\end{bmatrix} \\
|z+\rangle &= \begin{bmatrix}1\\0\end{bmatrix} \\
|z-\rangle &= \begin{bmatrix}0\\1\end{bmatrix}
\end{aligned}
\tag{5.115}
$$

We can easily find

$$
\begin{aligned}
|x+\rangle\langle x+| - |x+\rangle\langle x+| &= \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} = \sigma_x \\
|y+\rangle\langle y+| - |y+\rangle\langle y+| &= \begin{bmatrix}0 & -i\\i & 0\end{bmatrix} = \sigma_y \\
|z+\rangle\langle z+| - |z+\rangle\langle z+| &= \begin{bmatrix}1 & 0\\0 & -1\end{bmatrix} = \sigma_z
\end{aligned}
\tag{5.116}
$$

So we can write the density matrix in terms of any of the ensemble averages as

$$
\rho = \frac{1}{2}I + \frac{1}{\hbar}[S_i]\sigma_i = \frac{1}{2}(I + [\sigma_i]\sigma_i)
\tag{5.117}
$$

Alternatively, defining $\mathbf{P}_i = [\sigma_i]\mathbf{e}_i$, for any of the directions $i = 1, 2, 3$ we can write

$$\rho = \frac{1}{2}(I + \boldsymbol{\sigma} \cdot \mathbf{P}_i) \tag{5.118}$$

In equation (5.109) we had a similar result in terms of the polarization vector $\mathbf{P} = \langle\alpha| \boldsymbol{\sigma} |\alpha\rangle$, and the individual weights w_α, and w_β, but we see here that this $(w_\alpha - w_\beta)\mathbf{P}$ factor can be written exclusively in terms of the ensemble average. Actually, this is also a result in the text, down in (5.113), but we see it here in a more concrete form having picked specific spin directions.

Exercise 5.6 ([3] pr 5.6)

If a Hamiltonian is given by $\boldsymbol{\sigma} \cdot \mathbf{n}$ where $\mathbf{n} = (\sin\alpha\cos\beta, \sin\alpha\sin\beta, \cos\alpha)$, determine the time evolution operator as a 2 x 2 matrix. If a state at $t = 0$ is given by

$$|\phi(0)\rangle = \begin{bmatrix} a \\ b \end{bmatrix}, \tag{5.119}$$

then obtain $|\phi(t)\rangle$.

Answer for Exercise 5.6

Before diving into the meat of the problem, observe that a tidy factorization of the Hamiltonian is possible as a composition of rotations. That is

$$\begin{aligned} H &= \boldsymbol{\sigma} \cdot \mathbf{n} \\ &= \sin\alpha\sigma_1(\cos\beta + \sigma_1\sigma_2\sin\beta) + \cos\alpha\sigma_3 \\ &= \sigma_3\left(\cos\alpha + \sin\alpha\sigma_3\sigma_1 e^{i\sigma_3\beta}\right) \\ &= \sigma_3 \exp\left(\alpha i\sigma_2 \exp\left(\beta i\sigma_3\right)\right) \end{aligned} \tag{5.120}$$

So we have for the time evolution operator

$$U(\Delta t) = \exp(-i\Delta t H/\hbar) = \exp\left(-\frac{\Delta t}{\hbar} i\sigma_3 \exp\big(\alpha i\sigma_2 \exp\left(\beta i\sigma_3\right)\big)\right). \tag{5.121}$$

Does this really help? I guess not, but it is nice and tidy.

Returning to the specifics of the problem, we note that squaring the Hamiltonian produces the identity matrix

$$(\boldsymbol{\sigma} \cdot \mathbf{n})^2 = I\mathbf{n}^2 = I. \tag{5.122}$$

This allows us to exponentiate H by inspection utilizing

$$e^{i\mu(\boldsymbol{\sigma}\cdot\mathbf{n})} = I\cos\mu + i(\boldsymbol{\sigma}\cdot\mathbf{n})\sin\mu \tag{5.123}$$

Writing $\sin\mu = S_\mu$, and $\cos\mu = C_\mu$, we have

$$\boldsymbol{\sigma}\cdot\mathbf{n} = \begin{bmatrix} C_\alpha & S_\alpha e^{-i\beta} \\ S_\alpha e^{i\beta} & -C_\alpha \end{bmatrix}, \tag{5.124}$$

and thus

$$U(\Delta t) = \exp(-i\Delta t H/\hbar) = \begin{bmatrix} C_{\Delta t/\hbar} - iS_{\Delta t/\hbar}C_\alpha & -iS_{\Delta t/\hbar}S_\alpha e^{-i\beta} \\ -iS_{\Delta t/\hbar}S_\alpha e^{i\beta} & C_{\Delta t/\hbar} + iS_{\Delta t/\hbar}C_\alpha \end{bmatrix}. \tag{5.125}$$

Note that as a sanity check we can calculate that $U(\Delta t)U(\Delta t)^\dagger = 1$ as expected.
Now for $\Delta t = t$, we have

$$U(t,0)\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} aC_{t/\hbar} - aiS_{t/\hbar}C_\alpha - biS_{t/\hbar}S_\alpha e^{-i\beta} \\ -aiS_{t/\hbar}S_\alpha e^{i\beta} + bC_{t/\hbar} + biS_{t/\hbar}C_\alpha \end{bmatrix}. \tag{5.126}$$

It does not seem terribly illuminating to multiply this all out, but we can factor the results slightly to tidy it up. That gives us

$$U(t,0)\begin{bmatrix} a \\ b \end{bmatrix} = \cos(t/\hbar)\begin{bmatrix} a \\ b \end{bmatrix} + \sin(t/\hbar)\cos\alpha\begin{bmatrix} -a \\ b \end{bmatrix} + i\sin(t/\hbar)\sin\alpha\begin{bmatrix} be^{-i\beta} \\ -ae^{i\beta} \end{bmatrix} \tag{5.127}$$

Exercise 5.7 ([3] pr 5.7)

Consider a system of spin 1/2 particles in a mixed ensemble containing a mixture of 25% with spin given by $|z+\rangle$ and 75% with spin given by $|x-\rangle$. Determine the density matrix ρ and ensemble averages $\langle\boldsymbol{\sigma}_i\rangle_{\text{av}}$ for $i = x, y, z$.

Answer for Exercise 5.7

We have

$$\begin{aligned} \rho &= \frac{1}{4}\left|z+\right\rangle\left\langle z+\right| + \frac{3}{4}\left|x-\right\rangle\left\langle x-\right| \\ &= \frac{1}{4}\begin{bmatrix} 1 \\ 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \end{bmatrix} + \frac{3}{4}\frac{1}{2}\begin{bmatrix} 1 \\ -1 \end{bmatrix}\begin{bmatrix} 1 & -1 \end{bmatrix} \\ &= \frac{1}{4}\left(\frac{1}{2}\begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} + \frac{3}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\right) \end{aligned} \tag{5.128}$$

Giving us

$$\rho = \frac{1}{8}\begin{bmatrix} 5 & -3 \\ -3 & 3 \end{bmatrix}. \tag{5.129}$$

Note that we can also factor the identity out of this for

$$\begin{aligned}
\rho &= \frac{1}{2}\begin{bmatrix} 5/4 & -3/4 \\ -3/4 & 3/4 \end{bmatrix} \\
&= \frac{1}{2}\left(I + \begin{bmatrix} 1/4 & -3/4 \\ -3/4 & -1/4 \end{bmatrix}\right)
\end{aligned} \tag{5.130}$$

which is just:

$$\rho = \frac{1}{2}\left(I + \frac{1}{4}\sigma_z - \frac{3}{4}\sigma_x\right) \tag{5.131}$$

Recall that the ensemble average is related to the trace of the density and operator product

$$\begin{aligned}
\mathrm{Tr}(\rho A) &= \sum_\beta \langle\beta|\rho A|\beta\rangle \\
&= \sum_\beta \langle\beta|\left(\sum_\alpha w_\alpha |\alpha\rangle\langle\alpha|\right)A|\beta\rangle \\
&= \sum_{\alpha,\beta} w_\alpha \langle\beta|\alpha\rangle\langle\alpha|A|\beta\rangle \\
&= \sum_{\alpha,\beta} w_\alpha \langle\alpha|A|\beta\rangle\langle\beta|\alpha\rangle \\
&= \sum_\alpha w_\alpha \langle\alpha|A\left(\sum_\beta |\beta\rangle\langle\beta|\right)|\alpha\rangle \\
&= \sum_\alpha w_\alpha \langle\alpha|A|\alpha\rangle
\end{aligned} \tag{5.132}$$

But this, by definition of the ensemble average, is just

$$\mathrm{Tr}(\rho A) = \langle A\rangle_{\mathrm{av}}\,. \tag{5.133}$$

We can use this to compute the ensemble averages of the Pauli matrices

$$
\begin{aligned}
\langle \sigma_x \rangle_{\mathrm{av}} &= \mathrm{Tr}\left(\frac{1}{8} \begin{bmatrix} 5 & -3 \\ -3 & 3 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) = -\frac{3}{4} \\
\left\langle \sigma_y \right\rangle_{\mathrm{av}} &= \mathrm{Tr}\left(\frac{1}{8} \begin{bmatrix} 5 & -3 \\ -3 & 3 \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \right) = 0 \\
\langle \sigma_z \rangle_{\mathrm{av}} &= \mathrm{Tr}\left(\frac{1}{8} \begin{bmatrix} 5 & -3 \\ -3 & 3 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right) = \frac{1}{4}
\end{aligned}
\tag{5.134}
$$

We can also find without the explicit matrix multiplication from eq. (5.131)

$$
\begin{aligned}
\langle \sigma_x \rangle_{\mathrm{av}} &= \mathrm{Tr}\,\frac{1}{2}\left(\sigma_x + \frac{1}{4}\sigma_z\sigma_x - \frac{3}{4}\sigma_x^2 \right) = -\frac{3}{4} \\
\left\langle \sigma_y \right\rangle_{\mathrm{av}} &= \mathrm{Tr}\,\frac{1}{2}\left(\sigma_y + \frac{1}{4}\sigma_z\sigma_y - \frac{3}{4}\sigma_x\sigma_y \right) = 0 \\
\langle \sigma_z \rangle_{\mathrm{av}} &= \mathrm{Tr}\,\frac{1}{2}\left(\sigma_z + \frac{1}{4}\sigma_z^2 - \frac{3}{4}\sigma_x\sigma_z \right) = \frac{1}{4}.
\end{aligned}
\tag{5.135}
$$

(where to do so we observe that $\mathrm{Tr}\,\sigma_i\sigma_j = 0$ for $i \neq j$ and $\mathrm{Tr}\,\sigma_i = 0$, and $\mathrm{Tr}\,\sigma_i^2 = 2$.)

We see that the traces of the density operator and Pauli matrix products act very much like dot products extracting out the ensemble averages, which end up very much like the magnitudes of the projections in each of the directions.

Exercise 5.8 ([3] pr 5.8)

Show that the quantity $\boldsymbol{\sigma} \cdot \mathbf{p} V(r) \boldsymbol{\sigma} \cdot \mathbf{p}$, when simplified, has a term proportional to $\mathbf{L} \cdot \boldsymbol{\sigma}$.

Answer for Exercise 5.8

Consider the operation

$$
\begin{aligned}
\boldsymbol{\sigma} \cdot \mathbf{p} V(r) \Psi &= -i\hbar\sigma_k \partial_k V(r) \Psi \\
&= -i\hbar\sigma_k (\partial_k V(r)) \Psi + V(r)(\boldsymbol{\sigma} \cdot \mathbf{p}) \Psi
\end{aligned}
\tag{5.136}
$$

With $r = \sqrt{\sum_j x_j^2}$, we have

$$
\partial_k V(r) = \frac{1}{2}\frac{1}{r} 2 x_k \frac{\partial V(r)}{\partial r},
\tag{5.137}
$$

which gives us the commutator

$$\left[\boldsymbol{\sigma} \cdot \mathbf{p}, V(r)\right] = -\frac{i\hbar}{r}\frac{\partial V(r)}{\partial r}(\boldsymbol{\sigma} \cdot \mathbf{x}) \tag{5.138}$$

Insertion into the operator in question we have

$$\boldsymbol{\sigma} \cdot \mathbf{p} V(r) \boldsymbol{\sigma} \cdot \mathbf{p} = -\frac{i\hbar}{r}\frac{\partial V(r)}{\partial r}(\boldsymbol{\sigma} \cdot \mathbf{x})(\boldsymbol{\sigma} \cdot \mathbf{p}) + V(r)(\boldsymbol{\sigma} \cdot \mathbf{p})^2 \tag{5.139}$$

With decomposition of the $(\boldsymbol{\sigma} \cdot \mathbf{x})(\boldsymbol{\sigma} \cdot \mathbf{p})$ into symmetric and antisymmetric components, we should have in the second term our $\boldsymbol{\sigma} \cdot \mathbf{L}$

$$(\boldsymbol{\sigma} \cdot \mathbf{x})(\boldsymbol{\sigma} \cdot \mathbf{p}) = \frac{1}{2}\{\boldsymbol{\sigma} \cdot \mathbf{x}, \boldsymbol{\sigma} \cdot \mathbf{p}\} + \frac{1}{2}\left[\boldsymbol{\sigma} \cdot \mathbf{x}, \boldsymbol{\sigma} \cdot \mathbf{p}\right] \tag{5.140}$$

where we expect $\boldsymbol{\sigma} \cdot \mathbf{L} \propto \left[\boldsymbol{\sigma} \cdot \mathbf{x}, \boldsymbol{\sigma} \cdot \mathbf{p}\right]$. Alternately in components

$$\begin{aligned}
(\boldsymbol{\sigma} \cdot \mathbf{x})(\boldsymbol{\sigma} \cdot \mathbf{p}) &= \sigma_k x_k \sigma_j p_j \\
&= x_k p_k I + \sum_{j \neq k} \sigma_k \sigma_j x_k p_j \\
&= x_k p_k I + i \sum_m \epsilon_{kjm} \sigma_m x_k p_j \\
&= I(\mathbf{x} \cdot \mathbf{p}) + i(\boldsymbol{\sigma} \cdot \mathbf{L})
\end{aligned} \tag{5.141}$$

Exercise 5.9 ps III, p2.

A particle with intrinsic angular momentum or spin $s = 1/2$ is prepared in the spin-up with respect to the z-direction state $|f\rangle = |z+\rangle$. Determine

$$\left(\langle f| \left(S_z - \langle f| S_z |f\rangle \mathbf{1}\right)^2 |f\rangle\right)^{1/2} \tag{5.142}$$

and

$$\left(\langle f| \left(S_x - \langle f| S_x |f\rangle \mathbf{1}\right)^2 |f\rangle\right)^{1/2} \tag{5.143}$$

and explain what these relations say about the system.

Answer for Exercise 5.9

Solution: Uncertainty of S_z with respect to $|z+\rangle$ Noting that $S_z |f\rangle = S_z |z+\rangle = \hbar/2\, |z+\rangle$ we have

$$\langle f| S_z |f\rangle = \frac{\hbar}{2} \tag{5.144}$$

The average outcome for many measurements of the physical quantity associated with the operator S_z when the system has been prepared in the state $|f\rangle = |z+\rangle$ is $\hbar/2$.

$$(S_z - \langle f| S_z |f\rangle \mathbf{1}) |f\rangle = \frac{\hbar}{2} |f\rangle - \frac{\hbar}{2} |f\rangle = 0 \tag{5.145}$$

We could also compute this from the matrix representations, but it is slightly more work.

Operating once more with $S_z - \langle f| S_z |f\rangle \mathbf{1}$ on the zero ket vector still gives us zero, so we have zero in the root for eq. (5.142)

$$\left(\langle f| (S_z - \langle f| S_z |f\rangle \mathbf{1})^2 |f\rangle\right)^{1/2} = 0 \tag{5.146}$$

What does eq. (5.146) say about the state of the system? Given many measurements of the physical quantity associated with the operator $V = (S_z - \langle f| S_z |f\rangle \mathbf{1})^2$, where the initial state of the system is always $|f\rangle = |z+\rangle$, then the average of the measurements of the physical quantity associated with V is zero. We can think of the operator $V^{1/2} = S_z - \langle f| S_z |f\rangle \mathbf{1}$ as a representation of the observable, "how different is the measured result from the average $\langle f| S_z |f\rangle$".

So, given a system prepared in state $|f\rangle = |z+\rangle$, and performance of repeated measurements capable of only examining spin-up, we find that the system is never any different than its initial spin-up state. We have no uncertainty that we will measure any difference from spin-up on average, when the system is prepared in the spin-up state.

Solution: Uncertainty of S_x with respect to $|z+\rangle$ For this second part of the problem, we note that we can write

$$|f\rangle = |z+\rangle = \frac{1}{\sqrt{2}}(|x+\rangle + |x-\rangle). \tag{5.147}$$

So the expectation value of S_x with respect to this state is

$$\begin{aligned}
\langle f| S_x |f\rangle &= \frac{1}{2}(|x+\rangle + |x-\rangle) S_x (|x+\rangle + |x-\rangle) \\
&= \hbar(|x+\rangle + |x-\rangle)(|x+\rangle - |x-\rangle) \\
&= \hbar(1 + 0 + 0 - 1) \\
&= 0
\end{aligned} \tag{5.148}$$

After repeated preparation of the system in state $|f\rangle$, the average measurement of the physical quantity associated with operator S_x is zero. In terms of the eigenstates for that operator $|x+\rangle$ and $|x-\rangle$ we have equal probability of measuring either given this particular initial system state.

For the variance calculation, this reduces our problem to the calculation of $\langle f| S_x^2 |f\rangle$, which is

$$\begin{aligned} \langle f| S_x^2 |f\rangle &= \frac{1}{2}\left(\frac{\hbar}{2}\right)^2 (|x+\rangle + |x-\rangle)((+1)^2 |x+\rangle + (-1)^2 |x-\rangle) \\ &= \left(\frac{\hbar}{2}\right)^2, \end{aligned} \tag{5.149}$$

so for eq. (5.150) we have

$$\left(\langle f| \left(S_x - \langle f| S_x |f\rangle \mathbf{1}\right)^2 |f\rangle\right)^{1/2} = \frac{\hbar}{2} \tag{5.150}$$

The average of the absolute magnitude of the physical quantity associated with operator S_x is found to be $\hbar/2$ when repeated measurements are performed given a system initially prepared in state $|f\rangle = |z+\rangle$. We saw that the average value for the measurement of that physical quantity itself was zero, showing that we have equal probabilities of measuring either $\pm\hbar/2$ for this experiment. A measurement that would show the system was in the x-direction spin-up or spin-down states would find that these states are equi-probable.

6 GAUGE INVARIANCE, ANGULAR MOMENTUM AND SPIN

6.1 INTERACTION WITH ORBITAL ANGULAR MOMENTUM

In §6.5 it is stated that we take

$$\mathbf{A} = \frac{1}{2}(\mathbf{B} \times \mathbf{r}) \tag{6.1}$$

and that this reproduces the gauge condition $\boldsymbol{\nabla} \cdot \mathbf{A} = 0$, and the requirement $\boldsymbol{\nabla} \times \mathbf{A} = \mathbf{B}$.

These seem to imply that $\mathbf{B}$ is constant, which also accounts for the fact that he writes $\boldsymbol{\mu} \cdot \mathbf{L} = \mathbf{L} \cdot \boldsymbol{\mu}$.

Consider the gauge condition first, by expanding the divergence of a cross product

$$\begin{aligned}
\boldsymbol{\nabla} \cdot (\mathbf{F} \times \mathbf{G}) &= \left\langle \boldsymbol{\nabla} - I\frac{\mathbf{FG} - \mathbf{GF}}{2} \right\rangle \\
&= -\frac{1}{2}\langle I\boldsymbol{\nabla}\mathbf{FG} - I\boldsymbol{\nabla}\mathbf{GF}\rangle \\
&= -\frac{1}{2}\left\langle I\mathbf{G}(\overrightarrow{\boldsymbol{\nabla}}\mathbf{F}) - I\mathbf{F}(\overrightarrow{\boldsymbol{\nabla}}\mathbf{G}) + I(\mathbf{G}\overleftarrow{\boldsymbol{\nabla}})\mathbf{F} - I(\mathbf{F}\overleftarrow{\boldsymbol{\nabla}})\mathbf{G} \right\rangle \\
&= -\frac{1}{2}\left\langle I\mathbf{G}(\overrightarrow{\boldsymbol{\nabla}} \wedge \mathbf{F}) - I\mathbf{F}(\overrightarrow{\boldsymbol{\nabla}} \wedge \mathbf{G}) + I(\mathbf{G} \wedge \overleftarrow{\boldsymbol{\nabla}})\mathbf{F} - I(\mathbf{F} \wedge \overleftarrow{\boldsymbol{\nabla}})\mathbf{G} \right\rangle \\
&= \frac{1}{2}\left\langle \mathbf{G}(\overrightarrow{\boldsymbol{\nabla}} \times \mathbf{F}) - \mathbf{F}(\overrightarrow{\boldsymbol{\nabla}} \times \mathbf{G}) + (\mathbf{G} \times \overleftarrow{\boldsymbol{\nabla}})\mathbf{F} - (\mathbf{F} \times \overleftarrow{\boldsymbol{\nabla}})\mathbf{G} \right\rangle \\
&= \frac{1}{2}\left(\mathbf{G} \cdot (\boldsymbol{\nabla} \times \mathbf{F}) - \mathbf{F} \cdot (\boldsymbol{\nabla} \times \mathbf{G}) - \mathbf{F} \cdot (\boldsymbol{\nabla} \times \mathbf{G}) + \mathbf{G} \cdot (\boldsymbol{\nabla} \times \mathbf{F}) \right)
\end{aligned} \tag{6.2}$$

This gives us

$$\boldsymbol{\nabla} \cdot (\mathbf{F} \times \mathbf{G}) = \mathbf{G} \cdot (\boldsymbol{\nabla} \times \mathbf{F}) - \mathbf{F} \cdot (\boldsymbol{\nabla} \times \mathbf{G}) \tag{6.3}$$

With $\mathbf{A} = (\mathbf{B} \times \mathbf{r})/2$ we then have

$$\boldsymbol{\nabla} \cdot \mathbf{A} = \frac{1}{2}\mathbf{r} \cdot (\boldsymbol{\nabla} \times \mathbf{B}) - \frac{1}{2}\mathbf{B} \cdot (\boldsymbol{\nabla} \times \mathbf{r}) = \frac{1}{2}\mathbf{r} \cdot (\boldsymbol{\nabla} \times \mathbf{B}) \tag{6.4}$$

Unless $\boldsymbol{\nabla} \times \mathbf{B}$ is always perpendicular to $\mathbf{r}$ we can only have a zero divergence when $\mathbf{B}$ is constant.

Now, let us look at $\boldsymbol{\nabla} \times \mathbf{A}$. We need another auxiliary identity

$$\begin{aligned}
\boldsymbol{\nabla} \times (\mathbf{F} \times \mathbf{G}) &= -I\boldsymbol{\nabla} \wedge (\mathbf{F} \times \mathbf{G}) \\
&= -\frac{1}{2}\left\langle I\overrightarrow{\boldsymbol{\nabla}}(\mathbf{F} \times \mathbf{G}) - I(\mathbf{F} \times \mathbf{G})\overleftarrow{\boldsymbol{\nabla}}\right\rangle_1 \\
&= \frac{1}{2}\left(-\overrightarrow{\boldsymbol{\nabla}} \cdot (\mathbf{F} \wedge \mathbf{G}) + (\mathbf{F} \wedge \mathbf{G}) \cdot \overleftarrow{\boldsymbol{\nabla}}\right) \\
&= \frac{1}{2}\left(-(\overrightarrow{\boldsymbol{\nabla}} \cdot \mathbf{F})\mathbf{G} + (\overrightarrow{\boldsymbol{\nabla}} \cdot \mathbf{G})\mathbf{F} + \mathbf{F}(\mathbf{G} \cdot \overleftarrow{\boldsymbol{\nabla}}) - \mathbf{G}(\mathbf{F} \cdot \overleftarrow{\boldsymbol{\nabla}})\right) \\
&= \frac{1}{2}\left(-(\boldsymbol{\nabla} \cdot \mathbf{F})\mathbf{G} + (\boldsymbol{\nabla} \cdot \mathbf{G})\mathbf{F} + (\boldsymbol{\nabla} \cdot \mathbf{G})\mathbf{F} - (\boldsymbol{\nabla} \cdot \mathbf{F})\mathbf{G}\right)
\end{aligned} \tag{6.5}$$

Here the gradients are all still acting on both $\mathbf{F}$ and $\mathbf{G}$. Expanding this out by chain rule we have

$$\begin{aligned}
2\boldsymbol{\nabla} \times (\mathbf{F} \times \mathbf{G}) = &- (\mathbf{F} \cdot \boldsymbol{\nabla})\mathbf{G} - \mathbf{G}(\boldsymbol{\nabla} \cdot \mathbf{F}) + \mathbf{F}(\boldsymbol{\nabla} \cdot \mathbf{G}) + (\mathbf{G} \cdot \boldsymbol{\nabla})\mathbf{F} \\
&+ \mathbf{F}(\boldsymbol{\nabla} \cdot \mathbf{G}) + (\mathbf{G} \cdot \boldsymbol{\nabla})\mathbf{F} - (\mathbf{F} \cdot \boldsymbol{\nabla})\mathbf{G} - \mathbf{G}(\boldsymbol{\nabla} \cdot \mathbf{F})
\end{aligned} \tag{6.6}$$

or

$$\boldsymbol{\nabla} \times (\mathbf{F} \times \mathbf{G}) = \mathbf{F}(\boldsymbol{\nabla} \cdot \mathbf{G}) - (\mathbf{F} \cdot \boldsymbol{\nabla})\mathbf{G} + (\mathbf{G} \cdot \boldsymbol{\nabla})\mathbf{F} - \mathbf{G}(\boldsymbol{\nabla} \cdot \mathbf{F}) \tag{6.7}$$

With $\mathbf{F} = \mathbf{B}/2$, and $\mathbf{G} = \mathbf{r}$, we have

$$\boldsymbol{\nabla} \times \mathbf{A} = \frac{1}{2}\mathbf{B}(\boldsymbol{\nabla} \cdot \mathbf{r}) - \frac{1}{2}(\mathbf{B} \cdot \boldsymbol{\nabla})\mathbf{r} + \frac{1}{2}(\mathbf{r} \cdot \boldsymbol{\nabla})\mathbf{B} - \frac{1}{2}\mathbf{r}(\boldsymbol{\nabla} \cdot \mathbf{B}) \tag{6.8}$$

We note that $\boldsymbol{\nabla} \cdot \mathbf{r} = 3$, and

$$\begin{aligned}
(\mathbf{B} \cdot \boldsymbol{\nabla})\mathbf{r} &= B_k \partial_k x_m \mathbf{e}_m \\
&= B_k \delta_{km} \mathbf{e}_m \\
&= \mathbf{B}
\end{aligned} \tag{6.9}$$

If $\mathbf{B}$ is constant, we have

$$\boldsymbol{\nabla} \times \mathbf{A} = \frac{3\mathbf{B}}{2} - \frac{\mathbf{B}}{2} = \mathbf{B}, \tag{6.10}$$

as desired. Now this would all likely be a lot more intuitive if one started with constant $\mathbf{B}$ and derived from that what the vector potential was. That is probably worth also thinking about.

7 STERN-GERLACH

7.1 LECTURE: STERN GERLACH

Short class today since 43 minutes was wasted since the feedback given the Prof was so harsh that he wants to cancel the mid-term because students have said they are not prepared. How ironic that this wastes more time that could be getting us prepared!

7.2 WHY DO THIS (DIRAC NOTATION) MATH?

Because of the Stern-Gerlach Experiment. Explaining the Stern-Gerlach experiment is just not possible with wave functions and the "old style" Schrödinger equation that operates on wave functions

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\Psi(\mathbf{x},t) + V(\mathbf{x})\Psi(\mathbf{x},t) = i\hbar\frac{\partial\Psi(\mathbf{x},t)}{\partial t}. \tag{7.1}$$

Review all of Chapter I so that you understand the idea of a Hermitian operator and its associated eigenvalues and eigenvectors.

Hermitian operation A is associated with a measurable quantity.

Example 7.1: Spin-up

S_z is associated with the measurement of "spin-up" $|z+\rangle$ or "spin-down" $|z-\rangle$ states in silver atoms in the Stern-Gerlach experiment.

Each operator has associated with it a set of eigenvalues, and those eigenvalues are the outcomes of possible measurements.

S_z can be represented as

$$S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{7.2}$$

or

$$S_z = \frac{\hbar}{2} \left(|z+\rangle \langle z+| - |z-\rangle \langle z-| \right) . \tag{7.3}$$

Find the eigenvalues of S_z in order to establish the possible outcomes of measurements of the z-component of the intrinsic angular momentum.

This is the point of the course. It is to find the possible outcomes. You have to appreciate that the measurement in the Stern-Gerlach experiment are trying to find the possible outcomes of the z-component measurement. The eigenvalues of this operator give us those possible outcomes.

Example 7.2: What if you put a brick in the experiment?

In the Stern-Gerlach experiment the "spin down" along the z-direction are atoms are blocked. Diagram: silver going through a hole, with a brick between the detector and the spin-down location on the screen:

FIXME: scan it. Oct 26, Fig 1.

What is the probability of measuring an outcome of $+\hbar/2$ along the x-direction?

Recall from Chapter I

$$|\phi\rangle = \sum_n c_n |a_n\rangle \tag{7.4}$$

We can express an arbitrary state $|\phi\rangle$ in terms of basis vectors (could be eigenstates of an operator A, but could be for example the eigenstates of the operator B, say.) Note that here in physics we will only work with orthonormal basis sets. The generality. To calculate the $c_n' s$ we take inner products

$$\langle a_m|\phi\rangle = \sum_n c_n \langle a_m|a_n\rangle = \sum_n c_n \delta_{mn} = c_m \tag{7.5}$$

The probability for measured outcome a_m is

$$|c_m|^2 = |\langle a_m|\phi\rangle|^2 \tag{7.6}$$

In the end we have to appreciate that part of QM is figuring out what the possible outcomes are and the probabilities of those outcomes.

Appreciate that $|\phi\rangle = |z+\rangle$ in this case. This is a superposition of eigenstates of S_z. Why is it a superposition? Because one of the coefficients is 1, and the other is 0.

$$|\phi\rangle = c_1\,|z+\rangle + c_2\,|z-\rangle = c_1\,|z+\rangle + 0\,|z-\rangle \tag{7.7}$$

So

$$c_1 = 1 \tag{7.8}$$

recall that

$$\begin{aligned} S_z &= \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ |z+\rangle &\leftrightarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ |z+\rangle &\leftrightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{aligned} \tag{7.9}$$

Also recall that

$$\begin{aligned} S_x &= \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ |x+\rangle &\leftrightarrow \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} \\ |x-\rangle &\leftrightarrow \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} \end{aligned} \tag{7.10}$$

(with eigenvalues $\pm\hbar/2$).
These eigenvectors are expressed in terms of $|z+\rangle$ and $|z-\rangle$, so that

$$\begin{aligned} |x+\rangle &= \frac{1}{\sqrt{2}}\left(|z+\rangle + |z-\rangle\right) \\ |x-\rangle &= \frac{1}{\sqrt{2}}\left(|z+\rangle - |z-\rangle\right). \end{aligned} \tag{7.11}$$

Outcome $+\hbar/2$ along the x-direction has an associated state $|x+\rangle$. That probability is

$$\begin{aligned}
|\langle x+|\phi\rangle|^2 &= \left|\frac{1}{\sqrt{2}}\left(\langle z+| + \langle z-|\right)|\phi\rangle\right|^2 \\
&= \frac{1}{2}|\langle z+|\phi\rangle + \langle z-|\phi\rangle|^2 \\
&= \frac{1}{2}|\langle z+|z+\rangle + \langle z-|z+\rangle|^2 \\
&= \frac{1}{2}|1+0|^2 \\
&= \frac{1}{2}
\end{aligned} \tag{7.12}$$

Example 7.3: Variation. With a third splitter (SGZ)

The probability for outcome $+\hbar/2$ along z after the second SGZ magnets is

$$\begin{aligned}
\left|\langle z+|\phi'\rangle\right|^2 &= |\langle z+|x+\rangle|^2 \\
&= \left|\langle z+|\frac{1}{\sqrt{2}}\left(|z+\rangle + |z-\rangle\right)\right|^2 \\
&= \frac{1}{2}|\langle z+|z+\rangle + \langle z+|z-\rangle|^2 \\
&= \frac{1}{2}
\end{aligned} \tag{7.13}$$

My question: what is the point of the brick when the second splitter is already only being fed by the “spin up” stream. Answer: just to ensure that the states are prepared in the expected way. If the beams are two close together, without the brick perhaps we end up with some spin up in the upper stream. Note that the beam separation here is on the order of centimeters. ie: imagine that it is hard to redirect just one of the beams to the next stage splitter without blocking one of the beams or else the next splitter inevitably gets fed with some of both. Might be nice to see a real picture of the Stern-Gerlach apparatus complete with scale.

Why silver? Silver has 47 electrons, all of which but one are in spin pairs. Only the “outermost” electron is free to have independent spin.

Aside: Note that we have the term "Collapse" to describe the now-known state after measurement. There is some debate about the applicability of this term, and the interpretation that this imposes. Will not be discussed here.

7.3 ON SECTION 5.11, THE COMPLETE WAVEFUNCTION

Aside: section 5.12 (Pauli exclusion principle and Fermi energy) excluded.

The complete wavefunction

$$\begin{aligned} |\phi\rangle &= \text{the complete state of an atomic in the Stern-Gerlach experiment} \\ &= |u\rangle \otimes |\chi\rangle \end{aligned} \tag{7.14}$$

We also write

$$|u\rangle \otimes |\chi\rangle = |u\rangle \, |\chi\rangle \tag{7.15}$$

where $|u\rangle$ is associate with translation, and $|\chi\rangle$ is associated with spin. This is a product state where the $\otimes$ is a symbol for states in two or more different spaces.

8 LECTURE: MAKING SENSE OF QUANTUM MECHANICS

8.0.1 *Discussion*

Desai: "Quantum Theory is a linear theory ..."

We can discuss SHM without using sines and cosines or complex exponentials, say, only using polynomials, but it would be HARD to do so, and much more work. We want the framework of Hilbert space, linear operators and all the rest to make our life easier.

Dirac: "All the same the Mathematics is only a tool and one should learn to hold the physical ideas on one's mind without reference to the mathematical form"

You have to be able to understand the concepts and apply the concepts as well as the mathematics.

Deyirmenjian: "Think before you compute."

Joke: With his name included it is the 3Ds. There is a lot of information included in the question, so read it carefully.

Q: The equation $A\,|a_n\rangle = a_n\,|a_n\rangle$ for operator A, eigenvalue a_n, $n = 1, 2$ and eigenvector $|a_n\rangle$ that is identified by the eigenvalue a_n says that

- (a) measuring the physical quantity associated with A gives result a_n
- (b) A acting on the state $|a_n\rangle$ gives outcome a_n
- (c) the possible outcomes of measuring the physical quantity associated with A are the eigenvalues a_n
- (d) Quantum mechanics is hard.

$|a_n\rangle$ is a vector in a vector space or Hilbert space identified by some quantum number $a_n, n \in 1, 2, \cdots$.

The a_n values could be expressions. Example, Angular momentum is describe by states $|lm\rangle\,, l = 0, 1, 2, \cdots$ and $m = 0, \pm 1, \pm 2$

Recall that the problem is

$$\begin{aligned}\mathbf{L}^2 \left|lm\right\rangle &= l(l+1)\,\hbar^2 \left|lm\right\rangle \\ L_z \left|lm\right\rangle &= m\,\hbar \left|lm\right\rangle\end{aligned} \tag{8.1}$$

We have respectively eigenvalues $l(l+1)\,\hbar^2$, and $m\,\hbar$.

A: Answer is (c). a_n is not a measurement itself. These represent possibilities. Contrast this to classical mechanics where time evolution is given without probabilities

$$\begin{aligned}\mathbf{F}_{\text{net}} &= m\mathbf{a} \\ \mathbf{x}(0), \mathbf{x}'(0) &\implies \mathbf{x}(t), \mathbf{x}'(t)\end{aligned} \tag{8.2}$$

The eigenvalues are the possible outcomes, but we only know statistically that these are the possibilities.

(a),(b) are incorrect because we do not know what the initial state is, nor what the final outcome is. We also can not say "gives result a_n". That statement is too strong!

Q: We would not say that A acts on pure state $\left|a_n\right\rangle$, instead. If the state of the system is $\left|\psi\right\rangle = \left|a_5\right\rangle$, the probability of measuring outcome a_5 is

- (a) a_5
- (b) a_5^2
- (c) $\left\langle a_5 | \psi \right\rangle = \left\langle a_5 | a_5 \right\rangle = 1$.
- (d) $\left|\left\langle a_5 | \psi \right\rangle\right|^2 = \left|\left\langle a_5 | a_5 \right\rangle\right|^2 = |1|^2 = 1$.

A: (d) The eigenformula equation does not say anything about any specific outcome. We want to talk about probability amplitudes. When the system is prepared in a particular pure eigenstate, then we have a guarantee that the probability of measuring that state is unity. We would not say (c) because the probability amplitudes are the absolute square of the complex number $\left\langle a_n | a_n \right\rangle$.

The probability of outcome a_n, given initial state $\left|\Psi\right\rangle$ is $\left|\left\langle a_n | \Psi \right\rangle\right|^2$.

Wave function collapse: When you make a measurement of the physical quantity associated with A, then the state of the system will be the value $\left|a_5\right\rangle$. The state is not the number (eigenvalue) a_5.

Example: SGZ. With a "spin-up" measurement in the z-direction, the state of the system is $\left|z+\right\rangle$. The state before the measurement, by the magnet, was $\left|\Psi\right\rangle$. After the measurement, the state describing the system is $|\phi\rangle = |z+\rangle$. The measurement outcome is $+\frac{\hbar}{2}$ for the spin angular momentum along the z-direction.

FIXME: SGZ picture here.

There is an interaction between the magnet and the silver atoms coming out of the oven. Before that interaction we have a state described by $|\Psi\rangle$. After the measurement, we have a new state $|\phi\rangle$. We call this the collapse of the wave function. In a future course (QM interpretations) the language used and interpretations associated with this language can be discussed.

Q: Express Hermitian operator A in terms of its eigenvectors.

Q: The above question is vague because

- (a) The eigenvectors may form a discrete set.
- (b) The eigenvectors may form a continuous set.
- (c) The eigenvectors may not form a complete set.
- (d) The eigenvectors are not given.

A: None of the above. A Hermitian operator is guaranteed to have a complete set of eigenvectors. The operator may also be both discrete and continuous (example: the complete spin wave function).

discrete:

$$\begin{aligned}
A &= A\mathbf{1} \\
&= A\left(\sum_n |a_n\rangle \langle a_n|\right) \\
&= \sum_n (A\,|a_n\rangle)\,\langle a_n| \\
&= \sum_n (a_n\,|a_n\rangle)\,\langle a_n| \\
&= \sum_n a_n\,|a_n\rangle \langle a_n|
\end{aligned} \tag{8.3}$$

continuous:

$$\begin{aligned} A &= A\mathbf{1} \\ &= A\left(\int d\alpha\, |\alpha\rangle\langle\alpha|\right) \\ &= \int d\alpha (A\,|\alpha\rangle)\langle\alpha| \\ &= \int d\alpha (\alpha\,|\alpha\rangle)\langle\alpha| \\ &= \int d\alpha\alpha\,|\alpha\rangle\langle\alpha| \end{aligned} \tag{8.4}$$

An example is the position eigenstate $|x\rangle$, eigenstate of the Hermitian operator X. α is a label indicating the summation.

general case with both discrete and continuous:

$$\begin{aligned} A &= A\mathbf{1} \\ &= A\left(\sum_n |a_n\rangle\langle a_n| + \int d\alpha\, |\alpha\rangle\langle\alpha|\right) \\ &= \sum_n (A\,|a_n\rangle)\langle a_n| + \int d\alpha\,(A\,|\alpha\rangle)\langle\alpha| \\ &= \sum_n (a_n\,|a_n\rangle)\langle a_n| + \int d\alpha\,(\alpha\,|\alpha\rangle)\langle\alpha| \\ &= \sum_n a_n\,|a_n\rangle\langle a_n| + \int d\alpha\alpha\,|\alpha\rangle\langle\alpha| \end{aligned} \tag{8.5}$$

Problem Solving

- MODEL – Quantum, linear vector space
- VISUALIZE – Operators can have discrete, continuous or both discrete and continuous eigenvectors.
- SOLVE – Use the identity operator.
- CHECK – Does the above expression give $A\,|a_n\rangle = a_n\,|a_n\rangle$.

Check

$$\begin{aligned} A\left|a_m\right\rangle &= \sum_n a_n \left|a_n\right\rangle \left\langle a_n | a_m\right\rangle + \int d\alpha\alpha \left|\alpha\right\rangle \left\langle \alpha | a_n\right\rangle \\ &= \sum_n a_n \left|a_n\right\rangle \delta_{nm} \\ &= a_m \left|a_m\right\rangle \end{aligned} \tag{8.6}$$

What remains to be shown, used above, is that the continuous and discrete eigenvectors are orthonormal. He has an example vector space, not yet discussed.

Q: what is $\langle \Psi_1 | A | \Psi_1 \rangle$, where A is a Hermitian operator, and $|\Psi_1\rangle$ is a general state.

A: $\langle \Psi_1 | A | \Psi_1 \rangle$ = average outcome for <u>many measurements</u> of the physical quantity associated with A such that the system is prepared in state $|\Psi_1\rangle$ prior to each measurement.

Q: What if the preparation is $|\Psi_2\rangle$. This is not necessarily an eigenstate of A, it is some linear combination of eigenstates. It is a general state.

A: $\langle \Psi_2 | A | \Psi_2 \rangle$ = average of the physical quantity associated with A, but the preparation is $|\Psi_2\rangle$, not $|\Psi_1\rangle$.

Q: What if our initial state is a little bit of $|\Psi_1\rangle$, and a little bit of $|\Psi_2\rangle$, and a little bit of $|\Psi_N\rangle$. ie: how to describe what comes out of the oven in the Stern-Gerlach experiment. That spin is a statistical mixture. We could understand this as only a statistical mix. This is a physical relevant problem.

A: To describe that statistical situation we have the following.

$$\langle A \rangle_{\text{average}} = \sum_j w_j \left\langle \Psi_j \middle| A \middle| \Psi_j \right\rangle \tag{8.7}$$

We sum up all the expectation values modified by statistical weighting factors. These w_j's are statistical weighting factors for a preparation associated with $\left|\Psi_j\right\rangle$, real numbers (that sum to unity). Note that these states $\left|\Psi_j\right\rangle$ are not necessarily orthonormal.

With insertion of the identity operator we have

$$\begin{aligned}
\langle A\rangle_{\text{average}} &= \sum_j w_j \left\langle \Psi_j \right| \mathbf{1} A \left| \Psi_j \right\rangle \\
&= \sum_j w_j \left\langle \Psi_j \right| \left(\sum_n |a_n\rangle \langle a_n| \right) A \left| \Psi_j \right\rangle \\
&= \sum_j \sum_n w_j \left\langle \Psi_j | a_n \right\rangle \langle a_n| A \left| \Psi_j \right\rangle \\
&= \sum_j \sum_n w_j \langle a_n| A \left| \Psi_j \right\rangle \left\langle \Psi_j | a_n \right\rangle \\
&= \sum_n \langle a_n| A \left(\sum_j w_j \left| \Psi_j \right\rangle \left\langle \Psi_j \right| \right) |a_n\rangle
\end{aligned} \tag{8.8}$$

This inner bit is called the density operator ρ

$$\rho \equiv \sum_j w_j \left| \Psi_j \right\rangle \left\langle \Psi_j \right| \tag{8.9}$$

Returning to the average we have

$$\langle A\rangle_{\text{average}} = \sum_n \langle a_n| A\rho \,|a_n\rangle \equiv \operatorname{Tr}(A\rho) \tag{8.10}$$

The trace of an operator A is

$$\operatorname{Tr}(A) = \sum_j \left\langle a_j \right| A \left| a_j \right\rangle = \sum_j A_{jj} \tag{8.11}$$

8.1 PROJECTION OPERATOR

Returning to the last lecture. From chapter 1, we have

$$P_n = |a_n\rangle \langle a_n| \tag{8.12}$$

is called the projection operator. This is physically relevant. This takes a general state and gives you the component of that state associated with that eigenvector. Observe

$$P_n |\phi\rangle = |a_n\rangle \langle a_n|\phi\rangle = \overbrace{\boxed{\langle a_n|\phi\rangle}}^{\text{coefficient}} |a_n\rangle \tag{8.13}$$

Example 8.1: Projection operator for the $|z+\rangle$ state

$$P_{z+} = |z+\rangle\langle z+| \tag{8.14}$$

We see that the density operator

$$\rho \equiv \sum_j w_j \left|\Psi_j\right\rangle\left\langle\Psi_j\right|, \tag{8.15}$$

can be written in terms of the Projection operators

$$\left|\Psi_j\right\rangle\left\langle\Psi_j\right| = \text{Projection operator for state} \left|\Psi_j\right\rangle \tag{8.16}$$

The projection operator is like a dot product, determining the quantity of a state that lines in the direction of another state.

Q: What is the projection operator for spin-up along the z-direction.

A:

$$P_{z+} = |z+\rangle\langle z+| \tag{8.17}$$

Or in matrix form with

$$\begin{aligned}\langle z+| &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ \langle z-| &= \begin{bmatrix} 0 \\ 1 \end{bmatrix},\end{aligned} \tag{8.18}$$

so

$$P_{z+} = |z+\rangle\langle z+| = \begin{bmatrix} 1 \\ 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \tag{8.19}$$

Example 8.2: A harder problem.

What is P_χ, where

$$|\chi\rangle = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \tag{8.20}$$

Note: We want normalized states, with $\langle\chi|\chi\rangle = |c_1|^2 + |c_2|^2 = 1$.

A:

$$P_\chi = |\chi\rangle\langle\chi| = \begin{bmatrix} c_1^* \\ c_2^* \end{bmatrix} \begin{bmatrix} c_1 & c_2 \end{bmatrix} = \begin{bmatrix} c_1^* c_1 & c_1^* c_2 \\ c_2^* c_1 & c_2^* c_2 \end{bmatrix} \tag{8.21}$$

Observe that this has the proper form of a projection operator is that the square is itself

$$\begin{aligned} (|\chi\rangle\langle\chi|)(|\chi\rangle\langle\chi|) &= |\chi\rangle(\langle\chi|\chi\rangle)\langle\chi| \\ &= |\chi\rangle\langle\chi| \end{aligned} \tag{8.22}$$

Example 8.3: Projection

Show that $P_\chi = a_0 \mathbf{1} + \mathbf{a}\cdot\boldsymbol{\sigma}$, where $\mathbf{a} = (a_x, a_y, a_z)$ and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$.

A: See Section 5.9. Note the following about computing $(\boldsymbol{\sigma}\cdot\mathbf{a})^2$.

$$\begin{aligned} (\boldsymbol{\sigma}\cdot\mathbf{a})^2 &= (a_x\sigma_x + a_y\sigma_y + a_z\sigma_z)(a_x\sigma_x + a_y\sigma_y + a_z\sigma_z) \\ &= a_x a_x \sigma_x\sigma_x + a_x a_y \sigma_x\sigma_y + a_x a_z \sigma_x\sigma_z \\ &\quad + a_y a_x \sigma_y\sigma_x + a_y a_y \sigma_y\sigma_y + a_y a_z \sigma_y\sigma_z \\ &\quad + a_z a_x \sigma_z\sigma_x + a_z a_y \sigma_z\sigma_y + a_z a_z \sigma_z\sigma_z \\ &= (a_x^2 + a_y^2 + a_z^2)I + a_x a_y(\sigma_x\sigma_y + \sigma_y\sigma_x) + a_y a_z(\sigma_y\sigma_z + \sigma_z\sigma_y) + a_z a_x(\sigma_z\sigma_x + \sigma_x\sigma_z) \\ &= |\mathbf{x}|^2 I \end{aligned} \tag{8.23}$$

So we have

$$(\boldsymbol{\sigma} \cdot \mathbf{a})^2 = (\mathbf{a} \cdot \mathbf{a})\mathbf{1} \equiv \mathbf{a}^2 \tag{8.24}$$

Where the matrix representations

$$\begin{aligned}\sigma_x &\leftrightarrow \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \sigma_y &\leftrightarrow \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \\ \sigma_z &\leftrightarrow \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},\end{aligned} \tag{8.25}$$

would be used to show that

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I \tag{8.26}$$

and

$$\begin{aligned}\sigma_x\sigma_y &= -\sigma_y\sigma_x \\ \sigma_y\sigma_z &= -\sigma_z\sigma_y \\ \sigma_z\sigma_x &= -\sigma_x\sigma_z\end{aligned} \tag{8.27}$$

9 BOUND STATE PROBLEMS

9.1 HYDROGEN LIKE ATOM, AND LAGUERRE POLYNOMIALS

For the hydrogen atom, after some variable substitutions the radial part of the Schrödinger equation takes the form

$$\frac{d^2 R_l}{d\rho^2} + \frac{2}{\rho}\frac{dR_l}{d\rho} + \left(\frac{\lambda}{\rho} - \frac{l(l+1)}{\rho^2} - \frac{1}{4}\right) R_l = 0 \tag{9.1}$$

In [3] §8.8 it is argued that the functions R_l are of the form

$$R_l = \rho^s L(\rho) e^{-\rho/2} \tag{9.2}$$

where L is a polynomial in ρ, specifically Laguerre polynomials. Let us look at some of those details a bit more closely.

The first part of the argument comes from considering the $\rho \to \infty$ case, where Schrödinger's equation is approximately

$$\frac{d^2 R_l}{d\rho^2} - \frac{1}{4} R_l \approx 0. \tag{9.3}$$

This large ρ approximation has solutions $e^{\pm\rho/2}$, and we take the negative sign case as physically meaningful in order for the wave function to be normalizable.

Next it is argued that polynomial multiples of this will also be approximate solutions. Utilizing monomial multiple of the decreasing exponential as a trial solution, let us compute how this fits into the radial Schrödinger's equation eq. (9.1) above. Write

$$R_l = \rho^s e^{-\rho/2} \tag{9.4}$$

The derivatives are

$$\begin{aligned} R_l' &= \rho^{s-1}\left(s - \frac{\rho}{2}\right) e^{-\rho/2} \\ R_l'' &= \rho^{s-2}\left(s(s-1) - s\rho + \frac{1}{4}\rho^2\right) e^{-\rho/2} \end{aligned} \tag{9.5}$$

and substitution yields

$$\rho^{s-2}e^{-\rho/2}\left((s-\rho)(s+1)+\lambda\rho-l(l+1)\right) \tag{9.6}$$

There are two things that this can show. The first is that for $\rho \to \infty$ this produces a polynomial with degree $s-2$ and $s-1$ terms multiplied by the exponential, and we have approximately

$$\rho^{s-1}e^{-\rho/2}(\lambda-s-1) \tag{9.7}$$

The $s-1$ terms will dominate the polynomial, but the exponential dominate all, approaching zero for $\rho \to \infty$, just as the non-polynomial multiplied $e^{-\rho/2}$ approximate solution will. This confirms that in the limit this polynomial multiplied exponential still has the desired behavior in the large ρ limit. Also observe that in the limit of small ρ we have approximately

$$\rho^{s-2}e^{-\rho/2}\left(s(s+1)-l(l+1)\right) \tag{9.8}$$

Since $\rho^{s-2} \to \infty$ as $\rho \to 0$, we require either a different trial solution, or $s = l$ to have a normalizable wavefunction.

Before settling on $s = l$ let us compute the derivatives for a more general trial function, of the form eq. (9.2), and substitute those. After a bit of computation we find

$$R_l' = \rho^{s-1}e^{-\rho/2}\left(\left(s-\frac{\rho}{2}\right)L+\rho L'\right) \tag{9.9}$$

$$R_l'' = \rho^{s-2}e^{-\rho/2}\left(\left(s(s-1)-s\rho+\frac{\rho^2}{4}\right)L+\left(2s\rho-\rho^2\right)L'+\rho^2L''\right) \tag{9.10}$$

Putting these together and substitution back into eq. (9.1) yields

$$0 = \rho^{s-2}e^{-\rho/2}\left(L\left((s-\rho)(s+1)+\rho\lambda-l(l+1)\right)+\rho L'\left(2(s+1)-\rho\right)+\rho^2L''\right) \tag{9.11}$$

In the $\rho \to 0$ limit where the ρ^{s-2} terms dominate eq. (9.12) becomes

$$0 \approx \rho^{s-2}L\left(s(s+1)-l(l+1)\right) \tag{9.12}$$

Again, this provides the $s = l$ or $s = -(l+1)$ possibilities from the text, and we discard $s = -(l+1)$ due to non-normalizability. A side question. How does one solve integer equations like this?

What remains? With $s = l$ killing off the ρ^{s-2} terms, what is our differential equation for L?

$$0 = \rho L'' + L' \left(2(l+1) - \rho\right) + L \left(\lambda - (l+1)\right) \tag{9.13}$$

Comparing this to [14] we have something pretty close to the stated differential equation for the Laguerre polynomial. Ours is of the form

$$0 = \rho L'' + L' \left(m + 1 - \rho\right) + Ln, \tag{9.14}$$

where the differential equation in the wikipedia article has $m = 0$. No change of variables involving a scalar multiplicative factor for ρ appears to be able to get it into that form, and I am guessing this is the differential equation for the associated Laguerre polynomial (something not stated in the wikipedia article).

Let us derive the recurrence relations for the coefficients, and work out the first few such polynomials to compare. Plugging in a polynomial of the form

$$L = \sum_{k=0}^{r} a_k \rho^k, \tag{9.15}$$

where a_r is assumed to be non-zero. We also assume that this polynomial is not an infinite series (ruling out the infinite series with convergence arguments is covered nicely in the text).

we have for eq. (9.14)

$$\begin{aligned}
0 &= \sum_{k=0}^{r} a_k \left(k(k-1)\rho^{k-1} + k(m+1)\rho^{k-1} - k\rho^k + n\rho^k\right) \\
&= \sum_{k'=1}^{r} \rho^{k'-1} a_{k'} k' \left(k' - 1 + (m+1)\right) + \sum_{k=0}^{r} \rho^k a_k \left(-k + n\right) \\
&= \sum_{k=0}^{r-1} \rho^k a_{k+1}(k+1)\left(k + (m+1)\right) + \sum_{k=0}^{r} \rho^k a_k \left(-k + n\right) \\
&= \sum_{k=0}^{r-1} \rho^k \left(a_{k+1}(k+1)(k+m+1) + a_k(n-k)\right) + a_r(n-r)\rho^r
\end{aligned} \tag{9.16}$$

Observe first that since we have assumed $a_r \neq 0$, we must have $r = n$. Requiring termwise equality with zero gives us the recurrence relation between the coefficients, for $k \in [0, n-1]$

$$a_{k+1} = a_k \frac{k-n}{(k+1)(k+m+1)}. \tag{9.17}$$

Repeated application shows the pattern for these coefficients, and with $a_0 = 1$ we have

$$\begin{aligned} a_1 &= -\frac{n-0}{(1)(m+1)} \\ a_2 &= \frac{(n-1)(n-0)}{(2)(1)(m+2)(m+1)} \\ a_3 &= -\frac{(n-2)(n-1)(n-0)}{(3)(2)(1)(m+3)(m+2)(m+1)}, \end{aligned} \tag{9.18}$$

With

$$\begin{aligned} a_k &= \frac{(-1)^k (n-(k-1)) \cdots (n-1)(n-0)}{k!\,(m+k)\cdots(m+2)(m+1)} \\ &= \frac{(-1)^k n!\,m!}{k!\,(m+k)!\,(n-(k-1)-1)!}, \end{aligned} \tag{9.19}$$

Or

$$a_k = \frac{(-1)^k n!\,m!}{k!\,(m+k)!\,(n-k)!}. \tag{9.20}$$

Forming the complete series, we can get at the form of the associated Laguerre polynomials in the wikipedia article without too much trouble

$$\begin{aligned} L_n^m(\rho) &\propto 1 + \sum_{k=1}^{n} \frac{(-1)^k}{k!} \frac{n!\,m!}{(n-k)!\,(m+k)!}\rho^k \\ &\propto \frac{(n+m)!}{n!\,m!} + \sum_{k=1}^{n} \frac{(-1)^k}{k!} \frac{(n+m)!}{(n-k)!\,(m+k)!}\rho^k. \end{aligned} \tag{9.21}$$

Dropping the proportionality, this simplifies to just

$$L_n^m(\rho) = \sum_{k=0}^{n} \frac{(-1)^k}{k!} \binom{n+m}{m+k} \rho^k \tag{9.22}$$

This is not necessarily the form of the polynomials used in the text. To see if that is the case, we need to check the normalization.

According to the wikipedia article we have for the associated Laguerre polynomials as defined above

$$\int_0^\infty \rho^m e^{-\rho} L_n^m(\rho) L_{n'}^m(\rho) d\rho = \frac{(n+m)!}{n!}\delta_{n,n'} \tag{9.23}$$

whereas in the text we have

$$\int_0^\infty \rho^{2l+2} e^{-\rho} \left(L_{n+l}^{2l+1}(\rho) \right)^2 d\rho = \frac{2n((n+l)!\,)^3}{(n-l-1)!}. \tag{9.24}$$

It seems clear that two different notations are being used. In this physical context of wave functions we want the normalization defined by

$$1 = \int_0^\infty \rho^2 R_l^2(\rho) d\rho = \int_0^\infty \rho^{2l+2} e^{-\rho} L^2(\rho) d\rho \tag{9.25}$$

Using the wikipedia notation, with

$$L(\rho) = A L_n^{2l+1}, \tag{9.26}$$

we want

$$\begin{aligned} 1 &= \int \rho^{2l+2} e^{-\rho} L^2(\rho) d\rho \\ &= A^2 \sum_{a,b=0}^{n} \frac{(-1)^{a+b}}{a!\,b!} \binom{n+2l+1}{2l+1+a} \binom{n+2l+1}{2l+1+b} \int_0^\infty d\rho \rho^{2l+2+a+b} e^{-\rho} \end{aligned} \tag{9.27}$$

Since $\int_0^\infty d\rho \rho^a e^{-\rho} = \Gamma(a+1) = a!$ we have

$$1 = A^2 \sum_{a,b=0}^{n} \frac{(-1)^{a+b}}{a!\,b!} \binom{n+m}{m+a} \binom{n+m}{m+b} (m+1+a+b)! \tag{9.28}$$

It looks like there is probably some way to simplify this, and if so we would be able to map the notation used (without definition) used in the text, to the notation used in the wikipedia article. If we do not care about that, nor the specifics of the normalization constant then there is not too much more to say.

This is an ugly kind of place to leave things, but that is enough for today. It is too bad that the text is not just more explicit, and it is probably best to refer elsewhere for any more detail. With no specifics about the functions themselves in any form, one has to do that anyways.

9.2 EXAMPLES

Motivation. Motivation for today's physics is Solar Cell technology and quantum dots.

Example 9.1

What are the eigenvalues and eigenvectors for an electron trapped in a 1D potential well?

MODEL Quantum state $|\Psi\rangle$ describes the particle. What $V(X)$ should we choose? Try a quantum well with infinite barriers first.

These spherical quantum dots are like quantum wells. When you trap electrons in this scale you will get energy quantization.

VISUALIZE Draw a picture for $V(X)$ with infinite spikes at $\pm a$. (ie: figure 8.1 in the text).

SOLVE First task is to solve the time independent Schrödinger equation.

$$H|\Psi\rangle = E|\Psi\rangle \tag{9.29}$$

derivable from

$$H|\Psi\rangle = i\hbar\frac{\partial}{\partial t}|\Psi\rangle \tag{9.30}$$

In the position representation, we project $\langle x|$ onto $H|\Psi\rangle$ and solve for $\langle x|\Psi\rangle = \Psi(x)$. For the problems in Chapter 8,

$$H = \frac{\mathbf{P}^2}{2m} + V(X, Y, Z), \tag{9.31}$$

where

$$\begin{aligned} P &= \text{momentum operator} \\ X &= \text{position operator} \\ m &= \text{electron mass} \end{aligned} \tag{9.32}$$

We should be careful to be strict about the notation, and not interchange the operators and their specific representations (ie: not interchanging "little-x" and "big-x") as we see in the text in this chapter.

Here the potential energy operator $V(X, Y, Z)$ is time independent.

If $i\hbar\frac{d|\Psi\rangle}{dt} = H|\Psi\rangle$ and H is time independent then $|\Psi\rangle = |u\rangle e^{-iEt/\hbar}$ implies

$$i\hbar\frac{-iE}{\hbar}|u\rangle e^{-iEt/\hbar} = H|u\rangle e^{-iEt/\hbar} \tag{9.33}$$

or

$$E\,|u\rangle = H\,|u\rangle \tag{9.34}$$

Here E is the energy eigenvalue, and $|u\rangle$ is the energy eigenstate. Our differential equation now becomes

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + V(x)u(x) = Eu(x) \tag{9.35}$$

where $V(x) = 0$ for $|x| < a$. We will not find anything like this for real, but this is our first approximation to the quantum dot.

Our differential equation in the well is now

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} = Eu(x) \tag{9.36}$$

or with $\alpha = \sqrt{2mE/\hbar^2}$

$$\frac{d^2u(x)}{dx^2}u(x) = -\frac{2mE}{\hbar^2}u(x) = -\alpha^2 u(x) \tag{9.37}$$

Our solution for $|x| < a$ is then

$$u(x) = A\cos\alpha x + B\sin\alpha x \tag{9.38}$$

and for $|x| > a$ we have $u(x) = 0$ since $V(x) = \infty$.

Setting $u(a) = u(-a) = 0$ we have

$$\begin{aligned} A\cos\alpha a + B\sin\alpha a &= 0\\ A\cos\alpha a - B\sin\alpha a &= 0 \end{aligned} \tag{9.39}$$

Type I $B = 0$, $A\cos\alpha a = 0$. For $A \neq 0$ we must have

$$\cos\alpha a = 0 \tag{9.40}$$

or $\alpha a = n\frac{\pi}{2}$, where $n = 1, 3, 5, ...$, so our solution is

$$u(x) = A\cos\left(\frac{n\pi}{2a}x\right) \tag{9.41}$$

Type II $A = 0$, $B\sin\alpha a = 0$. For $B \neq 0$ we must have

$$\sin\alpha a = 0 \tag{9.42}$$

or $\alpha a = n\frac{\pi}{2}$, where $n = 1, 2, 4, ...$, so our solution is

$$u(x) = B\sin\left(\frac{n\pi}{2a}x\right) \tag{9.43}$$

Via determinant We could also write

$$\begin{bmatrix}\cos\alpha a & \sin\alpha a \\ \cos\alpha a & -\sin\alpha a\end{bmatrix}\begin{bmatrix}A \\ B\end{bmatrix} = 0 \tag{9.44}$$

and then must have zero determinant, or

$$-2\sin\alpha a\cos\alpha a = -\sin 2\alpha a \tag{9.45}$$

so we must have

$$2\alpha a = n\pi \tag{9.46}$$

or

$$\alpha = \frac{n\pi}{2a} \tag{9.47}$$

regardless of A and B. We can then determine the solutions eq. (9.41), and eq. (9.43) simply by noting that this value for α kills off either the sine or cosine terms of eq. (9.38) depending on whether n is even or odd.

CHECK

$$
\begin{aligned}
u_n(x) &= A\cos\left(\frac{n\pi}{2a}x\right)\\
u_n(x) &= B\sin\left(\frac{n\pi}{2a}x\right)
\end{aligned}
\tag{9.48}
$$

satisfy the time independent Schrödinger equation, and the corresponding eigenvalues from from

$$
\alpha = \sqrt{\frac{2mE}{\hbar^2}}, \tag{9.49}
$$

or

$$
E = \frac{\hbar^2\alpha^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{2a}\right)^2 \tag{9.50}
$$

for $n = 1, 2, 3, \cdots$.

On the derivative of u at the boundaries Integrating

$$
-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}u(x) + V(x)u(x) = Eu(x), \tag{9.51}
$$

over $[a-\epsilon, a+\epsilon]$ we have

$$
\begin{aligned}
&-\frac{\hbar^2}{2m}\int_{a-\epsilon}^{a-\epsilon}\frac{d^2u(x)}{dx^2}dx + \int_{a-\epsilon}^{a-\epsilon}V(x)u(x)dx = \int_{a-\epsilon}^{a-\epsilon}Eu(x)dx\\
&-\frac{\hbar^2}{2m}\left(\left.\frac{du}{dx}\right|_{a-\epsilon}^{a+\epsilon} + 0 = 0\right)
\end{aligned}
\tag{9.52}
$$

which gives us

$$
\left.\frac{du}{dx}\right|_{a+\epsilon} - \left.\frac{du}{dx}\right|_{a-\epsilon} = 0 \tag{9.53}
$$

or

$$\left.\frac{du}{dx}\right|_{a+\epsilon} = \left.\frac{du}{dx}\right|_{a-\epsilon} \tag{9.54}$$

We can infer how the derivative behaves over the potential discontinuity, so in the limit where $\epsilon \to 0$ we must have wave function continuity at despite the potential discontinuity.

This sort of analysis, which is potential dependent, we see that for this infinite potential well, our derivative must be continuous at the boundary.

Example 9.2: Non-infinite step well potential.

Given a zero potential in the well $|x| < a$

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}u(x) + 0 = Eu(x), \tag{9.55}$$

and outside of the well $|x| > a$

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}u(x) + V_0 u(x) = Eu(x) \tag{9.56}$$

Inside of the well, we have the solution worked previously, with $\alpha = \sqrt{2mE/\hbar^2}$

$$u(x) = A\cos\alpha x + B\sin\alpha x \tag{9.57}$$

Then we have outside of the well the same form

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}u(x) = (E - V_0)u(x) \tag{9.58}$$

With $\beta = \sqrt{2m(V_0 - E)/\hbar^2}$, this is

$$\frac{d^2u(x)}{dx^2}u(x) = \beta^2 u(x) \tag{9.59}$$

If $V_0 - E > 0$, we have $V_0 > E$, and the states are "bound" or "localized" in the well.

Our solutions for this $V_0 > E$ case are then

$$\begin{aligned} u(x) &= De^{\beta x} \\ u(x) &= Ce^{-\beta x} \end{aligned} \tag{9.60}$$

for $x \leq a$, and $x \geq a$ respectively.

Question: Why can we not have

$$u(x) = De^{\beta x} + Ce^{-\beta x} \tag{9.61}$$

for $x \leq -a$?

Answer: As $x \to -\infty$ we would then have

$$u(x) \to Ce^{\beta\infty} \to \infty \tag{9.62}$$

This is a non-physical solution, and we discard it based on our normalization requirement.

Our total solution, in regions $x < -a$, $|x| \leq a$, and $x > a$ respectively

$$\begin{aligned} u_1(x) &= De^{\beta x} \\ u_2(x) &= A\cos\alpha x + B\sin\alpha x \\ u_3(x) &= Ce^{-\beta x} \end{aligned} \tag{9.63}$$

To find the coefficients, set $u_1(-a) = u_2(-a)$, $u_2(a) = u_3(a)$ $u_1'(-a) = u_2'(-a)$, $u_2'(a) = u_3'(a)$, and NORMALIZE $u(x)$.

Now, how about in region 2 ($x < -a$), $V_0 < E$ implies that our equation is

$$\frac{d^2u(x)}{dx^2}u(x) = -\frac{2m}{\hbar^2}(E - V_0)u(x) = -k^2u(x) \tag{9.64}$$

We no longer have quantized energy for such a solution. These correspond to the "unbound" or "continuum" states. Even though we do not have quantized energy we still have quantum effects. Our solution becomes

$$\begin{aligned} u_1(x) &= C_2 e^{ikx} + D_2 e^{-ikx} \\ u_2(x) &= A e^{i\alpha x} + B e^{-i\alpha x} \\ u_3(x) &= C_3 e^{ikx} \end{aligned} \tag{9.65}$$

Question. Why no $D_2 e^{-ikx}$, in the $u_3(x)$ term?

Answer. We can, but this is not physically relevant. Why is because we associate e^{ikx} with an incoming wave, with reflection in the $x < -a$ interval, and both $e^{\pm i\alpha x}$ in the $|x| < a$ interval, but just an outgoing wave e^{ikx} in the $x > a$ region.

FIXME: scan picture: 9.1 in my notebook.

Observe that this is not normalizable as is. We require "delta-function" normalization. What we can do is ask about current densities. How much passes through the barrier, and so forth.

Note to self. We probably really we want to consider a wave packet of states, something like:

$$\begin{aligned} \Psi_1(x) &= \int dk f_1(k) e^{ikx} \\ \Psi_2(x) &= \int d\alpha f_2(\alpha) e^{i\alpha x} \\ \Psi_3(x) &= \int dk f_3(k) e^{ikx} \end{aligned} \tag{9.66}$$

Then we would have something that we can normalize. Play with this later.

9.3 LECTURE: HYDROGEN ATOM

Introduce the center of mass coordinates We will want to solve this using the formalism we have discussed. The general problem is a proton, positively charged, with a nearby negative charge (the electron).

Our equation to solve is

$$\left(-\frac{\hbar^2}{2m_1}\boldsymbol{\nabla}_1^2 - \frac{\hbar^2}{2m_2}\boldsymbol{\nabla}_2^2\right)\bar{u}(\mathbf{r}_1, \mathbf{r}_2) + V(\mathbf{r}_1, \mathbf{r}_2)\bar{u}(\mathbf{r}_1, \mathbf{r}_2) = E\bar{u}(\mathbf{r}_1, \mathbf{r}_2). \tag{9.67}$$

Here $\left(-\frac{\hbar^2}{2m_1}\boldsymbol{\nabla}_1^2 - \frac{\hbar^2}{2m_2}\boldsymbol{\nabla}_2^2\right)$ is the total kinetic energy term. For hydrogen we can consider the potential to be the Coulomb potential energy function that depends only on $\mathbf{r}_1 - \mathbf{r}_2$. We can transform this using a center of mass transformation. Introduce the center of mass coordinate and relative coordinate vectors

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2} \tag{9.68}$$

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2. \tag{9.69}$$

The notation $\boldsymbol{\nabla}_k^2$ represents the Laplacian for the positions of the k'th particle, so that if $\mathbf{r}_1 = (x_1, x_2, x_3)$ is the position of the first particle, the Laplacian for this is:

$$\boldsymbol{\nabla}_1^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2} \tag{9.70}$$

Here $\mathbf{R}$ is the center of mass coordinate, and $\mathbf{r}$ is the relative coordinate. With this transformation we can reduce the problem to a single coordinate PDE.

We set $\bar{u}(\mathbf{r}_1, \mathbf{r}_2) = u(\mathbf{r})U(\mathbf{R})$ and $E = E_{rel} + E_{cm}$, and get

$$-\frac{\hbar^2}{2\mu}\boldsymbol{\nabla}_{\mathbf{r}}{}^2 u(\mathbf{r}) + V(\mathbf{r})u(\mathbf{r}) = E_{rel}u(\mathbf{r}) \tag{9.71}$$

and

$$-\frac{\hbar^2}{2M}\boldsymbol{\nabla}_{\mathbf{R}}{}^2 U(\mathbf{R}) = E_{cm}U(\mathbf{R}) \tag{9.72}$$

where $M = m_1 + m_2$ is the total mass, and $\mu = m_1 m_2/M$ is the reduced mass.

Aside: WHY do we care (slide of Hydrogen line spectrum shown)? This all started because when people looked at the spectrum for the hydrogen atom, a continuous spectrum was not found. Instead what was found was quantized frequencies. All this abstract Hilbert space notation with its bras and kets is a way of representing observable phenomena.

Also note that we have the same sort of problems in electrodynamics and mechanics, so we are able to recycle this sort of work, either applying it in those problems later, or using those techniques here.

In Electromagnetism these are the problems involving the solution to

$$\boldsymbol{\nabla} \cdot \mathbf{E} = 0 \tag{9.73}$$

or for

$$\mathbf{E} = -\boldsymbol{\nabla}\Phi \tag{9.74}$$

$$\boldsymbol{\nabla}^2\Phi = 0, \tag{9.75}$$

where $\mathbf{E}$ is the electric field and Φ is the electric potential.
We need sol solve eq. (9.71) for $u(\mathbf{r})$. In spherical coordinates

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}(rR_l) + \left(V(\mathbf{r}) + \frac{\hbar^2}{2m}l(l+1)\right)R_l = ER_l \tag{9.76}$$

where

$$u(\mathbf{r}) = R_l(\mathbf{r})Y_{lm}(\theta, \phi) \tag{9.77}$$

This all follows by the separation of variables technique that we will use here, in E and M, in PDEs, and so forth.

FIXME: picture drawn. Theta measured down from $\mathbf{e}_3$ axis to the position $\mathbf{r}$ and ϕ measured in the x, y plane measured in the $\mathbf{e}_1$ to $\mathbf{e}_2$ orientation.

For the hydrogen atom, we have

$$V(\mathbf{r}) = -\frac{Ze^2}{r} \tag{9.78}$$

Here is what this looks like.

We introduce

$$\rho = \alpha r \tag{9.79}$$

$$\alpha = \sqrt{\frac{-8mE}{\hbar^2}} \tag{9.80}$$

$$\lambda = \frac{2mZe^2}{\hbar^2\alpha} \tag{9.81}$$

$$\frac{2m(-E)}{\hbar^2\alpha^2} = \frac{1}{4} \tag{9.82}$$

and write

$$\frac{d^2R_l}{d\rho^2} + \frac{2}{\rho}\frac{dR_l}{d\rho} + \left(\frac{\lambda}{\rho} - \frac{l(l+1)}{\rho^2} - \frac{1}{4}\right)R_l = 0 \tag{9.83}$$

Large ρ limit For $\rho \to \infty$, eq. (9.83) becomes

$$\frac{d^2R_l}{d\rho^2} - \frac{1}{4}R_l = 0 \tag{9.84}$$

which implies solutions of the form

$$R_l(\rho) = e^{\pm\rho/2} \tag{9.85}$$

but keep $R_l(\rho) = e^{-\rho/2}$ and note that $R_l(\rho) = F(\rho)e^{-\rho/2}$ is also a solution in the limit of $\rho \to \infty$, where $F(\rho)$ is a polynomial.

Let $F(\rho) = \rho^s L(\rho)$ where $L(\rho) = a_0 + a_1\rho + \cdots a_\nu\rho^\nu + \cdots$.

Small ρ limit We also want to consider the small ρ limit, and piece together the information that we find. Think about the following. The small $\rho \to 0$ or $r \to 0$ limit gives

$$\frac{d^2R_l}{d\rho^2} - \frac{l(l+1)}{\rho^2}R_l = 0 \tag{9.86}$$

Question: Is this correct?

Not always. Also: we will also think about the $l = 0$ case later (where λ/ρ would probably need to be retained.)

We need:

$$\frac{d^2R_l}{d\rho^2} + \frac{2}{\rho}\frac{dR_l}{d\rho} - \frac{l(l+1)}{\rho^2}R_l = 0 \tag{9.87}$$

Instead of using eq. (9.86) as in the text, we must substitute $R_l = \rho^s$ into the above to find

$$s(s-1)\rho^{s-2} + 2s\rho^{s-2} - l(l+1)\rho^{s-2} = 0 \tag{9.88}$$

$$\big(s(s-1) + 2s - l(l+1)\big)\,\rho^{s-2} = \tag{9.89}$$

for this equality for all ρ we need

$$s(s-1) + 2s - l(l+1) = 0 \tag{9.90}$$

Solutions $s = l$ and $s = -(l+1)$ can be found to this, and we need s positive for normalizability, which implies

$$R_l(\rho) = \rho^l L(\rho)e^{-\rho/2}. \tag{9.91}$$

Now we need to find what restrictions we must have on $L(\rho)$. Recall that we have $L(\rho) = \sum a_\nu \rho^\nu$. Substitution into eq. (9.86) gives

$$\rho \frac{d^2 L}{d\rho} + \left(2(l+1) - \rho\right) \frac{dL}{d\rho} + (\lambda - l - 1)L = 0 \tag{9.92}$$

We get

$$A_0 + A_1\rho + \cdots A_\nu \rho^\nu + \cdots = 0 \tag{9.93}$$

For this to be valid for all ρ,

$$a_{\nu+1}\left((\nu+1)(\nu+2l+2)\right) - a_\nu\left(\nu - \lambda + l + 1\right) = 0 \tag{9.94}$$

or

$$\frac{a_{\nu+1}}{a_\nu} = \frac{\nu - \lambda + l + 1}{(\nu+1)(\nu+2l+2)} \tag{9.95}$$

For large ν we have

$$\frac{a_{\nu+1}}{a_\nu} = \frac{1}{\nu+1} \to \frac{1}{\nu} \tag{9.96}$$

Recall that for the exponential Taylor series we have

$$e^\rho = 1 + \rho + \frac{\rho^2}{2!} + \cdots \tag{9.97}$$

for which we have

$$\frac{a_{\nu+1}}{a_\nu} \to \frac{1}{\nu} \tag{9.98}$$

$L(\rho)$ is behaving like e^ρ, and if we had that

$$R_l(\rho) = \rho^l L(\rho) e^{-\rho/2} \to \rho^l e^\rho e^{-\rho/2} = \rho^l e^{\rho/2} \tag{9.99}$$

This is divergent, so for normalizable solutions we require $L(\rho)$ to be a polynomial of a finite number of terms.

The polynomial $L(\rho)$ must stop at $\nu = n'$, and we must have

$$a_{\nu+1} = a_{n'+1} = 0 \tag{9.100}$$

$$a_{n'} \neq 0 \tag{9.101}$$

From eq. (9.94) we have

$$a_{n'} \left(n' - \lambda + l + 1\right) = 0 \tag{9.102}$$

so we require

$$n' = \lambda - l - 1 \tag{9.103}$$

Let $\lambda = n$, an integer and $n' = 0, 1, 2, \cdots$ so that $n' + l + 1 = n$ says for $n = 1, 2, \cdots$

$$l \leq n - 1 \tag{9.104}$$

If

$$\lambda = n = \frac{2mZe^2}{\hbar^2 \alpha} \tag{9.105}$$

we have

$$E = E_n = -\frac{Z^2 e^2}{2a_0} \frac{1}{n^2} \tag{9.106}$$

where $a_0 = \hbar^2/me^2$ is the Bohr radius, and $\alpha = \sqrt{-8mE/\hbar^2}$. In the lecture m was originally used for the reduced mass. I have switched to μ earlier so that this cannot be mixed up with this use of m for the azimuthal quantum number associated with $L_z Y_{lm} = m\hbar Y_{lm}$.

PICTURE ON BOARD. Energy level transitions on $1/n^2$ graph with differences between $n = 2$ to $n = 1$ shown, and photon emitted as a result of the $n = 2$ to $n = 1$ transition.

From Chapter 4 and the story of the spherical harmonics, for a given l, the quantum number m varies between $-l$ and l in integer steps. The radial part of the solution of this separation of variables problem becomes

$$R_l = \rho^l L(\rho) e^{-\rho/2} \tag{9.107}$$

where the functions $L(\rho)$ are the Laguerre polynomials, and our complete wavefunction is

$$u_{nlm}(r, \theta, \phi) = R_l(\rho) Y_{lm}(\theta, \phi) \tag{9.108}$$

$$n = 1, 2, \cdots \tag{9.109}$$
$$l = 0, 1, 2, \cdots, n-1 \tag{9.110}$$
$$m = -l, -l+1, \cdots 0, 1, 2, \cdots, l-1, l \tag{9.111}$$

Note that for $n = 1, l = 0$, $R_{10} \propto e^{-r/a_0}$, as graphed here.

9.4 PROBLEMS

Exercise 9.1 ps 4, p1.

Is it possible to derive the eigenvalues and eigenvectors presented in Section 8.2 from those in Section 8.1.2? What does this say about the potential energy operator in these two situations?

For reference 8.1.2 was a finite potential barrier, $V(x) = V_0, |x| > a$, and zero in the interior of the well. This had trigonometric solutions in the interior, and died off exponentially past the boundary of the well.

On the other hand, 8.2 was a delta function potential $V(x) = -g\delta(x)$, which had the solution $u(x) = \sqrt{\beta}e^{-\beta|x|}$, where $\beta = mg/\hbar^2$.

Answer for Exercise 9.1

The pair of figures in the text [3] for these potentials does not make it clear that there are possibly any similarities. The attractive delta function potential is not illustrated (although the delta function is, but with opposite sign), and the scaling and the reference energy levels are different. Let us illustrate these using the same reference energy level and sign conventions to make the similarities more obvious.

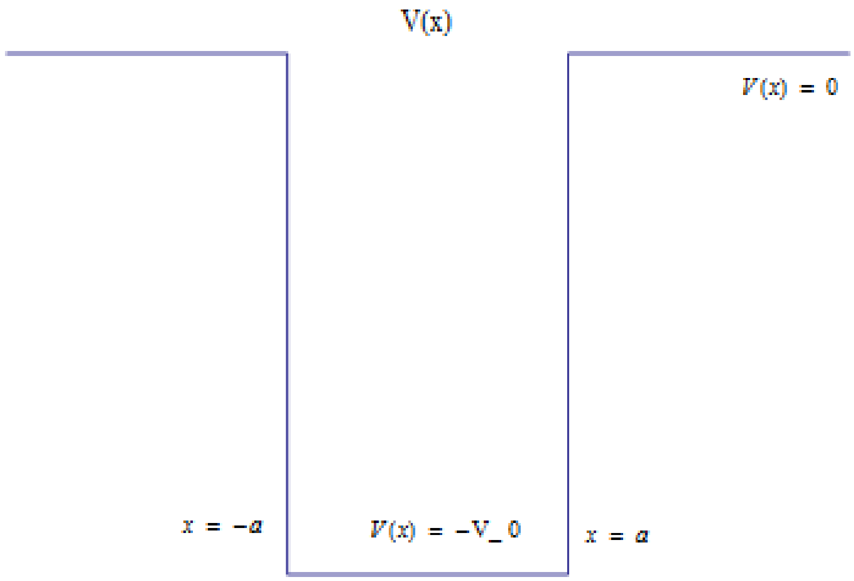

Figure 9.1: 8.1.2 Finite Well potential (with energy shifted downwards by V_0)

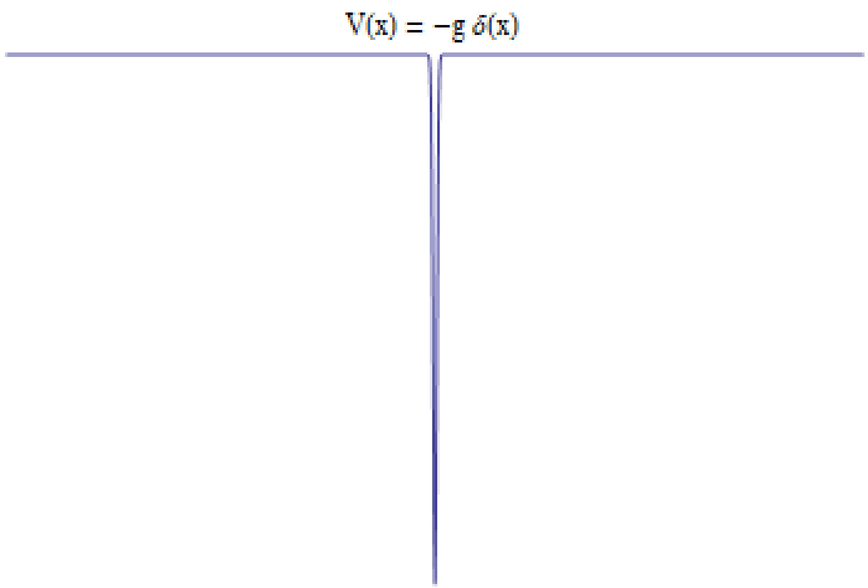

Figure 9.2: 8.2 Delta function potential

The physics is not changed by picking a different point for the reference energy level, so let us compare the two potentials, and their solutions using $V(x) = 0$ outside of the well for both cases. The method used to solve the finite well problem in the text is hard to follow, so re-doing this from scratch in a slightly tidier way does not hurt.

Schrödinger's equation for the finite well, in the $|x| > a$ region is

$$-\frac{\hbar^2}{2m}u'' = Eu = -E_B u, \tag{9.112}$$

where a positive bound state energy $E_B = -E > 0$ has been introduced.

Writing

$$\beta = \sqrt{\frac{2mE_B}{\hbar^2}}, \tag{9.113}$$

the wave functions outside of the well are

$$u(x) = \begin{cases} u(-a)e^{\beta(x+a)} & x < -a \\ u(a)e^{-\beta(x-a)} & x > a \end{cases} \tag{9.114}$$

Within the well Schrödinger's equation is

$$-\frac{\hbar^2}{2m}u'' - V_0 u = Eu = -E_B u, \tag{9.115}$$

or

$$\frac{\hbar^2}{2m}u'' = -\frac{2m}{\hbar^2}(V_0 - E_B)u, \tag{9.116}$$

Noting that the bound state energies are the $E_B < V_0$ values, let $\alpha^2 = 2m(V_0 - E_B)/\hbar^2$, so that the solutions are of the form

$$u(x) = Ae^{i\alpha x} + Be^{-i\alpha x}. \tag{9.117}$$

As was done for the wave functions outside of the well, the normalization constants can be expressed in terms of the values of the wave functions on the boundary. That provides a pair of equations to solve

$$\begin{bmatrix} u(a) \\ u(-a) \end{bmatrix} = \begin{bmatrix} e^{i\alpha a} & e^{-i\alpha a} \\ e^{-i\alpha a} & e^{i\alpha a} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}. \tag{9.118}$$

Inverting this and substitution back into eq. (9.117) yields

$$
\begin{aligned}
u(x) &= \begin{bmatrix} e^{i\alpha x} & e^{-i\alpha x} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} \\
&= \begin{bmatrix} e^{i\alpha x} & e^{-i\alpha x} \end{bmatrix} \frac{1}{e^{2i\alpha a} - e^{-2i\alpha a}} \begin{bmatrix} e^{i\alpha a} & -e^{-i\alpha a} \\ -e^{-i\alpha a} & e^{i\alpha a} \end{bmatrix} \begin{bmatrix} u(a) \\ u(-a) \end{bmatrix} \\
&= \begin{bmatrix} \frac{\sin(\alpha(a+x))}{\sin(2\alpha a)} & \frac{\sin(\alpha(a-x))}{\sin(2\alpha a)} \end{bmatrix} \begin{bmatrix} u(a) \\ u(-a) \end{bmatrix}.
\end{aligned}
\tag{9.119}
$$

Expanding the last of these matrix products the wave function is close to completely specified.

$$
u(x) = \begin{cases} u(-a)e^{\beta(x+a)} & x < -a \\ u(a)\frac{\sin(\alpha(a+x))}{\sin(2\alpha a)} + u(-a)\frac{\sin(\alpha(a-x))}{\sin(2\alpha a)} & |x| < a \\ u(a)e^{-\beta(x-a)} & x > a \end{cases}
\tag{9.120}
$$

There are still two unspecified constants $u(\pm a)$ and the constraints on E_B have not been determined (both α and β are functions of that energy level). It should be possible to eliminate at least one of the $u(\pm a)$ by computing the wavefunction normalization, and since the well is being narrowed the α term will not be relevant. Since only the vanishingly narrow case where $a \rightarrow 0, x \in [-a, a]$ is of interest, the wave function in that interval approaches

$$
u(x) \rightarrow \frac{1}{2}(u(a) + u(-a)) + \frac{x}{2}(u(a) - u(-a)) \rightarrow \frac{1}{2}(u(a) + u(-a)).
\tag{9.121}
$$

Since no discontinuity is expected this is just $u(a) = u(-a)$. Let us write $\lim_{a\rightarrow 0} u(a) = A$ for short, and the limited width well wave function becomes

$$
u(x) = \begin{cases} Ae^{\beta x} & x < 0 \\ Ae^{-\beta x} & x > 0 \end{cases}
\tag{9.122}
$$

This is now the same form as the delta function potential, and normalization also gives $A = \sqrt{\beta}$.

One task remains before the attractive delta function potential can be considered a limiting case for the finite well, since the relation between a, V_0, and g has not been established. To do so integrate the Schrödinger equation over the infinitesimal range $[-a, a]$. This was done in the text for the delta function potential, and that provided the relation

$$
\beta = \frac{mg}{\hbar^2}
\tag{9.123}
$$

For the finite well this is

$$\int_{-a}^{a} -\frac{\hbar^2}{2m}u'' - V_0 \int_{-a}^{a} u = -E_B \int_{-a}^{a} u \tag{9.124}$$

In the limit as $a \rightarrow 0$ this is

$$\frac{\hbar^2}{2m}(u'(a) - u'(-a)) + V_0 2au(0) = 2E_B au(0). \tag{9.125}$$

Some care is required with the $V_0 a$ term since $a \rightarrow 0$ as $V_0 \rightarrow \infty$, but the E_B term is unambiguously killed, leaving

$$\frac{\hbar^2}{2m}u(0)(-2\beta e^{-\beta a}) = -V_0 2au(0). \tag{9.126}$$

The exponential vanishes in the limit and leaves

$$\beta = \frac{m(2a)V_0}{\hbar^2} \tag{9.127}$$

Comparing to eq. (9.123) from the attractive delta function completes the problem. The conclusion is that when the finite well is narrowed with $a \rightarrow 0$, also letting $V_0 \rightarrow \infty$ such that the absolute area of the well $g = (2a)V_0$ is maintained, the finite potential well produces exactly the attractive delta function wave function and associated bound state energy.

Grading notes Lost 3/20 marks, all in the first question.

I did not show that $u(a) = u(-a)$.

I did not explain why the odd terms disappear in eq. (9.121).

I also did not get agreement with my statement that "but the E_B term is unambiguously killed", where I have assumed that it remains finite. Since $V_0 \rightarrow \infty$, E_B could tend to infinity too.

Some references Some references that I found helpful to provide some of the context for WHY to consider the delta function potential in the first place are [16], [2], [8], [5].

Exercise 9.2 ps4, p2.

For the hydrogen atom, determine $\langle nlm| (1/R) |nlm\rangle$ and $1/\langle nlm| R |nlm\rangle$ such that $(nlm) = (211)$ and R is the radial position operator $(X^2 + Y^2 + Z^2)^{1/2}$. What do these quantities represent physically and are they the same?

Answer for Exercise 9.2

Both of the computation tasks for the hydrogen like atom require expansion of a braket of the following form

$$\langle nlm| A(R) |nlm\rangle, \tag{9.128}$$

where $A(R) = R = (X^2 + Y^2 + Z^2)^{1/2}$ or $A(R) = 1/R$.

The spherical representation of the identity resolution is required to convert this braket into integral form

$$\mathbf{1} = \int r^2 \sin\theta dr d\theta d\phi |r\theta\phi\rangle \langle r\theta\phi|, \tag{9.129}$$

where the spherical wave function is given by the braket $\langle r\theta\phi|nlm\rangle = R_{nl}(r)Y_{lm}(\theta,\phi)$.

Additionally, the radial form of the delta function will be required, which is

$$\delta(\mathbf{x} - \mathbf{x}') = \frac{1}{r^2 \sin\theta}\delta(r - r')\delta(\theta - \theta')\delta(\phi - \phi') \tag{9.130}$$

Two applications of the identity operator to the braket yield

$$\begin{aligned}
&\langle nlm| A(R) |nlm\rangle \\
&= \langle nlm| \mathbf{1}A(R)\mathbf{1} |nlm\rangle \\
&= \int dr d\theta d\phi dr' d\theta' d\phi' r^2 \sin\theta r'^2 \sin\theta' \langle nlm|r\theta\phi\rangle \langle r\theta\phi| A(R) \left|r'\theta'\phi'\right\rangle \langle r'\theta'\phi'|nlm\rangle \\
&= \int dr d\theta d\phi dr' d\theta' d\phi' r^2 \sin\theta r'^2 \sin\theta' R_{nl}(r)Y^*_{lm}(\theta,\phi) \langle r\theta\phi| A(R) \left|r'\theta'\phi'\right\rangle R_{nl}(r')Y_{lm}(\theta',\phi')
\end{aligned} \tag{9.131}$$

To continue an assumption about the matrix element $\langle r\theta\phi| A(R) |r'\theta'\phi'\rangle$ is required. It seems reasonable that this would be

$$\langle r\theta\phi| A(R) \left|r'\theta'\phi'\right\rangle = \quad \delta(\mathbf{x} - \mathbf{x}')A(r) = \frac{1}{r^2 \sin\theta}\delta(r - r')\delta(\theta - \theta')\delta(\phi - \phi')A(r). \tag{9.132}$$

The braket can now be written completely in integral form as

$$\begin{aligned}
&\langle nlm| A(R) |nlm\rangle \\
&= \int dr d\theta d\phi dr' d\theta' d\phi' r^2 \sin\theta r'^2 \sin\theta' \\
&\quad R_{nl}(r)Y^*_{lm}(\theta,\phi)\frac{1}{r^2 \sin\theta}\delta(r - r')\delta(\theta - \theta')\delta(\phi - \phi')A(r)R_{nl}(r')Y_{lm}(\theta',\phi') \\
&= \int dr d\theta d\phi r'^2 \sin\theta' dr' d\theta' d\phi' R_{nl}(r)Y^*_{lm}(\theta,\phi)\delta(r - r')\delta(\theta - \theta')\delta(\phi - \phi')A(r)R_{nl}(r')Y_{lm}(\theta',\phi')
\end{aligned}$$

$$(9.133)$$

Application of the delta functions then reduces the integral, since the only θ, and ϕ dependence is in the (orthonormal) Y_{lm} terms they are found to drop out

$$\begin{aligned}
\langle nlm| A(R) |nlm\rangle &= \int drd\theta d\phi r^2 \sin\theta R_{nl}(r) Y^*_{lm}(\theta,\phi) A(r) R_{nl}(r) Y_{lm}(\theta,\phi) \\
&= \int drr^2 R_{nl}(r) A(r) R_{nl}(r) \overbrace{\boxed{\int \sin\theta d\theta d\phi Y^*_{lm}(\theta,\phi) Y_{lm}(\theta,\phi)}}^{=1}
\end{aligned} \tag{9.134}$$

This leaves just the radial wave functions in the integral

$$\langle nlm| A(R) |nlm\rangle = \int drr^2 R^2_{nl}(r) A(r) \tag{9.135}$$

As a consistency check, observe that with $A(r) = 1$, this integral evaluates to 1 according to equation (8.274) in the text, so we can think of $(rR_{nl}(r))^2$ as the radial probability density for functions of r.

The problem asks specifically for these expectation values for the $|211\rangle$ state. For that state the radial wavefunction is found in (8.277) as

$$R_{21}(r) = \left(\frac{Z}{2a_0}\right)^{3/2} \frac{Zr}{a_0\sqrt{3}} e^{-Zr/2a_0} \tag{9.136}$$

The braket can now be written explicitly

$$\langle 21m| A(R) |21m\rangle = \frac{1}{24}\left(\frac{Z}{a_0}\right)^5 \int_0^\infty drr^4 e^{-Zr/a_0} A(r) \tag{9.137}$$

Now, let us consider the two functions $A(r)$ separately. First for $A(r) = r$ we have

$$\begin{aligned}
\langle 21m| R |21m\rangle &= \frac{1}{24}\left(\frac{Z}{a_0}\right)^5 \int_0^\infty drr^5 e^{-Zr/a_0} \\
&= \frac{a_0}{24Z} \int_0^\infty duu^5 e^{-u}
\end{aligned} \tag{9.138}$$

The last integral evaluates to 120, leaving

$$\langle 21m| R |21m\rangle = \frac{5a_0}{Z}. \tag{9.139}$$

The expectation value associated with this $|21m\rangle$ state for the radial position is found to be proportional to the Bohr radius. For the hydrogen atom where $Z = 1$ this average value for repeated measurements of the physical quantity associated with the operator R is found to be 5 times the Bohr radius for $n = 2, l = 1$ states.

Our problem actually asks for the inverse of this expectation value, and for reference this is

$$1/\langle 21m|\, R\, |21m\rangle = \frac{Z}{5a_0} \tag{9.140}$$

Performing the same task for $A(R) = 1/R$

$$\begin{aligned}\langle 21m|\, 1/R\, |21m\rangle &= \frac{1}{24}\left(\frac{Z}{a_0}\right)^5 \int_0^\infty dr r^3 e^{-Zr/a_0} \\ &= \frac{1}{24}\frac{Z}{a_0}\int_0^\infty du u^3 e^{-u}.\end{aligned} \tag{9.141}$$

This last integral has value 6, and we have the second part of the computational task complete

$$\langle 21m|\, 1/R\, |21m\rangle = \frac{1}{4}\frac{Z}{a_0} \tag{9.142}$$

The question of whether or not eq. (9.140), and eq. (9.142) are equal is answered. They are not.

Still remaining for this problem is the question of the what these quantities represent physically.

The quantity $\langle nlm|\, R\, |nlm\rangle$ is the expectation value for the radial position of the particle measured from the center of mass of the system. This is the average outcome for many measurements of this radial distance when the system is prepared in the state $|nlm\rangle$ prior to each measurement.

Interestingly, the physical quantity that we associate with the operator R has a different measurable value than the inverse of the expectation value for the inverted operator $1/R$. Regardless, we have a physical (observable) quantity associated with the operator $1/R$, and when the system is prepared in state $|21m\rangle$ prior to each measurement, the average outcome of many measurements of this physical quantity produces this value $\langle 21m|\, 1/R\, |21m\rangle = Z/n^2 a_0$, a quantity inversely proportional to the Bohr radius.

ASIDE: Comparing to the general case As a confirmation of the results obtained, we can check eq. (9.140), and eq. (9.142) against the general form of the expectation values $\langle R^s\rangle$ for various powers s of the radial position operator. These can be found in locations such as farside.ph.utexas.edu which gives for $Z = 1$ (without proof), and in [9] (where these and harder looking ones expectation values are left as an exercise for the reader to prove). Both of those give:

$$\begin{aligned}\langle R\rangle &= \frac{a_0}{2}(3n^2 - l(l+1)) \\ \langle 1/R\rangle &= \frac{1}{n^2 a_0}\end{aligned} \tag{9.143}$$

It is curious to me that the general expectation values noted in eq. (9.143) we have a l quantum number dependence for $\langle R\rangle$, but only the n quantum number dependence for $\langle 1/R\rangle$. It is not obvious to me why this would be the case.

Exercise 9.3 Hydrogen atom (2007 PHY355H1F 4)

This problem deals with the hydrogen atom, with an initial ket

$$|\psi(0)\rangle = \frac{1}{\sqrt{3}}|100\rangle + \frac{1}{\sqrt{3}}|210\rangle + \frac{1}{\sqrt{3}}|211\rangle\,, \tag{9.144}$$

where

$$\langle \mathbf{r}|100\rangle = \Phi_{100}(\mathbf{r}), \tag{9.145}$$

etc.

Answer for Exercise 9.3

If no measurement is made until time $t = t_0$,

$$t_0 = \frac{\pi\hbar}{\frac{3}{4}(13.6\text{eV})} = \frac{4\pi\hbar}{3E_I}, \tag{9.146}$$

what is the ket $|\psi(t)\rangle$ just before the measurement is made?

A: Our time evolved state is

$$|\psi t_0\rangle = \frac{1}{\sqrt{3}}e^{-iE_1 t_0/\hbar}|100\rangle + \frac{1}{\sqrt{3}}e^{-iE_2 t_0/\hbar}(|210\rangle + |211\rangle). \tag{9.147}$$

Also observe that this initial time was picked to make the exponential values come out nicely, and we have

$$\begin{aligned}\frac{E_n t_0}{\hbar} &= -\frac{E_I \pi\hbar}{\frac{3}{4}E_I n^2\hbar} \\ &= -\frac{4\pi}{3n^2},\end{aligned} \tag{9.148}$$

so our time evolved state is just

$$|\psi(t_0)\rangle = \frac{1}{\sqrt{3}} e^{-i4\pi/3} |100\rangle + \frac{1}{\sqrt{3}} e^{-i\pi/3} (|210\rangle + |211\rangle). \tag{9.149}$$

Q: (b) Suppose that at time t_0 an L_z measurement is made, and the outcome 0 is recorded. What is the appropriate ket $\psi_{\text{after}}(t_0)$ right after the measurement?

A: A measurement with outcome 0, means that the L_z operator measurement found the state at that point to be the eigenstate for L_z eigenvalue 0. Recall that if $|\phi\rangle$ is an eigenstate of L_z we have

$$L_z |\phi\rangle = m\hbar |\phi\rangle, \tag{9.150}$$

so a measurement of L_z with outcome zero means that we have $m = 0$. Our measurement of L_z at time t_0 therefore filters out all but the $m = 0$ states and our new state is proportional to the projection over all $m = 0$ states as follows

$$\begin{aligned} |\psi_{\text{after}}(t_0)\rangle &\propto \left(\sum_{nl} |nl0\rangle \langle nl0| \right) |\psi(t_0)\rangle \\ &\propto \left(|100\rangle \langle 100| + |210\rangle \langle 210| \right) |\psi(t_0)\rangle \\ &= \frac{1}{\sqrt{3}} e^{-i4\pi/3} |100\rangle + \frac{1}{\sqrt{3}} e^{-i\pi/3} |210\rangle \end{aligned} \tag{9.151}$$

A final normalization yields

$$|\psi_{\text{after}}(t_0)\rangle = \frac{1}{\sqrt{2}} (|210\rangle - |100\rangle) \tag{9.152}$$

Q: (c) Right after this L_z measurement, what is $|\psi_{\text{after}}(t_0)|^2$?

A: Our amplitude is

$$\begin{aligned} \langle \mathbf{r} | \psi_{\text{after}}(t_0)\rangle &= \frac{1}{\sqrt{2}} (\langle \mathbf{r}|210\rangle - \langle \mathbf{r}|100\rangle) \\ &= \frac{1}{\sqrt{2\pi a_0^3}} \left(\frac{r}{4\sqrt{2} a_0} e^{-r/2a_0} \cos\theta - e^{-r/a_0} \right) \\ &= \frac{1}{\sqrt{2\pi a_0^3}} e^{-r/2a_0} \left(\frac{r}{4\sqrt{2} a_0} \cos\theta - e^{-r/2a_0} \right), \end{aligned} \tag{9.153}$$

so the probability density is

$$|\langle \mathbf{r}|\psi_{\text{after}}(t_0)\rangle|^2 = \frac{1}{2\pi a_0^3} e^{-r/a_0} \left(\frac{r}{4\sqrt{2}a_0} \cos\theta - e^{-r/2a_0} \right)^2 \tag{9.154}$$

Q: (d) If then a position measurement is made immediately, which if any components of the expectation value of **R** will be non-vanishing? Justify your answer.

A: The expectation value of this vector valued operator with respect to a radial state $|\psi\rangle = \sum_{nlm} a_{nlm} |nlm\rangle$ can be expressed as

$$\langle \mathbf{R} \rangle = \sum_{i=1}^{3} \mathbf{e}_i \sum_{nlm,n'l'm'} a^*_{nlm} a_{n'l'm'} \langle nlm| X_i \left| n'l'm' \right\rangle, \tag{9.155}$$

where $X_1 = X = R \sin\Theta \cos\Phi, X_2 = Y = R \sin\Theta \sin\Phi, X_3 = Z = R \cos\Phi$.
Consider one of the matrix elements, and expand this by introducing an identity twice

$$\begin{aligned}
\langle nlm| X_i \left| n'l'm' \right\rangle &= \int r^2 \sin\theta dr d\theta d\phi r'^2 \sin\theta' dr' d\theta' d\phi' \langle nlm|r\theta\phi\rangle \langle r\theta\phi| X_i \left| r'\theta'\phi' \right\rangle \langle r'\theta'\phi'|n'l'm'\rangle \\
&= \int r^2 \sin\theta dr d\theta d\phi r'^2 \sin\theta' dr' d\theta' d\phi' R_{nl}(r) Y^*_{lm}(\theta,\phi) \delta^3(\mathbf{x} - \mathbf{x}') x_i R_{n'l'}(r') Y_{l'm'}(\theta',\phi') \\
&= \int r^2 \sin\theta dr d\theta d\phi r'^2 \sin\theta' dr' d\theta' d\phi' R_{nl}(r) Y^*_{lm}(\theta,\phi) \\
&\qquad r'^2 \sin\theta' \delta(r - r') \delta(\theta - \theta') \delta(\phi - \phi') x_i R_{n'l'}(r') Y_{l'm'}(\theta',\phi') \\
&= \int r^2 \sin\theta dr d\theta d\phi dr' d\theta' d\phi' R_{nl}(r) Y^*_{lm}(\theta,\phi) \delta(r - r') \delta(\theta - \theta') \delta(\phi - \phi') x_i R_{n'l'}(r') Y_{l'm'}(\theta',\phi') \\
&= \int r^2 \sin\theta dr d\theta d\phi R_{nl}(r) R_{n'l'}(r) Y^*_{lm}(\theta,\phi) Y_{l'm'}(\theta,\phi) x_i
\end{aligned} \tag{9.156}$$

Because our state has only $m = 0$ contributions, the only ϕ dependence for the X and Y components of **R** come from those components themselves. For X, we therefore integrate $\int_0^{2\pi} \cos\phi d\phi = 0$, and for Y we integrate $\int_0^{2\pi} \sin\phi d\phi = 0$, and these terms vanish. Our expectation value for **R** for this state, therefore lies completely on the z axis.

10 HARMONIC OSCILLATOR

10.1 SETUP

Why study this problem?

It is relevant to describing the oscillation of molecules, quantum states of light, vibrations of the lattice structure of a solid, and so on.

FIXME: projected picture of masses on springs, with a ladle shaped well, approximately Harmonic about the minimum of the bucket.

The problem to solve is the one dimensional Hamiltonian

$$
\begin{aligned}
V(X) &= \frac{1}{2} K X^2 \\
K &= m\omega^2 \\
H &= \frac{P^2}{2m} + V(X)
\end{aligned}
\tag{10.1}
$$

where m is the mass, ω is the frequency, X is the position operator, and P is the momentum operator. Of these quantities, ω and m are classical quantities.

This problem can be used to illustrate some of the reasons why we study the different pictures (Heisenberg, Interaction and Schrödinger). This is a problem well suited to all of these (FIXME: lookup an example of this with the interaction picture. The book covers H and S methods.

We attack this with a non-intuitive, but cool technique. Introduce the raising $a^\dagger$ and lowering a operators:

$$
\begin{aligned}
a &= \sqrt{\frac{m\omega}{2\hbar}} \left(X + i \frac{P}{m\omega} \right) \\
a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}} \left(X - i \frac{P}{m\omega} \right)
\end{aligned}
\tag{10.2}
$$

Question: are we using the dagger for more than Hermitian conjugation in this case.

Answer: No, this is precisely the Hermitian conjugation operation.

Solving for X and P in terms of a and $a^\dagger$, we have

$$\begin{aligned} a + a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}2X \\ a - a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}2i\frac{P}{m\omega} \end{aligned} \tag{10.3}$$

or

$$\begin{aligned} X &= \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a) \\ P &= i\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a) \end{aligned} \tag{10.4}$$

Express H in terms of a and $a^\dagger$

$$\begin{aligned} H &= \frac{P^2}{2m} + \frac{1}{2}KX^2 \\ &= \frac{1}{2m}\left(i\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a)\right)^2 + \frac{1}{2}m\omega^2\left(\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)\right)^2 \\ &= \frac{-\hbar\omega}{4}\left(a^\dagger a^\dagger + a^2 - aa^\dagger - a^\dagger a\right) + \frac{\hbar\omega}{4}\left(a^\dagger a^\dagger + a^2 + aa^\dagger + a^\dagger a\right) \end{aligned} \tag{10.5}$$

$$H = \frac{\hbar\omega}{2}\left(aa^\dagger + a^\dagger a\right) = \frac{\hbar\omega}{2}\left(2a^\dagger a + \left[a, a^\dagger\right]\right) \tag{10.6}$$

Since $[X, P] = i\hbar\mathbf{1}$ then we can show that $\left[a, a^\dagger\right] = \mathbf{1}$. Solve for $\left[a, a^\dagger\right]$ as follows

$$\begin{aligned} i\hbar &= [X, P] \\ &= \left[\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a), i\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a)\right] \\ &= \sqrt{\frac{\hbar}{2m\omega}}i\sqrt{\frac{\hbar m\omega}{2}}\left[a^\dagger + a, a^\dagger - a\right] \\ &= \frac{i\hbar}{2}\left(\left[a^\dagger, a^\dagger\right] - \left[a^\dagger, a\right] + \left[a, a^\dagger\right] - [a, a]\right) \\ &= \frac{i\hbar}{2}\left(0 + 2\left[a, a^\dagger\right] - 0\right) \end{aligned} \tag{10.7}$$

Comparing LHS and RHS we have as stated

$$\left[a, a^{\dagger}\right] = \mathbf{1} \tag{10.8}$$

and thus from eq. (10.6) we have

$$H = \hbar\omega\left(a^{\dagger}a + \frac{\mathbf{1}}{2}\right) \tag{10.9}$$

Let $|n\rangle$ be the eigenstate of H so that $H|n\rangle = E_n|n\rangle$. From eq. (10.9) we have

$$H|n\rangle = \hbar\omega\left(a^{\dagger}a + \frac{\mathbf{1}}{2}\right)|n\rangle \tag{10.10}$$

or

$$a^{\dagger}a|n\rangle + \frac{|n\rangle}{2} = \frac{E_n}{\hbar\omega}|n\rangle \tag{10.11}$$

$$a^{\dagger}a|n\rangle = \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)|n\rangle = \lambda_n|n\rangle \tag{10.12}$$

We wish now to find the eigenstates of the "Number" operator $a^{\dagger}a$, which are simultaneously eigenstates of the Hamiltonian operator.

Observe that we have

$$\begin{aligned} a^{\dagger}a(a^{\dagger}|n\rangle) &= a^{\dagger}(aa^{\dagger}|n\rangle) \\ &= a^{\dagger}(\mathbf{1} + a^{\dagger}a)|n\rangle \end{aligned} \tag{10.13}$$

where we used $\left[a, a^{\dagger}\right] = aa^{\dagger} - a^{\dagger}a = \mathbf{1}$.

$$\begin{aligned} a^{\dagger}a(a^{\dagger}|n\rangle) &= a^{\dagger}\left(\mathbf{1} + \frac{E_n}{\hbar\omega} - \frac{\mathbf{1}}{2}\right)|n\rangle \\ &= a^{\dagger}\left(\frac{E_n}{\hbar\omega} + \frac{\mathbf{1}}{2}\right)|n\rangle, \end{aligned} \tag{10.14}$$

or

$$a^{\dagger}a(a^{\dagger}|n\rangle) = (\lambda_n + 1)(a^{\dagger}|n\rangle) \tag{10.15}$$

The new state $a^\dagger |n\rangle$ is presumed to lie in the same space, expressible as a linear combination of the basis states in this space. We can see the effect of the operator $aa^\dagger$ on this new state, we find that the energy is changed, but the state is otherwise unchanged. Any state $a^\dagger |n\rangle$ is an eigenstate of $a^\dagger a$, and therefore also an eigenstate of the Hamiltonian.

Play the same game and win big by discovering that

$$a^\dagger a(a|n\rangle) = (\lambda_n - 1)(a|n\rangle) \tag{10.16}$$

There will be some state $|0\rangle$ such that

$$a|0\rangle = 0\,|0\rangle \tag{10.17}$$

which implies

$$a^\dagger(a|0\rangle) = (a^\dagger a)|0\rangle = 0 \tag{10.18}$$

so from eq. (10.12) we have

$$\lambda_0 = 0 \tag{10.19}$$

Observe that we can identify $\lambda_n = n$ for

$$\lambda_n = \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right) = n, \tag{10.20}$$

or

$$\frac{E_n}{\hbar\omega} = n + \frac{1}{2} \tag{10.21}$$

or

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{10.22}$$

where $n = 0, 1, 2, \cdots$.

We can write

$$\begin{aligned} \hbar\omega\left(a^\dagger a + \frac{1}{2}\mathbf{1}\right)|n\rangle &= E_n\,|n\rangle \\ a^\dagger a\,|n\rangle + \frac{1}{2}\,|n\rangle &= \frac{E_n}{\hbar\omega}\,|n\rangle \end{aligned} \tag{10.23}$$

or

$$a^\dagger a\,|n\rangle = \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)|n\rangle = \lambda_n\,|n\rangle = n\,|n\rangle \tag{10.24}$$

We call this operator $a^\dagger a = N$, the number operator, so that

$$N\,|n\rangle = n\,|n\rangle \tag{10.25}$$

10.2 RELATING STATES

Recall the calculation we performed for

$$\begin{aligned} L_+\,|lm\rangle &= C_+\,|l, m+1\rangle \\ L_-\,|lm\rangle &= C_+\,|l, m-1\rangle \end{aligned} \tag{10.26}$$

Where C_+, and C_+ are constants. The next game we are going to play is to work out C_n for the lowering operation

$$a\,|n\rangle = C_n\,|n-1\rangle \tag{10.27}$$

and the raising operation

$$a^\dagger\,|n\rangle = B_n\,|n+1\rangle\,. \tag{10.28}$$

For the Hermitian conjugate of $a\,|n\rangle$ we have

$$(a\,|n\rangle)^\dagger = (C_n\,|n-1\rangle)^\dagger = C_n^*\,|n-1\rangle \tag{10.29}$$

So

$$(\langle n|\,a^\dagger)(a\,|n\rangle) = C_n C_n^*\,\langle n-1|n-1\rangle = |C_n|^2 \tag{10.30}$$

Expanding the LHS we have

$$\begin{aligned} |C_n|^2 &= \langle n|\,a^\dagger a\,|n\rangle \\ &= \langle n|\,n\,|n\rangle \\ &= n\,\langle n|n\rangle \\ &= n \end{aligned} \tag{10.31}$$

For

$$C_n = \sqrt{n} \tag{10.32}$$

Similarly

$$(\langle n|\, a^\dagger)(a\,|n\rangle) = B_n B_n^* \,\langle n+1|n+1\rangle = |B_n|^2 \tag{10.33}$$

and

$$aa^\dagger - a^\dagger a = \mathbf{1}$$

$$\begin{aligned}
|B_n|^2 &= \langle n|\boxed{aa^\dagger}|n\rangle \\
&= \langle n|\left(\mathbf{1} + a^\dagger a\right)|n\rangle \\
&= (1+n)\,\langle n|n\rangle \\
&= 1 + n
\end{aligned} \tag{10.34}$$

for

$$B_n = \sqrt{n+1} \tag{10.35}$$

10.3 HEISENBERG PICTURE

How does the lowering operator a evolve in time?

A: Recall that for a general operator A, we have for the time evolution of that operator

$$i\hbar \frac{dA}{dt} = [A, H] \tag{10.36}$$

Let us solve this one.

$$\begin{aligned}
i\hbar \frac{da}{dt} &= [a, H] \\
&= \left[a,\ \hbar\omega(a^\dagger a + \mathbf{1}/2)\right] \\
&= \hbar\omega \left[a, (a^\dagger a + \mathbf{1}/2)\right] \\
&= \hbar\omega \left[a, a^\dagger a\right] \\
&= \hbar\omega \left(aa^\dagger a - a^\dagger aa\right) \\
&= \hbar\omega \left((aa^\dagger)a - a^\dagger aa\right) \\
&= \hbar\omega \left((a^\dagger a + \mathbf{1})a - a^\dagger aa\right) \\
&= \hbar\omega a
\end{aligned} \tag{10.37}$$

Even though a is an operator, it can undergo a time evolution and we can think of it as a function, and we can solve for a in the differential equation

$$\frac{da}{dt} = -i\omega a \tag{10.38}$$

This has the solution

$$a = a(0)e^{-i\omega t} \tag{10.39}$$

here $a(0)$ is an operator, the value of that operator at $t = 0$. The exponential here is just a scalar (not effected by the operator so we can put it on either side of the operator as desired).

CHECK:

$$a' = a(0)\frac{d}{dt}e^{-i\omega t} = a(0)(-i\omega)e^{-i\omega t} = -i\omega a \tag{10.40}$$

10.4 A COUPLE COMMENTS ON THE SCHRÖDINGER PICTURE

We do not do this in class, but it is very similar to the approach of the hydrogen atom. See the text for full details.

In the Schrödinger picture,

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + \frac{1}{2}m\omega^2 x^2 u = Eu \tag{10.41}$$

This does directly to the wave function representation, but we can relate these by noting that we get this as a consequence of the identification $u = u(x) = \langle x|u\rangle$.

In eq. (10.41), we can switch to dimensionless quantities with

$$\xi = \text{“xi (z)”} = \alpha x \tag{10.42}$$

with

$$\alpha = \sqrt{\frac{m\omega}{\hbar}} \tag{10.43}$$

This gives, with $\lambda = 2E/\hbar\omega$,

$$\frac{d^2u}{d\xi^2} + (\lambda - \xi^2)u = 0 \tag{10.44}$$

We can use polynomial series expansion methods to solve this, and find that we require a terminating expression, and write this in terms of the Hermite polynomials (courtesy of the clever French once again).

When all is said and done we will get the energy eigenvalues once again

$$E = E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{10.45}$$

10.5 BACK TO THE HEISENBERG PICTURE

Let us express

$$\langle x|n\rangle = u_n(x) \tag{10.46}$$

With

$$a\,|0\rangle = 0, \tag{10.47}$$

we have

$$0 = \left(X + i\frac{P}{m\omega}\right)|0\rangle\,, \tag{10.48}$$

and

$$\begin{aligned} 0 &= \langle x|\left(X + i\frac{P}{m\omega}\right)|0\rangle \\ &= \langle x|\,X\,|0\rangle + i\frac{1}{m\omega}\,\langle x|\,P\,|0\rangle \\ &= x\,\langle x|0\rangle + i\frac{1}{m\omega}\,\langle x|\,P\,|0\rangle \end{aligned} \tag{10.49}$$

Recall that our matrix operator is

$$\langle x'|\,P\,|x\rangle = \delta(x - x')\left(-i\hbar\frac{d}{dx}\right) \tag{10.50}$$

$$\begin{aligned} \langle x|\,P\,|0\rangle &= \langle x|\,P\overbrace{\boxed{\int |x'\rangle\langle x'|\,dx'}}^{=\,\mathbf{1}}|0\rangle \\ &= \int \langle x|\,P\,|x'\rangle\,\langle x'|0\rangle\,dx' \\ &= \int \delta(x - x')\left(-i\hbar\frac{d}{dx}\right)\langle x'|0\rangle\,dx' \\ &= \left(-i\hbar\frac{d}{dx}\right)\langle x|0\rangle \end{aligned} \tag{10.51}$$

We have then

$$0 = xu_0(x) + \frac{\hbar}{m\omega}\frac{du_0(x)}{dx} \tag{10.52}$$

NOTE: picture of the solution to this LDE on slide.... but I did not look closely enough.

10.6 PROBLEMS

Exercise 10.1 ([3] pr 9.1)

Assume $x(t)$ and $p(t)$ to be Heisenberg operators with $x(0) = x_0$ and $p(0) = p_0$. For a Hamiltonian corresponding to the harmonic oscillator show that

$$\begin{aligned} x(t) &= x_0 \cos \omega t + \frac{p_0}{m\omega} \sin \omega t \\ p(t) &= p_0 \cos \omega t - m\omega x_0 \sin \omega t. \end{aligned} \tag{10.53}$$

Answer for Exercise 10.1

Recall that the Hamiltonian operators were defined by factoring out the time evolution from a set of states

$$\langle \alpha(t) | A | \beta(t) \rangle = \langle \alpha(0) | e^{iHt/\hbar} A e^{-iHt/\hbar} | \beta(0) \rangle . \tag{10.54}$$

So one way to complete the task is to compute these exponential sandwiches. Recall from the appendix of chapter 10, that we have

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!} [A, [A, B]] + \cdots \tag{10.55}$$

Perhaps there is also some smarter way to do this, but lets first try the obvious way.

Let us summarize the variables we will work with

$$\begin{aligned} \alpha &= \sqrt{\frac{m\omega}{\hbar}} \\ X &= \frac{1}{\alpha\sqrt{2}}(a + a^\dagger) \\ P &= -i\hbar \frac{\alpha}{\sqrt{2}}(a - a^\dagger) \\ H &= \hbar\omega(a^\dagger a + 1/2) \\ \left[a, a^\dagger\right] &= 1 \end{aligned} \tag{10.56}$$

The operator in the exponential sandwich is

$$A = iHt/\hbar = i\omega t(a^\dagger a + 1/2) \tag{10.57}$$

Note that the constant 1/2 factor will commute with all operators, which reduces the computation required

$$\left[iHt/\hbar, B\right] = (i\omega t)\left[a^\dagger a, B\right] \tag{10.58}$$

For $B = X$, or $B = P$, we will want some intermediate results

$$\begin{aligned}\left[a^\dagger a, a\right] &= a^\dagger a a - a a^\dagger a \\ &= a^\dagger a a - (a^\dagger a + 1)a \\ &= -a,\end{aligned} \tag{10.59}$$

and

$$\begin{aligned}\left[a^\dagger a, a^\dagger\right] &= a^\dagger a a^\dagger - a^\dagger a^\dagger a \\ &= a^\dagger a a^\dagger - a^\dagger(a a^\dagger - 1) \\ &= a^\dagger\end{aligned} \tag{10.60}$$

Using these we can evaluate the commutators for the position and momentum operators. For position we have

$$\begin{aligned}\left[iHt/\hbar, X\right] &= (i\omega t)\frac{1}{\alpha\sqrt{2}}\left[a^\dagger a, a + a^\dagger\right] \\ &= (i\omega t)\frac{1}{\alpha\sqrt{2}}(-a + a^\dagger) \\ &= \frac{\omega t}{\alpha^2}\frac{-i\hbar\alpha}{\sqrt{2}}(a - a^\dagger).\end{aligned} \tag{10.61}$$

Since $\alpha^2\hbar = m\omega$, we have

$$\left[iHt/\hbar, X\right] = (\omega t)\frac{P}{m\omega}. \tag{10.62}$$

For the momentum operator we have

$$\begin{aligned}\left[iHt/\hbar, P\right] &= (i\omega t)\frac{-i\hbar\alpha}{\sqrt{2}}\left[a^\dagger a, a - a^\dagger\right] \\ &= (i\omega t)\frac{i\hbar\alpha}{\sqrt{2}}(a + a^\dagger) \\ &= (\omega t)(\hbar\alpha^2)X\end{aligned} \tag{10.63}$$

So we have

$$\left[iHt/\hbar, P\right] = (-\omega t)(m\omega)X \tag{10.64}$$

The expansion of the exponential series of nested commutators can now be written down by inspection and we get

$$X_H = X + (\omega t)\frac{P}{m\omega} - \frac{(\omega t)^2}{2!}X - \frac{(\omega t)^3}{3!}\frac{P}{m\omega} + \cdots \tag{10.65}$$

$$P_H = P - (\omega t)(m\omega)X - \frac{(\omega t)^2}{2!}P + \frac{(\omega t)^3}{3!}(m\omega)X + \cdots \tag{10.66}$$

Collection of terms gives us the desired answer

$$X_H = X\cos(\omega t) + \frac{P}{m\omega}\sin(\omega t) \tag{10.67}$$

$$P_H = P\cos(\omega t) - (m\omega)X\sin(\omega t) \tag{10.68}$$

Exercise 10.2 ([3] pr X.2)

On the basis of the results already derived for the harmonic oscillator, determine the energy eigenvalues and the ground-state wavefunction for the truncated oscillator

$$V(x) = \frac{1}{2}Kx^2\theta(x) \tag{10.69}$$

Answer for Exercise 10.2

We require $u(0) = 0$, so our solutions are limited to the truncated odd harmonic oscillator solutions. The normalization will be different since only the $x > 0$ integration range is significant. Our energy eigenvalues are

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega, n = 1, 3, 5, \cdots \tag{10.70}$$

And its wave function is

$$v_1(x) \propto u_1(x)\theta(x) = Axe^{-\alpha^2 x^2/2}\theta(x) \tag{10.71}$$

where $u_1(x)$ is the first odd wavefunction for the non-truncated oscillator. Normalizing this we find $A^2 \sqrt{\pi}/4\alpha^3 = 1$, or

$$v_1(x) = 2 \left(\frac{\alpha^3}{\sqrt{\pi}} \right)^{1/2} xe^{-\alpha^2 x^2/2}\theta(x) \tag{10.72}$$

Exercise 10.3 ([3] pr X.3)

Show that for the harmonic oscillator in the state $|n\rangle$, the following uncertainty product holds.

$$\Delta x \Delta p = \left(n + \frac{1}{2} \right) \hbar \tag{10.73}$$

Answer for Exercise 10.3

I tried this first explicitly with the first two wave functions

$$\begin{aligned} u_0(x) &= \left(\frac{\alpha^2}{\pi} \right)^{1/4} e^{-\alpha^2 x^2/2} \\ u_1(x) &= \sqrt{2\alpha^2} \left(\frac{\alpha^2}{\pi} \right)^{1/4} xe^{-\alpha^2 x^2/2} \end{aligned} \tag{10.74}$$

For the $|0\rangle$ state we find easily that $\langle X \rangle = 0$

$$\begin{aligned}
\langle 0| X |0\rangle &= \int dx \langle 0| X |x\rangle \langle x|0\rangle \\
&= \int dx x |\langle x|0\rangle|^2 \\
&= \int dx x |u_0(x)|^2 \\
&\propto \int dx x e^{-\alpha^2 x^2}
\end{aligned} \tag{10.75}$$

and this is zero since we are integrating an odd function over an even range (presuming that we take the principle value of the integral).

For the $|1\rangle$ state this we have

$$\langle 0| X |0\rangle \propto \int dx x^5 e^{-\alpha^2 x^2} = 0 \tag{10.76}$$

Since each $u_n(x)$ is a polynomial times a $e^{-\alpha^2 x^2/2}$ factor we have $\langle X \rangle = 0$ for all states $|n\rangle$.

The momentum expectation values for states $|0\rangle$ and $|1\rangle$ are also fairly simple to compute. We have

$$\begin{aligned}
\langle n| P |n\rangle &= \int dx \langle n| P |x\rangle \langle x|n\rangle \\
&= \int dx' dx \langle n|x'\rangle \langle x| P |x\rangle \langle x|n\rangle \\
&= -i\hbar \int dx' dx u_n^*(x') \delta(x - x') \frac{\partial}{\partial x} u_n(x) \\
&= -i\hbar \int dx u_n^*(x) \frac{\partial}{\partial x} u_n(x)
\end{aligned} \tag{10.77}$$

For the $|0\rangle$ state our derivative is odd since a factor of x is brought down, and we are again integrating an odd function over an even range. For the $|1\rangle$ case our derivative is proportional to

$$\frac{\partial}{\partial x} u_1(x) \propto \frac{\partial}{\partial x} \left(x e^{-\alpha^2 x^2} \right) = \left(1 - 2\alpha^2 x^2 \right) e^{-\alpha^2 x^2} \tag{10.78}$$

Again, this is an even function, while $u_1(x)$ is odd, so we have zero. Noting that we can express each $u_n(x)$ in terms of Hankel functions

$$u_n(x) = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2} H_n(\alpha x) e^{-\alpha^2 x^2/2} \tag{10.79}$$

where $H_{2n}(x)$ is even and $H_{2n-1}(x)$ is odd, we note that this expectation value will always be zero since we will have an even times odd function in the integration kernel.

Knowing that the position and momentum expectation values are zero reduces this problem to the calculation of $\langle n| X^2 |n\rangle \langle n| P^2 |n\rangle$. Either of these expectation values are again not too hard to compute for $n = 0, 1$. However, we now have to keep track of the proportionality constants. As expected this yields

$$\begin{aligned}\langle 0| X^2 |0\rangle \langle 0| P^2 |0\rangle &= \hbar^2/4 \\ \langle 1| X^2 |1\rangle \langle 1| P^2 |1\rangle &= 9\hbar^2/4\end{aligned} \tag{10.80}$$

These are respectively

$$\begin{aligned}\Delta x \Delta p &= \left(0 + \frac{1}{2}\right)\hbar \\ \Delta x \Delta p &= \left(1 + \frac{1}{2}\right)\hbar\end{aligned} \tag{10.81}$$

However, these integrals were only straightforward (albeit tedious) to calculate because we had explicit representations for $u_0(x)$ and $u_1(x)$. For the general wave function, what we have to work with is either the Hankel function representation of eq. (10.79) or the derivative form

$$u_n(x) = (-1)^n \left(\frac{\alpha}{\sqrt{\pi} 2^n n!}\right)^{1/2} e^{\alpha^2 x^2/2} \frac{d^n}{d(\alpha x)^n} e^{-\alpha^2 x^2} \tag{10.82}$$

Expanding this explicitly for arbitrary n is not going to be feasible. We can reduce the scope of the problem by trying to be lazy and see how some work can be avoided. One possible trick is noting that we can express the squared momentum expectation in terms of the Hamiltonian

$$\begin{aligned}\langle n| P^2 |n\rangle &= \langle n| 2m\left(H - \frac{1}{2} m\omega^2 X^2\right)|n\rangle \\ &= \left(n + \frac{1}{2}\right) 2m\hbar\omega - m^2\omega^2 \langle n| X^2 |n\rangle \\ &= \left(n + \frac{1}{2}\right) 2\hbar^2\alpha^2 - \hbar^2\alpha^4 \langle n| X^2 |n\rangle\end{aligned} \tag{10.83}$$

So we can get away with only calculating $\langle n| X^2 |n\rangle$, an exercise in integration by parts

$$\begin{aligned}
\langle n| X^2 |n\rangle &= \frac{\alpha}{\sqrt{\pi}2^n n!} \int dx x^2 e^{\alpha^2 x^2} \left(\frac{d^n}{d(\alpha x)^n} e^{-\alpha^2 x^2} \right)^2 \\
&= \frac{1}{\alpha^2 \sqrt{\pi}2^n n!} \int dy y^2 e^{y^2} \left(\frac{d^n}{dy^n} e^{-y^2} \right)^2 \\
&= \frac{1}{\alpha^2 \sqrt{\pi}2^n n!} \int dy \frac{1}{2} y \frac{d}{dy} e^{y^2} \left(\frac{d^n}{dy^n} e^{-y^2} \right)^2 \\
&= \frac{1}{\alpha^2 \sqrt{\pi}2^n n!} \frac{1}{-2} \int dy e^{y^2} \frac{d}{dy} \left(y \left(\frac{d^n}{dy^n} e^{-y^2} \right)^2 \right) \\
&= \frac{1}{\alpha^2 \sqrt{\pi}2^n n!} \frac{1}{-2} \int dy e^{y^2} \left(\left(\frac{d^n}{dy^n} e^{-y^2} \right)^2 + 2y \frac{d^n}{dy^n} e^{-y^2} \frac{d^{n+1}}{dy^{n+1}} e^{-y^2} \right) \\
&= -\frac{1}{2\alpha^2} - \frac{1}{\alpha^2 \sqrt{\pi}2^n n!} \frac{1}{2} \int dy \frac{d}{dy} e^{y^2} \frac{d^n}{dy^n} e^{-y^2} \frac{d^{n+1}}{dy^{n+1}} e^{-y^2} \\
&= -\frac{1}{2\alpha^2} + \frac{1}{\alpha^2 \sqrt{\pi}2^n n!} \frac{1}{2} \int dy e^{y^2} \left(\frac{d^{n+1}}{dy^{n+1}} e^{-y^2} \frac{d^{n+1}}{dy^{n+1}} e^{-y^2} + \frac{d^n}{dy^n} e^{-y^2} \frac{d^{n+2}}{dy^{n+2}} e^{-y^2} \right)
\end{aligned} \tag{10.84}$$

The second term in this remaining integral is proportional to $\langle n|n+2\rangle = 0$, which leaves us with

$$\langle n| X^2 |n\rangle = -\frac{1}{2\alpha^2} + \frac{n+1}{\alpha^2} = \frac{1}{\alpha^2}\left(n + \frac{1}{2}\right) \tag{10.85}$$

Our squared momentum expectation value is then

$$\begin{aligned}
\langle n| P^2 |n\rangle &= \left(n + \frac{1}{2}\right) 2\hbar^2\alpha^2 - \hbar^2\alpha^4 \langle n| X^2 |n\rangle \\
&= \left(n + \frac{1}{2}\right) \hbar^2\alpha^2
\end{aligned} \tag{10.86}$$

This completes the problem, and we are left with

$$\Delta x \Delta p = \left(n + \frac{1}{2}\right) \hbar. \tag{10.87}$$

Exercise 10.4 **([3] *pr X.4*)**

Consider the following two-dimensional harmonic oscillator problem:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial x^2} - \frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial y^2} + \frac{1}{2}K_1 x^2 u + \frac{1}{2}K_2 y^2 u = Eu \tag{10.88}$$

where (x, y) are the coordinates of the particle. Use the separation of variables technique to obtain the energy eigenvalues. Discuss the degeneracy in the eigenvalues if $K_1 = K_2$.

Answer for Exercise 10.4

Write $u = A(x)B(y)$. Substitute and dividing throughout by u we have

$$\left(-\frac{\hbar^2}{2m}\frac{A''}{A} + \frac{1}{2}K_1 x^2\right) + \left(-\frac{\hbar^2}{2m}\frac{B''}{B} + \frac{1}{2}K_2 y^2\right) = E \tag{10.89}$$

Introduction of a pair of constants E_1, E_2 for each of the independent terms we have

$$\begin{aligned} H_1 A &= -\frac{\hbar^2}{2m}A'' + \frac{1}{2}K_1 x^2 A = E_1 A \\ H_2 B &= -\frac{\hbar^2}{2m}B'' + \frac{1}{2}K_1 y^2 B = E_2 B \\ H &= H_1 + H_2 \\ E &= E_1 + E_2 \end{aligned} \tag{10.90}$$

For each of these equations we have a set of quantized eigenvalues and can write

$$\begin{aligned} E_{1m} &= \left(m + \frac{1}{2}\right)\hbar\sqrt{\frac{K_1}{m}} \\ E_{2n} &= \left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{K_2}{m}} \\ H_1 A_m(x) &= E_{1m} A_m(x) \\ H_2 A_n(y) &= E_{2n} B_n(y) \end{aligned} \tag{10.91}$$

The complete eigenstates are then

$$u_{mn}(x, y) = A_m(x)B_n(y) \tag{10.92}$$

with total energy satisfying

$$Hu_{mn}(x, y) = \frac{\hbar}{\sqrt{m}}\left(\left(m + \frac{1}{2}\right)\sqrt{K_1} + \left(n + \frac{1}{2}\right)\sqrt{K_2}\right)u_{mn}(x, y) \tag{10.93}$$

A general state requires a double sum over the possible combinations of states $\Psi = \sum_{mn} c_{mn} u_{mn}$, however if $K_1 = K_2 = K$, we cannot distinguish between u_{mn} and u_{nm} based on the energy eigenvalues

$$Hu_{mn}(x,y) = \hbar\sqrt{\frac{K}{m}}\,(m+n+1)\,u_{mn}(x,y) = Hu_{nm}(x,y) \tag{10.94}$$

In this case, we can write the wave function corresponding to a general state for the system as just $\Psi = \sum_{m+n=\text{constant}} c_{mn} u_{mn}$. This reduction in the cardinality of this set of basis eigenstates is the degeneracy to be discussed.

Exercise 10.5 *([3] pr X.5,6)*

Consider now a variation on Problem 4 in which we have a coupled oscillator with the potential given by

$$V(x,y) = \frac{1}{2}K(x^2 + y^2 + 2\lambda xy) \tag{10.95}$$

Obtain the energy eigenvalues by changing variables (x,y) to (x',y') such that the new potential is quadratic in (x',y'), without the coupling term.

Answer for Exercise 10.5

This has the look of a diagonalization problem so we write the potential in matrix form

$$V(x,y) = \frac{1}{2}K\begin{bmatrix} x & y \end{bmatrix}\begin{bmatrix} 1 & \lambda \\ \lambda & 1 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \frac{1}{2}K\tilde{X}MX \tag{10.96}$$

The similarity transformation required is

$$M = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} 1+\lambda & 0 \\ 0 & 1-\lambda \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{10.97}$$

Our change of variables is therefore

$$X' = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}X = \frac{1}{\sqrt{2}}\begin{bmatrix} x+y \\ x-y \end{bmatrix} \tag{10.98}$$

Our Laplacian should also remain diagonal under this orthonormal transformation, but we can verify this by expanding out the partials explicitly

$$\begin{aligned} \frac{\partial}{\partial x} &= \frac{\partial x'}{\partial x}\frac{\partial}{\partial x'} + \frac{\partial y'}{\partial x}\frac{\partial}{\partial y'} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial x'} + \frac{\partial}{\partial y'}\right) \\ \frac{\partial}{\partial y} &= \frac{\partial x'}{\partial y}\frac{\partial}{\partial x'} + \frac{\partial y'}{\partial y}\frac{\partial}{\partial y'} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial x'} - \frac{\partial}{\partial y'}\right) \end{aligned} \tag{10.99}$$

Squaring and summing we have

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{1}{2}\left(\frac{\partial}{\partial x'} + \frac{\partial}{\partial y'}\right)^2 + \frac{1}{2}\left(\frac{\partial}{\partial x'} - \frac{\partial}{\partial y'}\right)^2 = \frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2} \tag{10.100}$$

Our transformed Hamiltonian operator is thus

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial x'^2} - \frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial y'^2} + \frac{1}{2}K(1+\lambda)x'^2 u + \frac{1}{2}K(1-\lambda)y'^2 u = Eu \tag{10.101}$$

So, provided $|\lambda| < 1$, the energy eigenvalue equation is given by eq. (10.93) with $K_1 = K(1+\lambda)$, and $K_2 = K(1-\lambda)$.

Exercise 10.6 ([3] pr X.7)

Consider two coupled harmonic oscillators in one dimension of natural length a and spring constant K connecting three particles located at x_1, x_2, and x_3. The corresponding Schrödinger equation is given as

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial {x_1}^2} - \frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial {x_2}^2} - \frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial {x_3}^2} + \frac{K}{2}\left((x_2 - x_1 - a)^2 + (x_3 - x_2 - a)^2\right)u = Eu \tag{10.102}$$

Obtain the energy eigenvalues using the matrix method.

Answer for Exercise 10.6

Let us start with an initial simplifying substitution to get rid of the factors of a. Write

$$\begin{aligned} r_1 &= x_1 + a \\ r_2 &= x_2 \\ r_3 &= x_3 - a \end{aligned} \tag{10.103}$$

These were picked so that the differences in our quadratic terms involve only factors of r_k

$$\begin{aligned} x_2 - x_1 - a &= r_2 - r_1 \\ x_3 - x_2 - a &= r_3 - r_2 \end{aligned} \tag{10.104}$$

Schrödinger's equation is now

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial {r_1}^2} - \frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial {r_2}^2} - \frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial {r_3}^2} + \frac{K}{2}\left((r_2 - r_1)^2 + (r_3 - r_2)^2\right)u = Eu \tag{10.105}$$

Putting our potential into matrix form, we have

$$V(r_1, r_2, r_3) = \frac{K}{2}\left((r_2 - r_1)^2 + (r_3 - r_2)^2\right) = \frac{K}{2}\begin{bmatrix} r_1 & r_2 & r_3 \end{bmatrix}\begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}\begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} \tag{10.106}$$

This symmetric matrix, let us call it M

$$M = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix} \tag{10.107}$$

has eigenvalues 0, 1, 3, with orthonormal eigenvectors

$$\begin{aligned} e_0 &= \frac{1}{\sqrt{3}}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \\ e_1 &= \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \\ e_3 &= \frac{1}{\sqrt{6}}\begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} \end{aligned} \tag{10.108}$$

Writing

$$U = [e_0 e_1 e_3] = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & 0 & -\frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \end{bmatrix} \tag{10.109}$$

$$M = U\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix}\tilde{U} = UD\tilde{U} \tag{10.110}$$

Writing $R' = \tilde{U}R$, and $\boldsymbol{\nabla}' = \tilde{U}\boldsymbol{\nabla}$, we see that the Laplacian has no mixed partial terms after transformation

$$\begin{aligned}
\boldsymbol{\nabla}' \cdot \boldsymbol{\nabla}' &= \widetilde{(\tilde{U}\boldsymbol{\nabla})}\tilde{U}\boldsymbol{\nabla} \\
&= \tilde{\boldsymbol{\nabla}}\boldsymbol{\nabla} \\
&= \boldsymbol{\nabla} \cdot \boldsymbol{\nabla}
\end{aligned} \tag{10.111}$$

Schrödinger's equation is then just

$$\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}'^2 + \frac{K}{2}\tilde{R}'DR'\right)u = Eu \tag{10.112}$$

Or

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial {r'_1}^2} - \frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial {r'_2}^2} - \frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial {r'_3}^2} + \frac{K}{2}\left({r'_2}^2 + 3{r'_3}^2\right)u = Eu \tag{10.113}$$

Separation of variables provides us with one free particle wave equation, and two harmonic oscillator equations

$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{\partial^2 u_1}{\partial {r'_1}^2} &= E_1 u_1 \\
-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial {r'_2}^2} + \frac{K}{2}{r'_2}^2 u_2 &= E_2 u_2 \\
-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial {r'_3}^2} + \frac{3K}{2}{r'_3}^2 u_3 &= E_3 u_3
\end{aligned} \tag{10.114}$$

We can borrow the Harmonic oscillator energy eigenvalues from problem 4 again with $K_1 = K$, and $K_2 = 3K$.

Exercise 10.7 ([3] pr X.8)

As a variation of Problem 7 assume that the middle particle at x_2 has a different mass M. Reduce this problem to the form of Problem 7 by a scale change in x_2 and then use the matrix method to obtain the energy eigenvalues.

Answer for Exercise 10.7

We write $\sqrt{M}x_2 = \sqrt{m}x'_2, x_1 + a = x'_1, x_3 - a = x'_3$, and then Schrödinger's equation takes the form

$$\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}'^2 + V(X')\right)u = Eu \tag{10.115}$$

$$V(X') = \frac{K}{2}\left(\left(\sqrt{\frac{m}{M}}x_2' - x_1'\right)^2 + \left(-\sqrt{\frac{m}{M}}x_2' + x_3'\right)^2\right) \tag{10.116}$$

With $\mu = \sqrt{m/M}$, we have

$$V(X') = \frac{K}{2}\tilde{X}'\begin{bmatrix} 1 & -\mu & 0 \\ -\mu & 2\mu^2 & -\mu \\ 0 & -\mu & 1 \end{bmatrix}X' \tag{10.117}$$

We find that this symmetric matrix has eigenvalues $0, 1, 1+2\mu^2$, and eigenvectors

$$\begin{aligned}
e_0 &= \frac{1}{\sqrt{1+2\mu^2}}\begin{bmatrix} \mu \\ 1 \\ \mu \end{bmatrix} \\
e_1 &= \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \\
e_{1+2\mu^2} &= \frac{1}{\sqrt{2+4\mu^2}}\begin{bmatrix} 1 \\ -2\mu \\ 1 \end{bmatrix}
\end{aligned} \tag{10.118}$$

The rest of the problem is now no different than the tail end of Problem 7, and we end up with $K_1 = K$, $K_2 = (1+2\mu^2)K$.

Exercise 10.8 ps V. p1.

A particle of mass m moves along the x-direction such that $V(X) = \frac{1}{2}KX^2$. Is the state

$$u(\xi) = B\xi e^{+\xi^2/2}, \tag{10.119}$$

where ξ is given by Eq. (9.60), B is a constant, and time $t = 0$, an energy eigenstate of the system? What is probability per unit length for measuring the particle at position $x = 0$ at $t = t_0 > 0$? Explain the physical meaning of the above results.

Answer for Exercise 10.8

Is this state an energy eigenstate? Recall that $\xi = \alpha x$, $\alpha = \sqrt{m\omega/\hbar}$, and $K = m\omega^2$. With this variable substitution Schrödinger's equation for this harmonic oscillator potential takes the form

$$\frac{d^2 u}{d\xi^2} - \xi^2 u = -\frac{2E}{\hbar\omega} u \tag{10.120}$$

While we can blindly substitute a function of the form $\xi e^{\xi^2/2}$ into this to get

$$\begin{aligned}\frac{1}{B}\left(\frac{d^2 u}{d\xi^2} - \xi^2 u\right) &= \frac{d}{d\xi}\left(1+\xi^2\right)e^{\xi^2/2} - \xi^3 e^{\xi^2/2} \\ &= \left(2\xi + \xi + \xi^3\right)e^{\xi^2/2} - \xi^3 e^{\xi^2/2} \\ &= 3\xi e^{\xi^2/2}\end{aligned} \tag{10.121}$$

and formally make the identification $E = -3\omega\hbar/2 = -(1+1/2)\omega\hbar$, this is not a normalizable wavefunction, and has no physical relevance, unless we set $B = 0$.

By changing the problem, this state could be physically relevant. We would require a potential of the form

$$V(x) = \begin{cases} f(x) & \text{if } x < a \\ \frac{1}{2}Kx^2 & \text{if } a < x < b \\ g(x) & \text{if } x > b \end{cases} \tag{10.122}$$

For example, $f(x) = V_1, g(x) = V_2$, for constant V_1, V_2. For such a potential, within the harmonic well, a general solution of the form

$$u(x,t) = \sum_n H_n(\xi)(A_n e^{-\xi^2/2} + B_n e^{\xi^2/2})e^{-iE_n t/\hbar}, \tag{10.123}$$

is possible since normalization would not prohibit non-zero B_n values in that situation. For the wave function to be a physically relevant, we require it to be (absolute) square integrable, and must also integrate to unity over the entire interval.

Probability per unit length at $x = 0$ We cannot answer the question for the probability that the particle is found at the specific $x = 0$ position at $t = t_0$ (that probability is zero in a continuous space), but we can answer the question for the probability that a particle is found in an interval surrounding a specific point at this time. By calculating the average of the probability to find the particle in an interval, and dividing by that interval's length, we arrive at plausible definition of probability per unit length for an interval surrounding $x = x_0$

$$P = \text{Probability per unit length near } x = x_0 = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{x_0 - \epsilon/2}^{x_0 + \epsilon/2} |\Psi(x, t_0)|^2 dx = |\Psi(x_0, t_0)|^2 \tag{10.124}$$

By this definition, the probability per unit length is just the probability density itself, evaluated at the point of interest.

Physically, for an interval small enough that the probability density is constant in magnitude over that interval, this probability per unit length times the length of this small interval, represents the probability that we will find the particle in that interval.

Probability per unit length for the non-normalizable state given It seems possible, albeit odd, that this question is asking for the probability per unit length for the non-normalizable E_1 wavefunction eq. (10.119). Since normalization requires $B = 0$, that probability density is simply zero (or undefined, depending on one's point of view).

Probability per unit length for some more interesting harmonic oscillator states Suppose we form the wavefunction for a superposition of all the normalizable states

$$u(x, t) = \sum_n A_n H_n(\xi) e^{-\xi^2/2} e^{-iE_n t/\hbar} \tag{10.125}$$

Here it is assumed that the A_n coefficients yield unit probability

$$\int |u(x, 0)|^2 dx = \sum_n |A_n|^2 = 1 \tag{10.126}$$

For the impure state of eq. (10.125) we have for the probability density

$$
\begin{aligned}
|u|^2 &= \sum_{m,n} A_n A_m^* H_n(\xi) H_m(\xi) e^{-\xi^2} e^{-i(E_n - E_m)t_0/\hbar} \\
&= \sum_n |A_n|^2 (H_n(\xi))^2 e^{-\xi^2} + \sum_{m \neq n} A_n A_m^* H_n(\xi) H_m(\xi) e^{-\xi^2} e^{-i(E_n - E_m)t_0/\hbar} \\
&= \sum_n |A_n|^2 (H_n(\xi))^2 e^{-\xi^2} + \sum_{m \neq n} A_n A_m^* H_n(\xi) H_m(\xi) e^{-\xi^2} e^{-i(E_n - E_m)t_0/\hbar} \\
&= \sum_n |A_n|^2 (H_n(\xi))^2 e^{-\xi^2} \\
&\quad + \sum_{m<n} H_n(\xi) H_m(\xi) \left(A_n A_m^* e^{-\xi^2} e^{-i(E_n - E_m)t_0/\hbar} + A_m A_n^* e^{-\xi^2} e^{-i(E_m - E_n)t_0/\hbar} \right) \\
&= \sum_n |A_n|^2 (H_n(\xi))^2 e^{-\xi^2} + 2 \sum_{m<n} H_n(\xi) H_m(\xi) e^{-\xi^2} \operatorname{Re}\left(A_n A_m^* e^{-i(E_n - E_m)t_0/\hbar} \right) \\
&= \sum_n |A_n|^2 (H_n(\xi))^2 e^{-\xi^2} \\
&\quad + 2 \sum_{m<n} H_n(\xi) H_m(\xi) e^{-\xi^2} \left(\operatorname{Re}(A_n A_m^*) \cos((n-m)\omega t_0) + \operatorname{Im}(A_n A_m^*) \sin((n-m)\omega t_0) \right)
\end{aligned}
\tag{10.127}
$$

Evaluation at the point $x = 0$, we have

$$
\begin{aligned}
|u(0, t_0)|^2 &= \sum_n |A_n|^2 (H_n(0))^2 \\
&\quad + 2 \sum_{m<n} H_n(0) H_m(0) \left(\operatorname{Re}(A_n A_m^*) \cos((n-m)\omega t_0) + \operatorname{Im}(A_n A_m^*) \sin((n-m)\omega t_0) \right)
\end{aligned}
\tag{10.128}
$$

It is interesting that the probability per unit length only has time dependence for a mixed state.

For a pure state and its wavefunction $u(x, t) = N_n H_n(\xi) e^{-\xi^2/2} e^{-iE_n t/\hbar}$ we have just

$$
|u(0, t_0)|^2 = N_n^2 (H_n(0))^2 = \frac{\alpha}{\sqrt{\pi} 2^n n!} H_n(0)^2 \tag{10.129}
$$

This is zero for odd n. For even n is appears that $(H_n(0))^2$ may equal 2^n (this is true at least up to n=4). If that is the case, we have for non-mixed states, with even numbered energy quantum numbers, at $x = 0$ a probability per unit length value of $|u(0, t_0)|^2 = \frac{\alpha}{\sqrt{\pi} n!}$.

Grading notes I lost 3/10 marks on this assignment. Two of these due to a sign error in eq. (10.120) (now corrected).

One mark lost for the sign error itself, and one for the conclusion that could have been drawn from the negative energy:

"Without that sign error, $E - -3\hbar\omega < V_{\text{min}} = 0$, so clearly not physical since a particle has to have at least as much energy as the potential."

It was also pointed out that in the discussion of probability per unit length, the $B = 0$ condition means no wave function, and thus no particle, and that undefined is the way to discuss this since it does not make sense to ask about a probability for this particle.

The last mark lost was due to my explaination associated with the modified potential eq. (10.122). I did not clearly explain that this modified potential would not have the wave function of eq. (10.119) since it must be different outside of the harmonic interval. What they wanted to see explained is that one must modify the wave function (for example, by introducing a cut off), for it to be normalizable. In my eyes, it then would not be a solution to the original Hamiltonian equation, so if you want solutions that include both positive and negative coefficients in the exponentials, you would also have to have a modified potential. Given the sign error that was also made, and the negative energy associated with the wave function eq. (10.119) I am not so sure that any modify-the-wave-function argument is even appropriate.

Also note that the question was not asking for elaboration on the "more interesting normalizable states". Basically, the intent was to to ask for just discussion on the un-normalizable aspects of the proposed wave function as if it was a real one. That seemed too easy to me (but obviously keeping track of my signs was not too easy).

Exercise 10.9 Free particle propagator (2007 PHY355H1F 1f)

For a free particle moving in one-dimension, the propagator (i.e. the coordinate representation of the evolution operator),

$$G(x, x'; t) = \langle x | U(t) \left| x' \right\rangle \tag{10.130}$$

is given by

$$G(x, x'; t) = \sqrt{\frac{m}{2\pi i \hbar t}} e^{im(x-x')^2/(2\hbar t)}. \tag{10.131}$$

Answer for Exercise 10.9

This problem is actually fairly straightforward, but it is nice to work it having had a similar problem set question where we were asked about this time evolution operator matrix element (ie: what it is physical meaning is). Here we have a concrete example of the form of this matrix operator.

Proceeding directly, we have

$$
\begin{aligned}
\langle x| U \left|x'\right\rangle &= \int \langle x|p'\rangle \left\langle p'\right| U |p\rangle \langle p|x'\rangle \, dp dp' \\
&= \int u_{p'}(x) \left\langle p'\right| e^{-iP^2 t/(2m\hbar)} |p\rangle \, u_p^*(x') dp dp' \\
&= \int u_{p'}(x) e^{-ip^2 t/(2m\hbar)} \delta(p - p') u_p^*(x') dp dp' \\
&= \int u_p(x) e^{-ip^2 t/(2m\hbar)} u_p^*(x') dp \\
&= \frac{1}{(\sqrt{2\pi\hbar})^2} \int e^{ip(x-x')/\hbar} e^{-ip^2 t/(2m\hbar)} dp \\
&= \frac{1}{2\pi\hbar} \int e^{ip(x-x')/\hbar} e^{-ip^2 t/(2m\hbar)} dp \\
&= \frac{1}{2\pi} \int e^{ik(x-x')} e^{-i\hbar k^2 t/(2m)} dk \\
&= \frac{1}{2\pi} \int dk e^{-\left(k^2 \frac{i\hbar t}{2m} - ik(x-x')\right)} \\
&= \frac{1}{2\pi} \int dk e^{-\frac{i\hbar t}{2m}\left(k - i\frac{2m}{i\hbar t}\frac{(x-x')}{2}\right)^2 - \frac{i^2 2m (x-x')^2}{4 i\hbar t}} \\
&= \frac{1}{2\pi} \sqrt{\pi} \sqrt{\frac{2m}{i\hbar t}} e^{\frac{im(x-x')^2}{2\hbar t}},
\end{aligned}
\tag{10.132}
$$

which is the desired result. Now, let us look at how this would be used. We can express our time evolved state using this matrix element by introducing an identity

$$
\begin{aligned}
\langle x|\psi(t)\rangle &= \langle x| U |\psi(0)\rangle \\
&= \int dx' \langle x| U \left|x'\right\rangle \langle x'|\psi(0)\rangle \\
&= \sqrt{\frac{m}{2\pi i\hbar t}} \int dx' e^{im(x-x')^2/(2\hbar t)} \langle x'|\psi(0)\rangle
\end{aligned}
\tag{10.133}
$$

This gives us

$$
\psi(x,t) = \sqrt{\frac{m}{2\pi i\hbar t}} \int dx' e^{im(x-x')^2/(2\hbar t)} \psi(x', 0)
\tag{10.134}
$$

However, note that our free particle wave function at time zero is

$$\psi(x,0) = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \tag{10.135}$$

So the convolution integral eq. (10.134) does not exist. We likely have to require that the solution be not a pure state, but instead a superposition of a set of continuous states (a wave packet in position or momentum space related by Fourier transforms). That is

$$\begin{aligned}
\psi(x,0) &= \frac{1}{\sqrt{2\pi\hbar}} \int \hat{\psi}(p,0) e^{ipx/\hbar} dp \\
\hat{\psi}(p,0) &= \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x'',0) e^{-ipx''/\hbar} dx''
\end{aligned} \tag{10.136}$$

The time evolution of this wave packet is then determined by the propagator, and is

$$\psi(x,t) = \sqrt{\frac{m}{2\pi i\hbar t}} \frac{1}{\sqrt{2\pi\hbar}} \int dx' dp e^{im(x-x')^2/(2\hbar t)} \hat{\psi}(p,0) e^{ipx'/\hbar}, \tag{10.137}$$

or in terms of the position space wave packet evaluated at time zero

$$\psi(x,t) = \sqrt{\frac{m}{2\pi i\hbar t}} \frac{1}{2\pi} \int dx' dx'' dk e^{im(x-x')^2/(2\hbar t)} e^{ik(x'-x'')} \psi(x'',0) \tag{10.138}$$

We see that the propagator also ends up with a Fourier transform structure, and we have

$$\begin{aligned}
\psi(x,t) &= \int dx' U(x,x';t) \psi(x',0) \\
U(x,x';t) &= \sqrt{\frac{m}{2\pi i\hbar t}} \frac{1}{2\pi} \int du dk e^{im(x-x'-u)^2/(2\hbar t)} e^{iku}
\end{aligned} \tag{10.139}$$

Does that Fourier transform exist? I had not be surprised if it ended up with a delta function representation. I will hold off attempting to evaluate and reduce it until another day.

Exercise 10.10 Eigenvectors of the Harmonic oscillator creation operator (2008 PHY355H1F final 1

Prove that the only eigenvector of the Harmonic oscillator creation operator is $|\text{null}\rangle$.

Answer for Exercise 10.10

Recall that the creation (raising) operator was given by

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}X - \frac{i}{\sqrt{2m\omega\hbar}}P = \frac{1}{\alpha\sqrt{2}}X - \frac{i\alpha}{\sqrt{2}\hbar}P, \tag{10.140}$$

where $\alpha = \sqrt{\hbar/m\omega}$. Now assume that $a^\dagger|\phi\rangle = \lambda|\phi\rangle$ so that

$$\langle x| a^\dagger |\phi\rangle = \langle x| \lambda |\phi\rangle. \tag{10.141}$$

Write $\langle x|\phi\rangle = \phi(x)$, and expand the LHS using eq. (10.140) for

$$\begin{aligned}\lambda\phi(x) &= \langle x| a^\dagger |\phi\rangle \\ &= \langle x| \left(\frac{1}{\alpha\sqrt{2}}X - \frac{i\alpha}{\sqrt{2}\hbar}P\right)|\phi\rangle \\ &= \frac{x\phi(x)}{\alpha\sqrt{2}} - \frac{i\alpha}{\sqrt{2}\hbar}(-i\hbar)\frac{\partial}{\partial x}\phi(x) \\ &= \frac{x\phi(x)}{\alpha\sqrt{2}} - \frac{\alpha}{\sqrt{2}}\frac{\partial\phi(x)}{\partial x}.\end{aligned} \tag{10.142}$$

As usual write $\xi = x/\alpha$, and rearrange. This gives us

$$\frac{\partial\phi}{\partial\xi} + \sqrt{2}\lambda\phi - \xi\phi = 0. \tag{10.143}$$

Observe that this can be viewed as a homogeneous LDE of the form

$$\frac{\partial\phi}{\partial\xi} - \xi\phi = 0, \tag{10.144}$$

augmented by a forcing term $\sqrt{2}\lambda\phi$. The homogeneous equation has the solution $\phi = Ae^{\xi^2/2}$, so for the complete equation we assume a solution

$$\phi(\xi) = A(\xi)e^{\xi^2/2}. \tag{10.145}$$

Since $\phi' = (A' + A\xi)e^{\xi^2/2}$, we produce a LDE of

$$\begin{aligned}0 &= (A' + A\xi - \xi A + \sqrt{2}\lambda A)e^{\xi^2/2} \\ &= (A' + \sqrt{2}\lambda A)e^{\xi^2/2},\end{aligned} \tag{10.146}$$

or

$$0 = A' + \sqrt{2}\lambda A. \tag{10.147}$$

This has solution $A = Be^{-\sqrt{2}\lambda\xi}$, so our solution for eq. (10.143) is

$$\phi(\xi) = Be^{\xi^2/2 - \sqrt{2}\lambda\xi} = B' e^{(\xi - \lambda\sqrt{2})^2/2}. \tag{10.148}$$

This wave function is an imaginary Gaussian with minimum at $\xi = \lambda\sqrt{2}$. It is also unnormalizable since we require $B' = 0$ for any λ if $\int |\phi|^2 < \infty$. Since $\langle \xi | \phi \rangle = \phi(\xi) = 0$, we must also have $|\phi\rangle = 0$, completing the exercise.

Exercise 10.11 One dimensional harmonic oscillator (2008 PHY355H1F final 3.)

Consider a one-dimensional harmonic oscillator with the Hamiltonian

$$H = \frac{1}{2m} P^2 + \frac{1}{2} m\omega^2 X^2 \tag{10.149}$$

Denote the ground state of the system by $|0\rangle$, the first excited state by $|1\rangle$ and so on.

a. Evaluate $\langle n| X |n\rangle$ and $\langle n| X^2 |n\rangle$ for arbitrary $|n\rangle$.

b. Suppose that at $t = 0$ the system is prepared in the state

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i\,|1\rangle). \tag{10.150}$$

If a measurement of position X were performed immediately, sketch the probability distribution $P(x)$ that a particle would be found within dx of x. Justify how you construct the sketch.

c. Now suppose the state given in (b) above were allowed to evolve for a time t, determine the expectation value of X and ΔX at that time.

d. Now suppose that initially the system were prepared in the ground state $|0\rangle$, and then the resonance frequency is changed abruptly from ω to ω' so that the Hamiltonian becomes

$$H = \frac{1}{2m} P^2 + \frac{1}{2} m{\omega'}^2 X^2. \tag{10.151}$$

Immediately, an energy measurement is performed ; what is the probability of obtaining the result $E = \hbar\omega'(3/2)$?

Answer for Exercise 10.11

Part a. Writing X in terms of the raising and lowering operators we have

$$X = \frac{\alpha}{\sqrt{2}}(a^\dagger + a), \tag{10.152}$$

so $\langle X \rangle$ is proportional to

$$\langle n| a^\dagger + a |n\rangle = \sqrt{n+1}\,\langle n|n+1\rangle + \sqrt{n}\,\langle n|n-1\rangle = 0. \tag{10.153}$$

For $\left\langle X^2 \right\rangle$ we have

$$\begin{aligned}
\left\langle X^2 \right\rangle &= \frac{\alpha^2}{2}\,\langle n|\,(a^\dagger + a)(a^\dagger + a)\,|n\rangle \\
&= \frac{\alpha^2}{2}\,\langle n|\,(a^\dagger + a)\Big(\sqrt{n+1}\,|n+1\rangle + \sqrt{n-1}\,|n-1\rangle\Big) \\
&= \frac{\alpha^2}{2}\,\langle n|\,\big((n+1)\,|n\rangle + \sqrt{n(n-1)}\,|n-2\rangle + \sqrt{(n+1)(n+2)}\,|n+2\rangle + n\,|n\rangle\big).
\end{aligned} \tag{10.154}$$

We are left with just

$$\left\langle X^2 \right\rangle = \frac{\hbar}{2m\omega}(2n+1). \tag{10.155}$$

Part b. The probability that we started in state $|\psi(0)\rangle$ and ended up in position x is governed by the amplitude $\langle x|\psi(0)\rangle$, and the probability of being within an interval Δx, surrounding the point x is given by

$$\int_{x'=x-\Delta x/2}^{x+\Delta x/2} \left|\langle x'|\psi(0)\rangle\right|^2 dx'. \tag{10.156}$$

In the limit as $\Delta x \to 0$, this is just the squared amplitude itself evaluated at the point x, so we are interested in the quantity

$$|\langle x|\psi(0)\rangle|^2 = \frac{1}{2}|\langle x|0\rangle + i\,\langle x|1\rangle|^2. \tag{10.157}$$

We are given these wave functions in the supplemental formulas. Namely,

$$\begin{aligned}\langle x|0\rangle &= \psi_0(x) = \frac{e^{-x^2/2\alpha^2}}{\sqrt{\alpha\sqrt{\pi}}}\\ \langle x|1\rangle &= \psi_1(x) = \frac{e^{-x^2/2\alpha^2}2x}{\alpha\sqrt{2\alpha\sqrt{\pi}}}.\end{aligned} \tag{10.158}$$

Substituting these into eq. (10.157) we have

$$|\langle x|\psi(0)\rangle|^2 = \frac{1}{2}e^{-x^2/\alpha^2}\frac{1}{\alpha\sqrt{\pi}}\left|1+\frac{2ix}{\alpha\sqrt{2}}\right|^2 = \frac{e^{-x^2/\alpha^2}}{2\alpha\sqrt{\pi}}\left(1+\frac{2x^2}{\alpha^2}\right). \tag{10.159}$$

This is parabolic near the origin and then quickly tapers off.

Part c. Our time evolved state is

$$U(t)|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(e^{-i\hbar\omega\left(0+\frac{1}{2}\right)t/\hbar}|0\rangle + ie^{-i\hbar\omega\left(1+\frac{1}{2}\right)t/\hbar}|0\rangle\right) = \frac{1}{\sqrt{2}}\left(e^{-i\omega t/2}|0\rangle + ie^{-3i\omega t/2}|1\rangle\right). \tag{10.160}$$

The position expectation is therefore

$$\langle\psi(t)|X|\psi(t)\rangle = \frac{\alpha}{2\sqrt{2}}\left(e^{i\omega t/2}\langle 0| - ie^{3i\omega t/2}\langle 1|\right)(a^\dagger + a)\left(e^{-i\omega t/2}|0\rangle + ie^{-3i\omega t/2}|1\rangle\right) \tag{10.161}$$

We have already demonstrated that $\langle n|X|n\rangle = 0$, so we must only expand the cross terms, but those are just $\langle 0|a^\dagger + a|1\rangle = 1$. This leaves

$$\langle\psi(t)|X|\psi(t)\rangle = \frac{\alpha}{2\sqrt{2}}\left(-ie^{i\omega t} + ie^{-i\omega t}\right) = \sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t) \tag{10.162}$$

For the squared position expectation

$$\begin{aligned}\langle\psi(t)|X^2|\psi(t)\rangle &= \frac{\alpha^2}{4(2)}\left(e^{i\omega t/2}\langle 0| - ie^{3i\omega t/2}\langle 1|\right)(a^\dagger + a)^2\left(e^{-i\omega t/2}|0\rangle + ie^{-3i\omega t/2}|1\rangle\right)\\ &= \frac{1}{2}(\langle 0|X^2|0\rangle + \langle 1|X^2|1\rangle) + i\frac{\alpha^2}{8}(-e^{i\omega t}\langle 1|(a^\dagger + a)^2|0\rangle + e^{-i\omega t}\langle 0|(a^\dagger + a)^2|1\rangle)\end{aligned}$$

$$(10.163)$$

Noting that $(a^\dagger + a)|0\rangle = |1\rangle$, and $(a^\dagger + a)^2 |0\rangle = (a^\dagger + a)|1\rangle = \sqrt{2}|2\rangle + |0\rangle$, so we see the last two terms are zero. The first two we can evaluate using our previous result eq. (10.155) which was $\left\langle X^2 \right\rangle = \frac{\alpha^2}{2}(2n+1)$. This leaves

$$\langle\psi(t)| X^2 |\psi(t)\rangle = \alpha^2 \tag{10.164}$$

Since $\langle X\rangle^2 = \alpha^2 \cos^2(\omega t)/2$, we have

$$(\Delta X)^2 = \left\langle X^2 \right\rangle - \langle X\rangle^2 = \alpha^2 \left(1 - \frac{1}{2}\cos^2(\omega t)\right) \tag{10.165}$$

Part d. This energy measurement $E = \hbar\omega'(3/2) = \hbar\omega'(1 + 1/2)$, corresponds to an observation of state $|1'\rangle$, after an initial observation of $|0\rangle$. The probability of such a measurement is

$$\left|\langle 1'|0\rangle\right|^2 \tag{10.166}$$

Note that

$$\begin{aligned}\langle 1'|0\rangle &= \int dx \langle 1'|x\rangle \langle x|0\rangle \\ &= \int dx \psi_{1'}^* \psi_0(x)\end{aligned} \tag{10.167}$$

The wave functions above are

$$\begin{aligned}\phi_{1'}(x) &= \frac{2xe^{-x^2/2\alpha'^2}}{\alpha'\sqrt{2\alpha'\sqrt{\pi}}} \\ \phi_0(x) &= \frac{e^{-x^2/2\alpha^2}}{\sqrt{\alpha\sqrt{\pi}}}\end{aligned} \tag{10.168}$$

Putting the pieces together we have

$$\langle 1'|0\rangle = \frac{2}{\alpha'\sqrt{2\alpha'\alpha\pi}} \int dx x e^{-\frac{x^2}{2}\left(\frac{1}{\alpha'^2} + \frac{1}{\alpha^2}\right)} \tag{10.169}$$

Since this is an odd integral kernel over an even range, this evaluates to zero, and we conclude that the probability of measuring the specified energy is zero when the system is initially prepared in the ground state associated with the original Hamiltonian. Intuitively this makes some sense, if one thinks of the Fourier coefficient problem: one cannot construct an even function from linear combinations of purely odd functions.

11

COHERENT STATES

11.1 INTERACTION WITH A ELECTRIC FIELD

In §10.3 (interaction with a electric field), Green's functions are introduced to solve the first order differential equation

$$\frac{da}{dt} + i\omega_0 a = -i\omega_0 \lambda(t) \tag{11.1}$$

A simpler way is to use the usual trick of assuming that we can take the constant term in the homogeneous solution and allow it to vary with time.

Since our homogeneous solution is of the form

$$a_H(t) = a_H(0)e^{-i\omega_0 t}, \tag{11.2}$$

we can look for a specific solution to the forcing term equation of the form

$$a_S(t) = f(t)e^{-i\omega_0 t} \tag{11.3}$$

We get

$$f' = -i\omega_0 \lambda(t) e^{i\omega_0 t} \tag{11.4}$$

which can be integrate directly to find the non-homogeneous solution

$$a_S(t) = a_S(t_0)e^{-i\omega_0(t-t_0)} - i\omega_0 \int_{t_0}^{t} \lambda(t')e^{-i\omega_0(t-t')}dt' \tag{11.5}$$

Setting $t_0 = -\infty$, with a requirement that $a_S(-\infty) = 0$ and adding in a general homogeneous solution one then has 10.92 without the complications of Green's functions or the associated contour integrals. I suppose the author wanted to introduce this as a general purpose tool and this was a simple way to do so.

His introduction of Green's functions this way I did not personally find very clear. Specifically, he does not actually define what a Green's function is, and the Appendix 20.13 he refers to only discusses the subtleties of the associated Contour integration. I did not understand where equation 10.83 came from in the first place.

Something like the following would have been helpful (the type of argument found in [13])

Given a linear operator L, such that $Lu(x) = f(x)$, we search for the Green's function $G(x, s)$ such that $LG(x, s) = \delta(x - s)$. For such a function we have

$$\begin{aligned} \int LG(x, s) f(s) ds &= \int \delta(x - s) f(s) ds \\ &= f(x) \end{aligned} \tag{11.6}$$

and by linearity we also have

$$\begin{aligned} f(x) &= \int LG(x, s) f(s) ds \\ &= L \int G(x, s) f(s) ds \end{aligned} \tag{11.7}$$

and can therefore identify $u(x) = \int G(x, s) f(s) ds$ as the desired solution to $Lu(x) = f(x)$ once the Green's function $G(x, s)$ associated with operator L has been determined.

12

ROTATIONS AND ANGULAR MOMENTUM

12.1 ROTATIONS (CHAPTER 26)

Why are we doing the math? Because it applies to physical systems. Slides of IBM's SEM quantum coral and others shown and discussed.

PICTURE: Standard right handed coordinate system with point (x, y, z). We would like to discuss how to represent this point in other coordinate systems, such as one with the x, y axes rotated to x', y' through an angle ϕ.

Our problem is to find in the rotated coordinate system from (x, y, z) to (x', y', z').

There is clearly a relationship between the representations. That relationship between x', y', z' and x, y, z for a counter-clockwise rotation about the z axis is

$$\begin{aligned} x' &= x\cos\phi - y\sin\phi \\ y' &= x\sin\phi + y\cos\phi \\ z' &= z \end{aligned} \tag{12.1}$$

Treat (x, y, z) and (x', y', z') like vectors and write

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \tag{12.2}$$

Or

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = R_z(\phi) \begin{bmatrix} x \\ y \\ z \end{bmatrix} \tag{12.3}$$

Q: Is $R_z(\phi)$ a unitary operator? Definition U is unitary if $U^\dagger U = \mathbf{1}$, where $\mathbf{1}$ is the identity operator. We take Hermitian conjugates, which in this case is just the transpose since all elements of the matrix are real, and multiply

$$
\begin{aligned}
(R_z(\phi))^\dagger R_z(\phi) &= \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} \cos^2\phi + \sin^2\phi & -\sin\phi\cos\phi + \sin\phi\cos\phi & 0 \\ -\cos\phi\sin\phi + \cos\phi\sin\phi & \cos^2\phi + \sin^2\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= \mathbf{1}
\end{aligned}
\tag{12.4}
$$

Apply the above to a vector $\mathbf{v} = (v_x, v_y, v_z)$ and write $\mathbf{v}' = (v'_x, v'_y, v'_z)$. These are related as

$$
\mathbf{v} = R_z(\phi)\mathbf{v}
\tag{12.5}
$$

Now we want to consider the infinitesimal case where we allow the rotation angle to get arbitrarily small. Consider this specific z axis rotation case, and assume that ϕ is very small. Let $\phi = \epsilon$ and write

$$
\begin{aligned}
\mathbf{v}' &= \begin{bmatrix} v'_x \\ v'_y \\ v'_z \end{bmatrix} = R_z(\phi) \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} = \begin{bmatrix} \cos\epsilon & -\sin\epsilon & 0 \\ \sin\epsilon & \cos\epsilon & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{v} \\
&\approx \begin{bmatrix} 1 & -\epsilon & 0 \\ \epsilon & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{v} = \left(\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & -\epsilon & 0 \\ \epsilon & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \right) \mathbf{v}
\end{aligned}
\tag{12.6}
$$

Define

$$
S_z = i\hbar \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}
\tag{12.7}
$$

which is the generator of infinitesimal rotations about the z axis.

Our rotated coordinate vector becomes

$$\begin{aligned}\mathbf{v}' &= \left(\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \frac{i\hbar\epsilon}{i\hbar} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \right) \mathbf{v} \\ &= \left(\mathbf{1} + \frac{\epsilon}{i\hbar} S_z \right) \mathbf{v}\end{aligned} \tag{12.8}$$

Or

$$\mathbf{v}' = \left(\mathbf{1} - \frac{i\epsilon}{\hbar} S_z \right) \mathbf{v} \tag{12.9}$$

Many infinitesimal rotations can be combined to create a finite rotation via

$$\lim_{N\to\infty} \left(1 + \frac{\alpha}{N} \right)^N = e^{\alpha} \tag{12.10}$$

$$\alpha = -i\phi S_z / \hbar \tag{12.11}$$

For a finite rotation

$$\mathbf{v}' = e^{-i\frac{\phi S_z}{\hbar}} \mathbf{v} \tag{12.12}$$

Now think about transforming $g(x, y, z)$, an arbitrary function. Take ϵ is very small so that

$$\begin{aligned} x' &= x\cos\phi - y\sin\phi = x\cos\epsilon - y\sin\epsilon \approx x - y\epsilon \\ y' &= x\sin\phi + y\cos\phi = x\sin\epsilon + y\cos\epsilon \approx x\epsilon + y \\ z' &= z \end{aligned} \tag{12.13}$$

Question: Why can we assume that ϵ is small?

Answer: We declare it to be small because it is simpler, and eventually build up to the general case where it is larger. We want to master the easy task before moving on to the more difficult ones.

Our function is now transformed

$$\begin{aligned} g(x', y', z') &\approx g(x - y\epsilon, y + x\epsilon, z) \\ &= g(x, y, z) - \epsilon y \frac{\partial g}{\partial x} + \epsilon x \frac{\partial g}{\partial y} + \cdots \\ &= \left(\mathbf{1} - \epsilon y \frac{\partial}{\partial x} + \epsilon x \frac{\partial}{\partial y} \right) g(x, y, z) \end{aligned} \tag{12.14}$$

Recall that the coordinate definition of the angular momentum operator is

$$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = xp_y - yp_x \tag{12.15}$$

We can now write

$$\begin{aligned}
g(x', y', z') &= \left(\mathbf{1} + \frac{-i\hbar\epsilon}{-i\hbar}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right) g(x, y, z) \\
&= \left(\mathbf{1} + \frac{i\epsilon}{\hbar}L_z\right) g(x, y, z)
\end{aligned} \tag{12.16}$$

For a finite rotation with angle ϕ we have

$$g(x', y', z') = e^{i\frac{\phi L_z}{\hbar}} g(x, y, z) \tag{12.17}$$

Question: Somebody says that the rotation is clockwise not counterclockwise?

I did not follow the reasoning briefly mentioned on the board since it looks right to me. Perhaps this is the age old mixup between rotating the coordinates and the basis vectors. Review what is in the text carefully. Can also check by

If you rotate a ket, and examine how the state representation of that ket changes under rotation, we have

$$\left|x', y', z'\right\rangle = |x - \epsilon y, y + \epsilon x, z\rangle \tag{12.18}$$

Or

$$\begin{aligned}
\left\langle \Psi|x', y', z'\right\rangle &= \Psi^*(x', y', z') \\
&= \Psi^*(x - \epsilon y, y + \epsilon x, z) \\
&= \Psi^*(x, y, z) - \epsilon\frac{\partial \Psi^*}{\partial y} + \epsilon\frac{\partial \Psi^*}{\partial x} \\
&= \left(\mathbf{1} + \frac{i\epsilon}{\hbar}L_z\right)\Psi^*(x, y, z)
\end{aligned} \tag{12.19}$$

Taking the complex conjugate we have

$$\Psi(x', y', z')\left(\mathbf{1} - \frac{i\epsilon}{\hbar}L_z\right)\Psi(x, y, z) \tag{12.20}$$

For infinitesimal rotations about the z axis we have for functions

$$\Psi(x', y', z') = e^{-\frac{i\epsilon}{\hbar}L_z}\Psi(x, y, z) \tag{12.21}$$

For finite rotations of a vector about the z axis we have

$$\mathbf{v}' = e^{-\frac{i\phi S_z}{\hbar}} \mathbf{v} \tag{12.22}$$

and for functions

$$\Psi(x', y', z') = e^{-\frac{i\phi L_z}{\hbar}} \Psi(x, y, z) \tag{12.23}$$

Vatche has mentioned some devices being researched right now where there is an attempt to isolate the spin orientation so that, say, only spin up or spin down electrons are allowed to flow. There are some possible interesting applications here to Quantum computation. Can we actually make a quantum computing device that is actually usable? We can make NAND devices as mentioned in the article above. Can this be scaled? We do not know how to do this yet.

Recall that one description of a "particle" that has both a position and spin representation is

$$|\Psi\rangle = |u\rangle \otimes |sm\rangle \tag{12.24}$$

where we have a tensor product of kets. One usually just writes the simpler

$$|u\rangle \otimes |sm\rangle \equiv |u\rangle |sm\rangle \tag{12.25}$$

An example of the above is

$$\begin{bmatrix} u_1(\mathbf{r}) \\ u_2(\mathbf{r}) \\ u_3(\mathbf{r}) \end{bmatrix} = \left(\langle \mathbf{r}| \langle sm|\right) |\Psi\rangle \tag{12.26}$$

where u_1 is spin component one. For $s = 1$ this would be $m = -1, 0, 1$.

Here we have also used

$$\begin{aligned} |\mathbf{r}\rangle &= |x\rangle \otimes |y\rangle \otimes |z\rangle \\ &= |x\rangle |y\rangle |z\rangle \\ &= |xyz\rangle \end{aligned} \tag{12.27}$$

We can now ask the question of how this thing transforms. We transform each component of this as a vector. The transformation of

$$\begin{bmatrix} u_1(\mathbf{r}) \\ u_2(\mathbf{r}) \\ u_3(\mathbf{r}) \end{bmatrix} \tag{12.28}$$

results in

$$\begin{bmatrix} u_1(\mathbf{r}) \\ u_2(\mathbf{r}) \\ u_3(\mathbf{r}) \end{bmatrix}' = e^{-i\phi(S_z+L_z)/\hbar} \begin{bmatrix} u_1(\mathbf{r}) \\ u_2(\mathbf{r}) \\ u_3(\mathbf{r}) \end{bmatrix} \tag{12.29}$$

Or with $J_z = S_z + L_z$

$$\left|\Psi'\right\rangle = e^{-i\phi J_z/\hbar} \left|\Psi\right\rangle \tag{12.30}$$

Observe that this separates out nicely with the S_z operation acting on the vector parts, and the L_z operator acting on the functional dependence.

12.2 TRIG RELATIONS

To verify equations 26.3-5 in the text it is worth noting that

$$\begin{aligned} \cos(a+b) &= \mathrm{Re}(e^{ia}e^{ib}) \\ &= \mathrm{Re}((\cos a + i\sin a)(\cos b + i\sin b)) \\ &= \cos a\cos b - \sin a\sin b \end{aligned} \tag{12.31}$$

and

$$\begin{aligned} \sin(a+b) &= \mathrm{Im}(e^{ia}e^{ib}) \\ &= \mathrm{Im}((\cos a + i\sin a)(\cos b + i\sin b)) \\ &= \cos a\sin b + \sin a\cos b \end{aligned} \tag{12.32}$$

So, for

$$\begin{aligned} x &= \rho\cos\alpha \\ y &= \rho\sin\alpha \end{aligned} \tag{12.33}$$

the transformed coordinates are

$$\begin{aligned} x' &= \rho\cos(\alpha+\phi) \\ &= \rho(\cos\alpha\cos\phi - \sin\alpha\sin\phi) \\ &= x\cos\phi - y\sin\phi \end{aligned} \tag{12.34}$$

and

$$\begin{aligned} y' &= \rho\sin(\alpha+\phi) \\ &= \rho(\cos\alpha\sin\phi + \sin\alpha\cos\phi) \\ &= x\sin\phi + y\cos\phi \end{aligned} \tag{12.35}$$

This allows us to read off the rotation matrix. Without all the messy trig, we can also derive this matrix with geometric algebra.

$$
\begin{aligned}
\mathbf{v}' &= e^{-\mathbf{e}_1\mathbf{e}_2\phi/2}\mathbf{v}e^{\mathbf{e}_1\mathbf{e}_2\phi/2} \\
&= v_3\mathbf{e}_3 + (v_1\mathbf{e}_1 + v_2\mathbf{e}_2)e^{\mathbf{e}_1\mathbf{e}_2\phi} \\
&= v_3\mathbf{e}_3 + (v_1\mathbf{e}_1 + v_2\mathbf{e}_2)(\cos\phi + \mathbf{e}_1\mathbf{e}_2\sin\phi) \\
&= v_3\mathbf{e}_3 + \mathbf{e}_1(v_1\cos\phi - v_2\sin\phi) + \mathbf{e}_2(v_2\cos\phi + v_1\sin\phi)
\end{aligned}
\tag{12.36}
$$

Here we use the Pauli-matrix like identities

$$
\begin{aligned}
\mathbf{e}_k^2 &= 1 \\
\mathbf{e}_i\mathbf{e}_j &= -\mathbf{e}_j\mathbf{e}_i, \quad i \neq j
\end{aligned}
\tag{12.37}
$$

and also note that $\mathbf{e}_3$ commutes with the bivector for the x, y plane $\mathbf{e}_1\mathbf{e}_2$. We can also read off the rotation matrix from this.

12.3 INFINITESIMAL TRANSFORMATIONS

Recall that in the problems of Chapter 5, one representation of spin one matrices were calculated 5.3. Since the choice of the basis vectors was arbitrary in that exercise, we ended up with a different representation. For S_x, S_y, S_z as found in (26.20) and (26.23) we can also verify easily that we have eigenvalues $0, \pm\hbar$. We can also show that our spin kets in this non-diagonal representation have the following column matrix representations:

$$
\begin{aligned}
|1, \pm 1\rangle_x &= \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ \pm i \end{bmatrix} \\
|1, 0\rangle_x &= \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \\
|1, \pm 1\rangle_y &= \frac{1}{\sqrt{2}} \begin{bmatrix} \pm i \\ 0 \\ 1 \end{bmatrix} \\
|1, 0\rangle_y &= \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \\
|1, \pm 1\rangle_z &= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm i \\ 0 \end{bmatrix} \\
|1, 0\rangle_z &= \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}
\end{aligned}
\tag{12.38}
$$

12.4 VERIFYING THE COMMUTATOR RELATIONS

Given the (summation convention) matrix representation for the spin one operators

$$
(S_i)_{jk} = -i\hbar\epsilon_{ijk}, \tag{12.39}
$$

let us demonstrate the commutator relation of (26.25).

$$\begin{aligned}
[S_i, S_j]_{rs} &= (S_i S_j - S_j S_i)_{rs} \\
&= \sum_t (S_i)_{rt}(S_j)_{ts} - (S_j)_{rt}(S_i)_{ts} \\
&= (-i\hbar)^2 \sum_t \epsilon_{irt}\epsilon_{jts} - \epsilon_{jrt}\epsilon_{its} \\
&= -(-i\hbar)^2 \sum_t \epsilon_{tir}\epsilon_{tjs} - \epsilon_{tjr}\epsilon_{tis}
\end{aligned} \tag{12.40}$$

Now we can employ the summation rule for sums products of antisymmetric tensors over one free index (4.179)

$$\sum_i \epsilon_{ijk}\epsilon_{iab} = \delta_{ja}\delta_{kb} - \delta_{jb}\delta_{ka}. \tag{12.41}$$

Continuing we get

$$\begin{aligned}
[S_i, S_j]_{rs} &= -(-i\hbar)^2 \left(\delta_{ij}\delta_{rs} - \delta_{is}\delta_{rj} - \delta_{ji}\delta_{rs} + \delta_{js}\delta_{ri}\right) \\
&= (-i\hbar)^2 \left(\delta_{is}\delta_{jr} - \delta_{ir}\delta_{js}\right) \\
&= (-i\hbar)^2 \sum_t \epsilon_{tij}\epsilon_{tsr} \\
&= i\hbar \sum_t \epsilon_{tij}(S_t)_{rs} \qquad \square
\end{aligned} \tag{12.42}$$

12.5 GENERAL INFINITESIMAL ROTATION

Equation (26.26) has for an infinitesimal rotation counterclockwise around the unit axis of rotation vector **n**

$$\mathbf{V}' = \mathbf{V} + \epsilon\mathbf{n} \times \mathbf{V}. \tag{12.43}$$

Let us derive this using the geometric algebra rotation expression for the same

$$\begin{aligned}
\mathbf{V}' &= e^{-I\mathbf{n}\alpha/2}\mathbf{V}e^{I\mathbf{n}\alpha/2} \\
&= e^{-I\mathbf{n}\alpha/2}\left((\mathbf{V}\cdot\mathbf{n})\mathbf{n} + (\mathbf{V}\wedge\mathbf{n})\mathbf{n}\right)e^{I\mathbf{n}\alpha/2} \\
&= (\mathbf{V}\cdot\mathbf{n})\mathbf{n} + (\mathbf{V}\wedge\mathbf{n})\mathbf{n}e^{I\mathbf{n}\alpha}
\end{aligned} \tag{12.44}$$

We note that $I\mathbf{n}$ and thus the exponential commutes with $\mathbf{n}$, and the projection component in the normal direction. Similarly $I\mathbf{n}$ anticommutes with $(\mathbf{V} \wedge \mathbf{n})\mathbf{n}$. This leaves us with

$$\mathbf{V}' = (\mathbf{V} \cdot \mathbf{n})\mathbf{n} \left(+(\mathbf{V} \wedge \mathbf{n})\mathbf{n}\right) (\cos\alpha + I\mathbf{n}\sin\alpha) \tag{12.45}$$

For $\alpha = \epsilon \rightarrow 0$, this is

$$\begin{aligned}\mathbf{V}' &= (\mathbf{V} \cdot \mathbf{n})\mathbf{n} + (\mathbf{V} \wedge \mathbf{n})\mathbf{n}(1 + I\mathbf{n}\epsilon) \\ &= (\mathbf{V} \cdot \mathbf{n})\mathbf{n} + (\mathbf{V} \wedge \mathbf{n})\mathbf{n} + \epsilon I^2 (\mathbf{V} \times \mathbf{n})\mathbf{n}^2 \\ &= \mathbf{V} + \epsilon(\mathbf{n} \times \mathbf{V}) \qquad \square\end{aligned} \tag{12.46}$$

12.6 POSITION AND ANGULAR MOMENTUM COMMUTATOR

Equation (26.71) is

$$\left[x_i, L_j\right] = i\hbar\epsilon_{ijk}x_k. \tag{12.47}$$

Let us derive this. Recall that we have for the position-momentum commutator

$$\left[x_i, p_j\right] = i\hbar\delta_{ij}, \tag{12.48}$$

and for each of the angular momentum operator components we have

$$L_m = \epsilon_{mab}x_a p_b. \tag{12.49}$$

The commutator of interest is thus

$$\begin{aligned}\left[x_i, L_j\right] &= x_i\epsilon_{jab}x_a p_b - \epsilon_{jab}x_a p_b x_i \\ &= \epsilon_{jab}x_a \left(x_i p_b - p_b x_i\right) \\ &= \epsilon_{jab}x_a i\hbar\delta_{ib} \\ &= i\hbar\epsilon_{jai}x_a \\ &= i\hbar\epsilon_{ija}x_a \qquad \square\end{aligned} \tag{12.50}$$

12.7 A NOTE ON THE ANGULAR MOMENTUM OPERATOR EXPONENTIAL SANDWICHES

In (26.73-74) we have

$$e^{i\epsilon L_z/\hbar} x e^{-i\epsilon L_z/\hbar} = x + \frac{i\epsilon}{\hbar}\left[L_z, x\right] \tag{12.51}$$

Observe that

$$[x, [L_z, x]] = 0 \tag{12.52}$$

so from the first two terms of (10.99)

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2}[A, [A, B]] \cdots \tag{12.53}$$

we get the desired result.

12.8 TRACE RELATION TO THE DETERMINANT

Going from (26.90) to (26.91) we appear to have a mystery identity

$$\det(\mathbf{1} + \mu \mathbf{A}) = 1 + \mu \operatorname{Tr} \mathbf{A} \tag{12.54}$$

According to wikipedia, under derivative of a determinant, [12], this is good for small μ, and related to something called the Jacobi identity. Someday I should really get around to studying determinants in depth, and will take this one for granted for now.

12.9 PROBLEMS

Exercise 12.1 A problem of spherical harmonics (2010 PHY356 final exam)

One of the PHY356 exam questions from the final I recall screwing up on, and figuring it out after the fact on the drive home. The question actually clarified a difficulty I had had, but unfortunately I had not had the good luck to perform such a question, to help figure this out before the exam.

From what I recall the question provided an initial state, with some degeneracy in m, perhaps of the following form

$$|\phi(0)\rangle = \sqrt{\frac{1}{7}}|12\rangle + \sqrt{\frac{2}{7}}|10\rangle + \sqrt{\frac{4}{7}}|20\rangle, \tag{12.55}$$

and a Hamiltonian of the form

$$H = \alpha L_z \tag{12.56}$$

Answer for Exercise 12.1

Evolved state One part of the question was to calculate the evolved state. Application of the time evolution operator gives us

$$|\phi(t)\rangle = e^{-i\alpha L_z t/\hbar}\left(\sqrt{\frac{1}{7}}\,|12\rangle + \sqrt{\frac{2}{7}}\,|10\rangle + \sqrt{\frac{4}{7}}\,|20\rangle\right). \tag{12.57}$$

Now we note that $L_z\,|12\rangle = 2\,\hbar\,|12\rangle$, and $L_z\,|l0\rangle = 0\,|l0\rangle$, so the exponentials reduce this nicely to just

$$|\phi(t)\rangle = \sqrt{\frac{1}{7}}e^{-2i\alpha t}\,|12\rangle + \sqrt{\frac{2}{7}}\,|10\rangle + \sqrt{\frac{4}{7}}\,|20\rangle\,. \tag{12.58}$$

Probabilities for L_z measurement outcomes I believe we were also asked what the probabilities for the outcomes of a measurement of L_z at this time would be. Here is one place that I think that I messed up, and it is really a translation error, attempting to get from the English description of the problem to the math description of the same. I had had trouble with this process a few times in the problems, and managed to blunder through use of language like "measure", and "outcome", but do not think I really understood how these were used properly.

What are the outcomes that we measure? We measure operators, but the result of a measurement is the eigenvalue associated with the operator. What are the eigenvalues of the L_z operator? These are the $m\,\hbar$ values, from the operation $L_z\,|lm\rangle = m\,\hbar\,|lm\rangle$. So, given this initial state, there are really two outcomes that are possible, since we have two distinct eigenvalues. These are $2\,\hbar$ and 0 for $m = 2$, and $m = 0$ respectively.

A measurement of the "outcome" $2\,\hbar$, will be the probability associated with the amplitude $\langle 12|\phi(t)\rangle$ (ie: the absolute square of this value). That is

$$|\langle 12|\phi(t)\rangle|^2 = \frac{1}{7}. \tag{12.59}$$

Now, the only other outcome for a measurement of L_z for this state is a measurement of $0\,\hbar$, and the probability of this is then just $1 - \frac{1}{7} = \frac{6}{7}$. On the exam, I think I listed probabilities for three outcomes, with values $\frac{1}{7}, \frac{2}{7}, \frac{4}{7}$ respectively, but in retrospect that seems blatantly wrong.

Probabilities for $\mathbf{L}^2$ measurement outcomes What are the probabilities for the outcomes for a measurement of $\mathbf{L}^2$ after this? The first question is really what are the outcomes. That is really a question of what are the possible eigenvalues of $\mathbf{L}^2$ that can be measured at this point. Recall that we have

$$\mathbf{L}^2\,|lm\rangle = \hbar^2 l(l+1)\,|lm\rangle \tag{12.60}$$

So for a state that has only $l = 1, 2$ contributions before the measurement, the eigenvalues that can be observed for the $\mathbf{L}^2$ operator are respectively $2\hbar^2$ and $6\hbar^2$ respectively.

For the $l = 2$ case, our probability is $4/7$, leaving $3/7$ as the probability for measurement of the $l = 1$ ($2\hbar^2$) eigenvalue. We can compute this two ways, and it seems worthwhile to consider both. This first method makes use of the fact that the L_z operator leaves the state vector intact, but it also seems like a bit of a cheat. Consider instead two possible results of measurement after the L_z observation. When an L_z measurement of $0\hbar$ is performed our state will be left with only the $m = 0$ kets. That is

$$|\psi_a\rangle = \frac{1}{\sqrt{3}}\left(|10\rangle + \sqrt{2}\,|20\rangle\right), \tag{12.61}$$

whereas, when a $2\hbar$ measurement of L_z is performed our state would then only have the $m = 2$ contribution, and would be

$$|\psi_b\rangle = e^{-2i\alpha t}\,|12\rangle\,. \tag{12.62}$$

We have two possible ways of measuring the $2\hbar^2$ eigenvalue for $\mathbf{L}^2$. One is when our state was $|\psi_a\rangle$ (, and the resulting state has a $|10\rangle$ component, and the other is after the $m = 2$ measurement, where our state is left with a $|12\rangle$ component.

The resulting probability is then a conditional probability result

$$\frac{6}{7}|\langle 10|\psi_a\rangle|^2 + \frac{1}{7}|\langle 12|\psi_b\rangle|^2 = \frac{3}{7} \tag{12.63}$$

The result is the same, as expected, but this is likely a more convincing argument.

Part II

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BIBLIOGRAPHY

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Part III

INDEX

INDEX