# 1 Mathematical Introduction

## 1.1 Linear Vector Spaces: Basics

1.1.1. Verify these claims. For the first consider $|0\rangle + |0'\rangle$ and use the advertised properties of the two null vectors in turn. For the second start with $|0\rangle = (0+1)|V\rangle + |-V\rangle$. For the third, begin with $|V\rangle + (-|V\rangle) = 0|V\rangle = |0\rangle$. For the last, let $|W\rangle$ also satisfy $|V\rangle + |W\rangle = |0\rangle$. Since $|0\rangle$ is unique, this means $|V\rangle + |W\rangle = |V\rangle + |-V\rangle$. Take it from here.

If both $|0\rangle$ and $|0'\rangle$ have the properties of the null vector, then

$$|0\rangle + |0'\rangle = |0\rangle = |0'\rangle,$$

i.e. they must be the same vector.

To verify that $0|V\rangle = |0\rangle$, consider

$$\begin{aligned}
|0\rangle &= |V\rangle + |-V\rangle \\
&= (0+1)|V\rangle + |-V\rangle \\
&= 0|V\rangle + |V\rangle + |-V\rangle \\
&= 0|V\rangle + |0\rangle \\
&= 0|V\rangle
\end{aligned}$$

From the fact that $0|V\rangle = |0\rangle$, we may write

$$\begin{aligned}
|0\rangle &= 0|V\rangle \\
&= (1-1)|V\rangle \\
&= |V\rangle + (-|V\rangle)
\end{aligned}$$

which implies that $-|V\rangle = |-V\rangle$.

Finally, consider two vectors that satisfy the property of being the inverse of $|V\rangle$, $|W\rangle$ and $|-V\rangle$. Then, since the addition of either of these to $|V\rangle$ equals $|0\rangle$, we have

$$\begin{aligned}
|V\rangle + |-V\rangle &= |V\rangle + |W\rangle \\
|-V\rangle &= |W\rangle
\end{aligned}$$

1.1.2. Consider the set of all entities of the form $(a, b, c)$ where the entries are real numbers. Addition and scalar multiplication are defined as follows:

$$\begin{aligned}
(a, b, c) + (d, e, f) &= (a+d, b+e, c+f) \\
\alpha(a, b, c) &= (\alpha a, \alpha b, \alpha c).
\end{aligned}$$

Write down the null vector and inverse of $(a, b, c)$. Show that vectors of the form $(a, b, 1)$ do not form a vector space.

The null vector is clearly given by

$$(0, 0, 0)$$

as this preserves any vector to which it is added.

Vectors of the form $(a, b, 1)$ do not form a space because, among other things, addition among them is not closed. That is, if $(a, b, 1) \in \mathbb{V}$, then

$$(a, b, 1) + (c, d, 1) = (a + c, b + d, 2) \notin \mathbb{V}$$

1.1.3. Do functions that vanish at the end points $x = 0$ and $x = L$ form a vector space? How about *periodic functions* obeying $f(0) = f(L)$? How about functions that obey $f(0) = 4$? If the functions do not qualify, list the things that go wrong.

Functions that satisfy $f(0) = f(L) = 0$ do indeed form a vector space, as do those that generically satisfy $f(0) = f(L)$. Under these conditions, the identifying characteristic of functions within the vector space is preserved: if $f(x)$ and $g(x)$ separately satisfy periodicity, then $f(x) + g(x)$ satisfies periodicity. All other vector space axioms are satisfied trivially.

Functions obeying $f(0) = 4$ do *not* form a vector space because they are not closed under addition.

1.1.4. Consider three elements from the vector space of real $2 \times 2$ matrices:

$$|1\rangle = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \qquad |2\rangle = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \qquad |3\rangle = \begin{bmatrix} -2 & -1 \\ 0 & -2 \end{bmatrix}$$

Are they linearly independent? Support your answer with details. (Notice we are calling these matrices vectors and using kets to represent them to emphasize their role as elements of a vector space.)

These three vectors are not linearly independent, because

$$-2|2\rangle + |1\rangle = \begin{bmatrix} -2 & -1 \\ 0 & -2 \end{bmatrix} = |3\rangle.$$

1.1.5. Show that the following row vectors are linearly dependent: $(1, 1, 0)$, $(1, 0, 1)$, and $(3, 2, 1)$. Show the opposite for $(1, 1, 0)$, $(1, 0, 1)$, and $(0, 1, 1)$.

For the first case, notice that

$$2(1, 1, 0) + (1, 0, 1) = (3, 2, 1),$$

showing the linear dependence of these three vectors.

For the second case, observe that linear dependence would imply a nontrivial solution to the system of equations

$$x + y = 0,$$

$$x + z = 0,$$
$$y + z = 0.$$

From this system, we see $x = -y$, and hence $y = z$, which implies $z = y = x = 0$. Because this system has the same number of equations as unknowns, this is the unique solution, and hence the original three vectors are linearly independent.

## 1.3 Dual Spaces and the Dirac Notation

1.3.1. Form an orthonormal basis in two dimensions starting with $\vec{A} = 3\vec{i} + 4\vec{j}$ and $\vec{B} = 2\vec{i} - 6\vec{j}$. Can you generate another orthonormal basis starting with these two vectors? If so, produce another.

Following the Gram-Schmidt procedure, we first determine the length of $\vec{A}$, which is $\sqrt{\vec{A} \cdot \vec{A}} = \sqrt{9 + 16} = 5$. We can then normalize $\vec{A}$ to obtain

$$\vec{A}' = \frac{3}{5}\vec{i} + \frac{4}{5}\vec{j}.$$

The projection of $\vec{B}$ along $\vec{A}'$ is $\vec{A}' \cdot \vec{B} = 6/5 - 24/5 = -18/5$. From this, we can find

$$\vec{B}'' = 2\vec{i} - 6\vec{j} + \frac{18}{5}\left(\frac{3}{5}\vec{i} + \frac{4}{5}\vec{j}\right) = \frac{104}{25}\vec{i} - \frac{78}{25}\vec{j}$$

which has a length of $\sqrt{\vec{B}'' \cdot \vec{B}''} = 26/5$. Using this, we may normalize our second basis vector as

$$\vec{B}' = \frac{4}{5}\vec{i} - \frac{3}{5}\vec{j}.$$

We may form another orthonormal basis from these two vectors by starting with $\vec{B}$. In this case, $\sqrt{\vec{B} \cdot \vec{B}} = 2\sqrt{10}$, and so

$$\vec{B}' = \frac{1}{\sqrt{10}}\vec{i} - \frac{3}{\sqrt{10}}\vec{j}.$$

The projection of $\vec{A}$ along this is $\vec{B}' \cdot \vec{A} = -9/\sqrt{10}$, and so

$$\vec{A}'' = 3\vec{i} + 4\vec{j} + \frac{9}{\sqrt{10}}\left(\frac{1}{\sqrt{10}}\vec{i} - \frac{3}{\sqrt{10}}\vec{j}\right) = \frac{39}{10}\vec{i} + \frac{13}{10}\vec{j}.$$

This has a length of $\sqrt{\vec{A}'' \cdot \vec{A}''} = 13/\sqrt{10}$, giving a normalized vector

$$\vec{A}' = \frac{3}{\sqrt{10}}\vec{i} + \frac{1}{\sqrt{10}}\vec{j}.$$

1.3.2. Show how to go from the basis

$$|I\rangle = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix} \qquad |II\rangle = \begin{bmatrix} 0 \\ 1 \\ 2 \end{bmatrix} \qquad |III\rangle = \begin{bmatrix} 0 \\ 2 \\ 5 \end{bmatrix}$$

to the orthonormal basis

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \qquad |2\rangle = \begin{bmatrix} 0 \\ 1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix} \qquad |3\rangle = \begin{bmatrix} 0 \\ -2/\sqrt{5} \\ 1/\sqrt{5} \end{bmatrix}$$

$|I\rangle$ clearly reduces to $|1\rangle$. Since $|II\rangle$ is already orthogonal to $|1\rangle$, we simply need to normalize it. Because $\langle II|II\rangle = 5$, we have

$$|2\rangle = \begin{bmatrix} 0 \\ 1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix}.$$

Since $|III\rangle$ is orthogonal to $|1\rangle$, we can find it via

$$\begin{aligned} |3'\rangle &= |III\rangle - |2\rangle\langle 2|III\rangle \\ &= \begin{bmatrix} 0 \\ 2 \\ 5 \end{bmatrix} - \left(\frac{12}{\sqrt{5}}\right) \begin{bmatrix} 0 \\ 1/\sqrt{5} \\ 2/\sqrt{5} \end{bmatrix} \\ &= \begin{bmatrix} 0 \\ -2/5 \\ 1/5 \end{bmatrix}. \end{aligned}$$

Because $\langle 2'|2'\rangle = 1/5$, our normalized third vector becomes

$$|3\rangle = \begin{bmatrix} 0 \\ -2/\sqrt{5} \\ 1/\sqrt{5} \end{bmatrix}.$$

1.3.3. When will this equality be satisfied? Does this agree with your experience with arrows?

The Schwarz inequality will be satisfied when $|W\rangle = \alpha|V\rangle$, because then we have

$$\begin{aligned} |\langle V|\alpha V\rangle| &= |V||\alpha V| \\ |\alpha||\langle V|V\rangle| &= |\alpha||V||V| \\ |\alpha||V|^2 &= |\alpha||V|^2. \end{aligned}$$

If we consider the case where our vectors are arrows, $\langle V|W\rangle = \vec{V} \cdot \vec{W} = |V||W|\cos\theta$, which equals $|V||W|$ when $\theta = 0$, i.e. when $\vec{W} = \alpha\vec{V}$.

1.3.4. Prove the triangle inequality starting with $|V+W|^2$. You must use $\mathrm{Re}\langle V|W\rangle \leq |\langle V|W\rangle|$ and the Schwarz inequality. Show that the final inequality becomes na equality only if $|V\rangle = a|W\rangle$ where $a$ is a real positive scalar.

We have

$$|V+W|^2 = \langle V+W|V+W\rangle,$$

$$
\begin{aligned}
&= \langle V|V\rangle + \langle W|V\rangle + \langle V|W\rangle + \langle W|W\rangle, \\
&= |V|^2 + |W|^2 + \langle V|W\rangle + \langle V|W\rangle^*, \\
&= |V|^2 + |W|^2 + 2\mathrm{Re}\langle V|W\rangle, \\
&\leq |V|^2 + |W|^2 + 2|\langle V|W\rangle|, \\
&\leq |V|^2 + |W|^2 + 2|V||W|, \\
&= (|V| + |W|)^2,
\end{aligned}
$$

where the second to last line invokes the Schwarz inequality. Taking the square root of both sides yields the triangle inequality,

$$|V + W| \leq |V| + |W|.$$

## 1.4 Subspaces

1.4.1. In a space $\mathbb{V}^n$, prove that the set of all vectors $\{|V_\perp^1\rangle, |V_\perp^2\rangle, \dots\}$, orthogonal to any $|V\rangle \neq |0\rangle$, form a subspace $\mathbb{V}^{n-1}$.

Clearly, the set of all vectors orthogonal to $|V\rangle$ is closed under addition, as

$$\langle V|W\rangle = \langle V|\Big(\sum_i \alpha_i |V_\perp^i\rangle\Big) = \sum_i \alpha_i \langle V|V_\perp^i\rangle = |0\rangle.$$

Also trivial is the fact that the suggested set contains $|0\rangle$, as $\langle V|0\rangle = |0\rangle$. All that is left is to show that the space must span $n-1$ dimensions.

Consider an orthogonal basis for $\mathbb{V}^n$ with $|V\rangle$ as one of its vectors. Removing $|V\rangle$ leaves $n-1$ linearly independent vectors orthogonal to $|V\rangle$. If there were vectors in $\mathbb{V}^n$ orthogonal to $|V\rangle$ incapable of being expressed in terms of these, $\mathbb{V}^n$ would have a dimension larger than $n$. On the other hand, if the space of vector spanned by all those orthogonal to $|V\rangle$ was smaller than $n-1$, our reduced set would be linearly dependent, contradicting our initial assumption of an orthogonal basis. Therefore, the subspace spanned by such a set must have dimension $n+1$.

1.4.2. Suppose $\mathbb{V}_1^{n_1}$ and $\mathbb{V}_2^{n_2}$ are two subspaces such that any element of $\mathbb{V}_1$ is orthogonal to any element of $\mathbb{V}_2$. Show that the dimensionality of $\mathbb{V}_1 \oplus \mathbb{V}_2$ is $n_1 + n_2$. (Hint: Theorem 4.)

Because every possible basis of either space is orthogonal to the possible bases of the other space, Theorem 4 tells us that the span of $\mathbb{V}_1 \oplus \mathbb{V}_2$ is the sum of the dimensions spanned by both, i.e. $n_1 + n_2$.

## 1.6 Matrix Elements of Linear Operators

1.6.1. An operator $\Omega$ is given by the matrix

$$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

What is its action?

$\Omega$ simply permutes the components of vectors expressed in its basis.

1.6.2. Given $\Omega$ and $\Lambda$ are Hermitian what can you say about (1) $\Omega\Lambda$; (2) $\Omega\Lambda+\Lambda\Omega$; (3) $[\Omega,\Lambda]$; and (4) $i[\Omega,\Lambda]$?

For (1), we see that $(\Omega\Lambda)^\dagger = \Lambda^\dagger\Omega^\dagger = \Lambda\Omega$, and so $\Omega\Lambda$ is *not* Hermitian.

This problem is alleviated by the configuration of operators expressed in (2), as now we have

$$(\Omega\Lambda+\Lambda\Omega)^\dagger = \Lambda^\dagger\Omega^\dagger + \Omega^\dagger\Lambda^\dagger = \Lambda\Omega+\Omega\Lambda = \Omega\Lambda+\Lambda\Omega,$$

which is clearly Hermitian.

For (3), we see

$$(\Omega\Lambda-\Lambda\Omega)^\dagger = \Lambda^\dagger\Omega^\dagger - \Omega^\dagger\Lambda^\dagger = \Lambda\Omega-\Omega\Lambda = -(\Omega\Lambda-\Lambda\Omega),$$

which is anti-Hermitian.
Finally, taking the adjoint of (4) shows that

$$(i\Omega\Lambda-i\Lambda\Omega)^\dagger = -i\Lambda^\dagger\Omega^\dagger + i\Omega^\dagger\Lambda^\dagger = -i\Lambda\Omega+i\Omega\Lambda = i\Omega\Lambda-i\Lambda\Omega,$$

is Hermitian.

1.6.3. Show that a product of unitary operators is unitary.

Suppose $\Omega$ and $\Lambda$ are both unitary. Then we have

$$(\Omega\Lambda)(\Omega\Lambda)^\dagger = \Omega\Lambda\Lambda^\dagger\Omega^\dagger = \Omega I\Omega^\dagger = \Omega\Omega^\dagger = I,$$

which shows that their product is unitary.

1.6.4. It is assumed that you know (1) what a *determinant* is, (2) that $\det\Omega^T = \det\Omega$ ($T$ denotes transpose), (3) that the determinant of a product of matrices is the product of the determinants. [If you do not, verify these properties for a two-dimensional case]

$$\Omega = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

with $\det\Omega = (\alpha\delta-\beta\gamma)$.] Prove that the determinant of a unitary matrix is a complex number of unit modulus.

Taking the determinant of $UU^\dagger = I$, we find

$$|\det UU^\dagger| = |\det U||\det U^\dagger| = |\det U|^2 = |\det I| = 1,$$

which, upon taking the square root, yields $|\det U| = \pm 1$. This is satisfied when the determinant of $U$ is of the form $e^{i\phi}$.

1.6.5. Verify that $R(\frac{1}{2}\pi\hat{\mathbf{i}})$ is unitary (orthogonal) by examining its matrix.

The matrix for $R(\frac{1}{2}\pi\hat{\mathbf{i}})$ in a Cartesian basis is given by

$$R(\frac{1}{2}\pi\hat{\mathbf{i}}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix},$$

which clearly has a determinant of 1. That it is unitary is easily verified by the fact that both its rows and columns form orthonormal bases and that

$$R(\frac{1}{2}\pi\hat{\mathbf{i}})R(\frac{1}{2}\pi\hat{\mathbf{i}})^\dagger = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = I.$$

1.6.6. Verify that the following matrices are unitary:

$$\frac{1}{2^{1/2}} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix}, \qquad \frac{1}{2} \begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix}$$

Verify that the determinant is of the form $e^{i\theta}$ in each case. Are any of the above matrices Hermitian?

The determinant of the first matrix is 1, and its unitarity can be verified via

$$\frac{1}{2} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix} \begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1+1 & -i+i \\ i-i & 1+1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

This determinant of the second matrix is

$$\frac{1}{4}\big((1+i)^2 - (1-i)^2\big) = \frac{1}{4}(1 + 2i - 1 - 1 + 2i + 1) = i,$$

while its unitarity is shown with

$$\begin{aligned} \frac{1}{4} \begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix} \begin{bmatrix} 1-i & 1+i \\ 1+i & 1-i \end{bmatrix} &= \frac{1}{4} \begin{bmatrix} 2(1+i)(1-i) & (1+i)^2 + (1-i)^2 \\ (1-i)^2 + (1+i)^2 & 2(1+i)(1-i) \end{bmatrix} \\ &= \frac{1}{4} \begin{bmatrix} 2+2 & 1+2i-1+1-2i-1 \\ 1+2i-1+1-2i-1 & 2+2 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \end{aligned}$$

Neither of the above matrices are Hermitian.

## 1.7 Active and Passive Transformations

1.7.1. The *trace* of a matrix is defined to be the sum of its diagonal matrix elements

$$\mathrm{Tr}\Omega = \sum_i \Omega_{ii}$$

Show that

(1) $\mathrm{Tr}(\Omega\Lambda) = \mathrm{Tr}(\Lambda\Omega)$

(2) $\text{Tr}(\Omega\Lambda\theta) = \text{Tr}(\Lambda\theta\Omega) = \text{Tr}(\theta\Omega\Lambda)$ (The permutations are *cyclic*.)

(3) The trace of an operator is unaffected by a unitary change of basis $|i\rangle \to U|i\rangle$. [Equivalently, show $\text{Tr}(\Omega) = \text{Tr}(U^\dagger\Omega U)$.

If we write matrix multiplication in component form,

$$[\Omega\Lambda]_{ij} = \sum_k \Omega_{ik}\Lambda_{kj},$$

we can easily show (1) and (2). For the first case, we have

$$\text{Tr}(\Omega\Lambda) = \sum_i \sum_k \Omega_{ik}\Lambda_{ki} = \sum_k \sum_i \Lambda_{ki}\Omega_{ik} = \text{Tr}(\Lambda\Omega).$$

For the second case, matrix multiplication becomes,

$$[\Omega\Lambda\theta]_{ij} = \sum_k \sum_l \Omega_{ik}\Lambda_{kl}\theta_{lj},$$

and so the expression for the trace is

$$\begin{aligned}\text{Tr}(\Omega\Lambda\theta) = \sum_i \sum_k \sum_l \Omega_{ik}\Lambda_{kl}\theta_{li} &= \sum_k \sum_l \sum_i \Lambda_{kl}\theta_{li}\Omega_{ik} = \text{Tr}(\Lambda\theta\Omega) \\ &= \sum_l \sum_i \sum_k \theta_{li}\Omega_{ik}\Lambda_{kl} = \text{Tr}(\theta\Omega\Lambda)\end{aligned}$$

Using the results above, we can immediately see

$$\text{Tr}(U^\dagger\Omega U) = \text{Tr}(UU^\dagger\Omega) = \text{Tr}(I\Omega) = \text{Tr}(\Omega).$$

1.7.2. Show that the determinant of a matrix is unaffected by a unitary change of basis. [Equivalently show $\det\Omega = \det(U^\dagger\Omega U)$.]

Since the determinant of a product is the product of the determinants, we have

$$\det(U^\dagger\Omega U) = \det(U^\dagger)\det(\Omega)\det(U) = e^{-i\phi}\det(\Omega)e^{i\phi} = e^{-i\phi}e^{i\phi}\det(\Omega) = \det(\Omega),$$

because the determinant of a unitary matrix is a complex number of unit modulus.

## 1.8 The Eigenvalue Problem

1.8.1. (1) Find the eigenvalues and normalized eigenvectors of the matrix

$$\Omega = \begin{bmatrix} 1 & 3 & 1 \\ 0 & 2 & 0 \\ 0 & 1 & 4 \end{bmatrix}$$

(2) Is the matrix Hermitian? Are the eigenvectors orthogonal?

The characteristic equation of the above matrix is given by

$$\det(\Omega - \omega I) = \begin{vmatrix} 1-\omega & 3 & 1 \\ 0 & 2-\omega & 0 \\ 0 & 1 & 4-\omega \end{vmatrix} = (1-\omega)(2-\omega)(4-\omega) = 0,$$

from which we immediately see $\omega = 1, 2, 4$. By inspection, it is clear that

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

For $\omega = 2$, $\Omega - \omega I$ becomes

$$\Omega - 2I = \begin{bmatrix} -1 & 3 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & 2 \end{bmatrix}$$

One possible vector that spans the null space of this matrix is

$$|2'\rangle = \begin{bmatrix} 5 \\ 2 \\ -1 \end{bmatrix}.$$

We can normalize this to find

$$|2\rangle = \frac{1}{30^{1/2}} \begin{bmatrix} 5 \\ 2 \\ -1 \end{bmatrix}$$

Finally, for $\omega = 4$, $\Omega - \omega I$ is

$$\Omega - 4I = \begin{bmatrix} -3 & 3 & 1 \\ 0 & -2 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

which is associated with eigenvectors parallel to

$$|3\rangle = \frac{1}{10^{1/2}} \begin{bmatrix} 1 \\ 0 \\ 3 \end{bmatrix}$$

It is clear that the original matrix is not Hermitian and that the eigenvectors are not pairwise orthogonal.

1.8.2. Consider the matrix

$$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

(1) Is it Hermitian?
(2) Find its eigenvalues and eigenvectors.
(3) Verify that $U^\dagger \Omega U$ is diagonal, $U$ being the matrix of eigenvectors of $\Omega$.

Yes, the given matrix is Hermitian. Its eigenvalues are the solutions to

$$\det(\Omega - \omega I) = \begin{vmatrix} -\omega & 0 & 1 \\ 0 & -\omega & 0 \\ 1 & 0 & -\omega \end{vmatrix} = -\omega^3 + \omega = \omega(1-\omega^2) = 0,$$

which are $\omega = 0, 1, -1$. Clearly, the normalized eigenvector corresponding to $\omega = 0$ is

$$|0\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

The remaining eigenvectors are also found by inspection,

$$|1\rangle = \frac{1}{2^{1/2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

$$|-1\rangle = \frac{1}{2^{1/2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

If we define

$$U = \frac{1}{2^{1/2}} \begin{bmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix}$$

then we see

$$\begin{aligned} U^\dagger \Omega U &= \frac{1}{2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \end{aligned}$$

1.8.3. Consider the Hermitian matrix

$$\Omega = \frac{1}{2} \begin{bmatrix} 2 & 0 & 0 \\ 0 & 3 & -1 \\ 0 & -1 & 3 \end{bmatrix}$$

(1) Show that $\omega_1 = \omega_2 = 1$; $\omega_3 = 2$.
(2) Show that $|\omega = 2\rangle$ is any vector of the form

$$\frac{1}{(2a^2)^{1/2}} \begin{bmatrix} 0 \\ a \\ -a \end{bmatrix}$$

(3) Show that the $\omega = 1$ eigenspace contains all vectors of the form

$$\frac{1}{(b^2 + 2c^2)^{1/2}} \begin{bmatrix} b \\ c \\ c \end{bmatrix}$$

either by feeding $\omega = 1$ into the equations or by requiring that the $\omega = 1$ eigenspace be orthogonal to $|\omega = 2\rangle$.

We begin by examining the characteristic equation,

$$\begin{aligned}
\det(\Omega - \omega I) &= \begin{vmatrix} 1-\omega & 0 & 0 \\ 0 & 1.5-\omega & -0.5 \\ 0 & -0.5 & 1.5-\omega \end{vmatrix}, \\
&= (1-\omega)[(1.5-\omega)^2 - 0.25], \\
&= (1-\omega)(2.25 - 3\omega + \omega^2 - 0.25), \\
&= (1-\omega)(\omega^2 - 3\omega + 2) \\
&= (1-\omega)^2(2-\omega) = 0
\end{aligned}$$

which clearly shows a repeated root at 1 and an single root at 2.

Let us examine $\Omega - 2I$,

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -0.5 & -0.5 \\ 0 & -0.5 & -0.5 \end{bmatrix}$$

Clearly, any vector of the form

$$|2'\rangle = \begin{bmatrix} 0 \\ a \\ -a \end{bmatrix}$$

will reside in the null space of this matrix. If we normalize this vector, we find

$$|2\rangle = \frac{1}{(2a^2)^{1/2}} \begin{bmatrix} 0 \\ a \\ -a \end{bmatrix}$$

For $\omega = 1$, we examine

$$\Omega - I = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0.5 & -0.5 \\ 0 & -0.5 & 0.5 \end{bmatrix}$$

In this case, all vectors within the null space of the above matrix will take the form

$$|1'\rangle = \begin{bmatrix} b \\ c \\ c \end{bmatrix}$$

Normalizing this gives

$$|1\rangle = \frac{1}{(b^2 + 2c^2)^{1/2}} \begin{bmatrix} b \\ c \\ c \end{bmatrix}$$

1.8.4. An arbitrary $n \times n$ matrix need not have $n$ eigenvectors. Consider as an example

$$\begin{bmatrix} 4 & 1 \\ -1 & 2 \end{bmatrix}$$

(1) Show that $\omega_1 = \omega_2 = 3$. (2) By feeding in this value show we get only one eigenvector of the form

$$\frac{1}{(2a^2)^{1/2}}\begin{bmatrix}+a\\-a\end{bmatrix}$$

We cannot find another one that is LI.

We begin, as always, by investigating the solutions of the characteristic equation,

$$\begin{aligned}\det(\Omega-\omega I) &= \begin{vmatrix}4-\omega & 1\\ -1 & 2-\omega\end{vmatrix},\\ &= (4-\omega)(2-\omega)+1,\\ &= 8-4\omega-2\omega+\omega^2+1,\\ &= \omega^2-6\omega+9,\\ &= (\omega-3)^2=0.\end{aligned}$$

Armed with the single solution of a repeated root at $\omega = 3$, we examine the null space of

$$\Omega - 3I = \begin{bmatrix}1 & 1\\ -1 & -1\end{bmatrix}$$

This is spanned by any (normalized) vector of the form

$$|\omega\rangle = \frac{1}{(2a^2)^{1/2}}\begin{bmatrix}+a\\-a\end{bmatrix}$$

1.8.5. Consider the matrix

$$\Omega = \begin{bmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{bmatrix}$$

(1) Show that it is unitary.
(2) Show that its eigenvalues are $e^{i\theta}$ and $e^{-i\theta}$.
(3) Find the corresponding eigenvectors; show that they are orthogonal.
(4) Verify that $U^\dagger\Omega U =$ (diagonal matrix), where $U$ is the matrix of eigenvectors of $\Omega$.

To show the unitarity of the above matrix, we need only consider the product of $\Omega$ with its conjugate transpose,

$$\begin{aligned}\Omega\Omega^\dagger &= \begin{bmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{bmatrix}\begin{bmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{bmatrix}\\ &= \begin{bmatrix}\cos^2\theta+\sin^2\theta & -\sin\theta\cos\theta+\sin\theta\cos\theta\\ -\cos\theta\sin\theta+\cos\theta\sin\theta & \sin^2\theta+\cos^2\theta\end{bmatrix}\\ &= \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\end{aligned}$$

This has the characteristic feature $\Omega\Omega^\dagger = I$ of a unitary matrix. To find the eigenvalues of this matrix, we examine its characteristic equation,

$$\det(\Omega-\omega I) = \begin{vmatrix}\cos\theta-\omega & \sin\theta\\ -\sin\theta & \cos\theta-\omega\end{vmatrix}$$

$$
\begin{aligned}
&= (\cos\theta - \omega)^2 + \sin^2\theta \\
&= \cos^2\theta - 2\omega\cos\theta + \omega^2 + \sin^2\theta \\
&= \omega^2 - 2\omega\cos\theta + 1 = 0
\end{aligned}
$$

The solutions to this are given by

$$
\begin{aligned}
\omega = & \frac{2\cos\theta \pm \sqrt{4\cos^2\theta - 4}}{2} \\
& \cos\theta \pm \sqrt{\cos^2 - 1} \\
& = \cos\theta \pm i\sin\theta \\
& = \frac{1}{2}e^{i\theta} + \frac{1}{2}e^{-i\theta} \pm \frac{1}{2}e^{i\theta} \mp \frac{1}{2}e^{-i\theta} \\
& = e^{\pm i\theta}
\end{aligned}
$$

To find the $|e^{i\theta}\rangle$ and $|e^{-i\theta}\rangle$, we may look at

$$
\begin{aligned}
\Omega - e^{i\theta}I &= \frac{1}{2}\begin{bmatrix} -(e^{i\theta} - e^{-i\theta}) & -i(e^{i\theta} - e^{-i\theta}) \\ i(e^{i\theta} - e^{-i\theta}) & -(e^{i\theta} - e^{-i\theta}) \end{bmatrix} \\
\Omega - e^{-i\theta} &= \frac{1}{2}\begin{bmatrix} e^{i\theta} - e^{-i\theta} & -i(e^{i\theta} - e^{-i\theta}) \\ i(e^{i\theta} - e^{-i\theta}) & e^{i\theta} - e^{-i\theta} \end{bmatrix}
\end{aligned}
$$

The null space each matrix is spanned by

$$
|e^{i\theta}\rangle = \frac{1}{2^{1/2}}\begin{bmatrix} i \\ 1 \end{bmatrix} \qquad |e^{-i\theta}\rangle = \frac{1}{2^{1/2}}\begin{bmatrix} -i \\ 1 \end{bmatrix}
$$

Finally, to confirm the diagonal nature of $U^\dagger\Omega U$, we compute

$$
\begin{aligned}
U^\dagger\Omega U &= \frac{1}{4}\begin{bmatrix} -i & 1 \\ i & 1 \end{bmatrix}\begin{bmatrix} e^{i\theta} + e^{-i\theta} & -i(e^{i\theta} - e^{-i\theta}) \\ i(e^{i\theta} - e^{-i\theta}) & e^{i\theta} + e^{-i\theta} \end{bmatrix}\begin{bmatrix} i & -i \\ 1 & 1 \end{bmatrix} \\
&= \frac{1}{2}\begin{bmatrix} -i & 1 \\ i & 1 \end{bmatrix}\begin{bmatrix} ie^{-i\theta} & -ie^{i\theta} \\ e^{-i\theta} & e^{i\theta} \end{bmatrix} \\
&= \begin{bmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{bmatrix}
\end{aligned}
$$

1.8.6. (1) We have seen that the determinant of a matrix is unchanged under a unitary change of basis. Argue now that

$$
\det\Omega = \text{product of eigenvalues of } \Omega = \prod_{i=1}^{n}\omega_i
$$

for a Hermitian or unitary $\Omega$.

(2) Using the invariance of the trace under the same transformation, show that

$$
\operatorname{Tr}\Omega = \sum_{i=1}^{n}\omega_i
$$

We know that $\det(\Omega) = \det(U^\dagger \Omega U)$. Because $U^\dagger \Omega U$ is a diagonal matrix consisting of the eigenvalues of $\Omega$, we have

$$\det(\Omega) = \det(U^\dagger \Omega U) = \begin{vmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_n \end{vmatrix} = \prod_{i=1}^{n} \omega_i.$$

By a similar argument, we have

$$\mathrm{Tr}(\Omega) = \mathrm{Tr}(U^\dagger \Omega U) = \mathrm{Tr} \begin{bmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_n \end{bmatrix} = \sum_{i=1}^{n} \omega_i.$$

1.8.7. By using the results on the trace and determinant from the last problem, show that the eigenvalues of the matrix

$$\Omega = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$$

are 3 and $-1$. Verify this by explicit computation. Note that the Hermitian nature of the matrix is an essential ingredient.

By inspection, we see $\det(\Omega) = -3$ and $\mathrm{Tr}(\Omega) = 2$, therefore $\omega_1\omega_2 = -3$ and $\omega_1 + \omega_2 = 2$. This holds when $\omega_1 = 3$ and $\omega_2 = -1$.

We may verify this by explicit computation. The roots of

$$\det(\Omega - \omega I) = \begin{vmatrix} 1-\omega & 2 \\ 2 & 1-\omega \end{vmatrix} = (1-\omega)^2 - 4 = \omega^2 - 2\omega - 3 = (\omega - 3)(\omega + 1)$$

are clearly $\omega_1 = 3$ and $\omega_2 = -1$.

1.8.8. Consider Hermitian matrices $M^1$, $M^2$, $M^3$, $M^4$ that obey

$$M^i M^j + M^j M^i = 2\delta^{ij} I, \qquad i, j = 1, \ldots, 4$$

(1) Show that the eigenvalues of $M^i$ are $\pm 1$. (Hint: go to the eigenbasis of $M^i$ and use the equation for $i = j$.)
(2) By considering the relation

$$M^i M^j = -M^j M^i \quad \text{for } i \neq j$$

show that $M^i$ are traceless. [Hint: $\mathrm{Tr}(ACB) = \mathrm{Tr}(CBA)$.]
(3) Show that they cannot be odd-dimensional matrices.

When $i = j$, the above relation becomes

$$(M^i)^2 = I.$$

In the eigenbasis of $M^i$, this becomes

$$\begin{bmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_n \end{bmatrix}^2 = \begin{bmatrix} \omega_1^2 & 0 & \cdots & 0 \\ 0 & \omega_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_n^2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

Put another way, for each $\omega_i$ we have the equation $\omega_i^2 = 1$. This has the solutions $\pm 1$, showing that each eigenvalue of $M^i$ is one of the two values.

Taking the trace of the relation in part (2) gives

$$\mathrm{Tr}(M^i M^j) = \mathrm{Tr}(M^j M^i) = -\mathrm{Tr}(M^j M^i) = 0,$$

where we have made use of the invariance of the trace under cyclic permutations in the second equality.

Since the trace of a matrix is also the sum of its eigenvalues, each $M^i$ must have an even number of dimensions. If it did not, we would find that its eigenvalues do not exactly cancel.

1.8.9. A collection of masses $m_\alpha$, located at $\mathbf{r}_\alpha$ and rotating with angular velocity $\omega$ around a common axis has an angular momentum

$$\mathbf{l} = \sum_\alpha m_\alpha (\mathbf{r}_\alpha \times \mathbf{v}_\alpha)$$

where $\mathbf{v}_\alpha = \omega \times \mathbf{r}_\alpha$ is the velocity of $m_\alpha$. By using the identity

$$\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B})$$

show that each Cartesian component $l_i$ of $\mathbf{l}$ is given by

$$l_i = \sum_j M_{ij} \omega_j$$

where

$$M_{ij} = \sum_\alpha m_\alpha [r_\alpha^2 \delta_{ij} - (\mathbf{r}_\alpha)_i (\mathbf{r}_\alpha)_j]$$

or in Dirac notation

$$|l\rangle = M|\omega\rangle$$

(1) Will the angular momentum and angular velocity always be parallel?
(2) Show that the moment of inertia matrix $M_{ij}$ is Hermitian.
(3) Argue now that there exist three directions for $\omega$ such that $\mathbf{l}$ and $\omega$ will be parallel. How are these directions to be found?
(4) Consider the moment of inertia matrix of a sphere. Due to the complete symmetry of the sphere, it is clear that every direction is its eigendirection for rotation. What does this say about the given three eigenvalues of the matrix $M$?

A simple application of the above identity yields

$$\begin{aligned} \mathbf{l} &= \sum_\alpha m_\alpha (\mathbf{r}_\alpha \times (\omega \times \mathbf{r}_\alpha)) \\ &= \sum_\alpha m_\alpha [\omega (r_\alpha^2) - \mathbf{r}_\alpha (\mathbf{r}_\alpha \cdot \omega)] \end{aligned}$$

which has a component form of

$$
\begin{aligned}
l_i &= \sum_\alpha m_\alpha(r_\alpha^2 \omega_i - (\mathbf{r}_\alpha)_i(\mathbf{r}_\alpha \cdot \omega)) \\
&= \sum_j \sum_\alpha m_\alpha(r_\alpha^2 \omega_i - (\mathbf{r}_\alpha)_i[(\mathbf{r}_\alpha)_j \omega_j]) \\
&= \sum_j \Big( \sum_\alpha m_\alpha [r_\alpha^2 \delta_{ij} - (\mathbf{r}_\alpha)_i(\mathbf{r}_\alpha)_j] \Big) \omega_j \\
&= \sum_j M_{ij}\omega_j
\end{aligned}
$$

From this, there is no reason to expect that the angular momentum and angular velocity will always be parallel. This would imply that all angular velocity vectors are eigenvectors of the moment of intertia matrix.

As all of the values of $M_{ij}$ are real, its Hermiticity is equivalent to it being a symmetric matrix. Since $\delta_{ij}$ and $(\mathbf{r}_\alpha)_i(\mathbf{r}_\alpha)_j$ are symmetric, so is $M_{ij}$; therefore it is Hermitian.

The three directions for which $\mathbf{l}$ and $\omega$ are parallel are those denoted by the eigenvectors of $M_{ij}$. They can be found using the same methods we have used in previous problems.

Due to the symmetry of the system, the eigenvalues of its moment of inertia matrix must be identical. If this were otherwise, a preferred direction would be implied.

1.8.10. By considering the commutator, show that the following Hermitian matrices may be simultaneously diagonalized. Find the eigenvectors common to both and verify that under a unitary transformation to this basis, both matrices are diagonalized.

$$
\Omega = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix} \qquad \Lambda = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{bmatrix}
$$

Since $\Omega$ is degenerate and $\Lambda$ is not, you must be prudent in deciding which matrix dictates the choice of basis.

We calculate each product in turn

$$
\begin{aligned}
\Omega\Lambda &= \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{bmatrix} \\
&= \begin{bmatrix} 3 & 0 & 3 \\ 0 & 0 & 0 \\ 3 & 0 & 3 \end{bmatrix} \\
\Lambda\Omega &= \begin{bmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & -1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} 3 & 0 & 3 \\ 0 & 0 & 0 \\ 3 & 0 & 3 \end{bmatrix}
\end{aligned}
$$

and so $[\Omega, \Lambda] = \Omega\Lambda - \Lambda\Omega = 0$. Since $\Lambda$ is not degenerate, we will work in its eigenbasis. We begin by finding its eigenvalues, the solutions to

$$\begin{aligned}
\det(\Lambda - \lambda I) &= \begin{vmatrix} 2-\lambda & 1 & 1 \\ 1 & -\lambda & -1 \\ 1 & -1 & 2-\lambda \end{vmatrix} \\
&= (2-\lambda)(\lambda^2 - 2\lambda - 1) - (3-\lambda) + (\lambda - 1) \\
&= -\lambda^3 + 4\lambda^2 - \lambda - 6 \\
&= -(\lambda - 3)(\lambda - 2)(\lambda + 1) = 0
\end{aligned}$$

which are $\lambda = -1, 2, 3$. The relevant degenerate matrices are

$$\begin{aligned}
\Lambda + I &= \begin{bmatrix} 3 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 3 \end{bmatrix} \\
\Lambda - 2I &= \begin{bmatrix} 0 & 1 & 1 \\ 1 & -2 & -1 \\ 1 & -1 & 0 \end{bmatrix} \\
\Lambda - 3I &= \begin{bmatrix} -1 & 1 & 1 \\ 1 & -3 & -1 \\ 1 & -1 & -1 \end{bmatrix}
\end{aligned}$$

Solving for the null space of each tells us the eigenvectors

$$\begin{aligned}
|-1\rangle &= \frac{1}{6^{1/2}} \begin{bmatrix} 1 \\ -2 \\ -1 \end{bmatrix} \\
|2\rangle &= \frac{1}{3^{1/2}} \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} \\
|3\rangle &= \frac{1}{2^{1/2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}
\end{aligned}$$

We can collect these together into a unitary matrix,

$$U = \begin{bmatrix} 1/\sqrt{6} & 1/\sqrt{3} & 1/\sqrt{2} \\ -2/\sqrt{6} & 1/\sqrt{3} & 0 \\ -1/\sqrt{6} & -1/\sqrt{3} & 1/\sqrt{2} \end{bmatrix}$$

After some tedious matrix algebra, we find

$$\begin{aligned}
U^\dagger \Lambda U &= \begin{bmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix} \\
U^\dagger \Omega U &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2 \end{bmatrix}
\end{aligned}$$

which shows that we can simultaneously diagonalize both $\Omega$ and $\Lambda$.

1.8.11. Consider the coupled mass problem discussed above.

(1) Given that the initial state is $|1\rangle$, in which the first mass is displaced by unity and the second is left alone, calculate $|1(t)\rangle$ by following the algorithm.

(2) Compare your result with that following from Eq. (1.8.39).

This amounts to resolving the above problem. By Newton's laws, it is clear that

$$m\ddot{x}_1 = -2kx_1 + kx_2$$
$$m\ddot{x}_2 = kx_1 - 2kx_2$$

Dividing by $m$ and using ket notation, this can be rewritten as

$$|\ddot{x}\rangle = \Omega|x\rangle$$

where

$$\Omega = \begin{bmatrix} -\frac{2k}{m} & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} \end{bmatrix}$$

The characteristic equation for the above matrix is

$$\det(\Omega - \omega I) = \begin{vmatrix} -\frac{2k}{m} - \omega & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} - \omega \end{vmatrix} = \left(-\frac{2k}{m} - \omega\right)^2 - \frac{k^2}{m^2} = \left(\omega + \frac{3k}{m}\right)\left(\omega + \frac{k}{m}\right) = 0$$

which has the solutions $\omega_{\text{I}} = -k/m$ and $\omega_{\text{II}} = -3k/m$. By inspection, we see that the associated eigenvectors are

$$|\omega_{\text{I}}\rangle = \frac{1}{2^{1/2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} \qquad |\omega_{\text{II}}\rangle = \frac{1}{2^{1/2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Expressing $|x\rangle$ in this basis gives the equation

$$\begin{aligned} |\omega_I\rangle\ddot{x}_{\text{I}} + |\omega_{\text{II}}\rangle\ddot{x}_{\text{II}} &= \Omega(|\omega_{\text{I}}\rangle x_{\text{I}} + |\omega_{\text{II}}\rangle x_{\text{II}}) \\ &= -\frac{k}{m}|\omega_{\text{I}}\rangle x_{\text{I}} - \frac{3k}{m}|\omega_{\text{II}}\rangle x_{\text{II}} \end{aligned}$$

or, consolidating terms,

$$|\omega_{\text{I}}\rangle\left(\ddot{x}_{\text{I}} + \frac{k}{m}x_{\text{I}}\right) + |\omega_{\text{II}}\rangle\left(\ddot{x}_{\text{II}} + \frac{3k}{m}x_{\text{II}}\right) = 0.$$

As $|\omega_{\text{I}}\rangle$ and $|\omega_{\text{II}}\rangle$ are linearly independent, this shows

$$\ddot{x}_{\text{I}} = -\frac{k}{m}x_{\text{I}}$$
$$\ddot{x}_{\text{II}} = -\frac{3k}{m}x_{\text{II}}$$

The solutions to the above equations that obey $\dot{x}_i(0) = 0$ are

$$x_{\text{I}}(t) = x_{\text{I}}(0)\cos\left[\left(\frac{k}{m}\right)^{1/2}t\right]$$
$$x_{\text{II}}(t) = x_{\text{II}}(0)\cos\left[\left(\frac{3k}{m}\right)^{1/2}t\right]$$

In vector form, this becomes

$$|x(t)\rangle = \left(|\omega_{\text{I}}\rangle\langle\omega_{\text{I}}|\cos\left[\left(\frac{k}{m}\right)^{1/2}t\right] + |\omega_{\text{II}}\rangle\langle\omega_{\text{II}}|\cos\left[\left(\frac{3k}{m}\right)^{1/2}t\right]\right)|x(0)\rangle$$

From the above, we can immediately identify

$$U(t) = |\omega_{\rm I}\rangle\langle\omega_{\rm I}| \cos\left[\left(\frac{k}{m}\right)^{1/2} t\right] + |\omega_{\rm II}\rangle\langle\omega_{\rm II}| \cos\left[\left(\frac{3k}{m}\right)^{1/2} t\right]$$
$$= \sum_{i=\rm I}^{\rm II} |\omega_i\rangle\langle\omega_i| \cos(\omega_i t)$$

To find $|1(t)\rangle$, we need to contract $U(t)$ with $|1\rangle$, then project it onto the $|1\rangle, |2\rangle$ basis.

$$\sum_{j=1}^{2} |j\rangle\langle j|U(t)|1\rangle = \frac{1}{2}\Big( \cos\left[\left(\frac{k}{m}\right)^{1/2} t\right] + | \cos\left[\left(\frac{3k}{m}\right)^{1/2} t\right]\Big)|1\rangle$$
$$+ \frac{1}{2}\Big( \cos\left[\left(\frac{k}{m}\right)^{1/2} t\right] - | \cos\left[\left(\frac{3k}{m}\right)^{1/2} t\right]\Big)|2\rangle$$

This is the same as what we would have gotten were we to directly use Eq. (1.8.39).

1.8.12. Consider once again the problem discussed in the previous example.

(1) Assuming that

$$|\ddot{x}\rangle = \Omega|x\rangle$$

has a solution

$$|x(t)\rangle = U(t)|x(0)\rangle$$

find the differential equation satisfied by $U(t)$. Use the fact that $|x(0)\rangle$ is arbitrary.

(2) Assuming (as is the case) that $\Omega$ and $U$ can be simultaneously diagonalized, solve for the elements of the matrix $U$ in this common basis and regain Eq. (1.8.43). Assume $|\dot{x}(0)\rangle = 0$.

Substituting the second equation into the first gives

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} U(t)|x(0)\rangle = \Omega|x\rangle$$

Recognizing that $|x\rangle = |x(t)\rangle = U(t)|x(0)\rangle$, we find

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} U(t)|x(0)\rangle = \Omega U(t)|x(0)\rangle$$

which encodes the condition

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} U(t) = \Omega U(t)$$

$U(t)$ satisfies the above equation when

$$U(t) = A\exp(\sqrt{\Omega}t) + B\exp(-\sqrt{\Omega}t)$$

where the exponential and square root of $\Omega$ are defined in terms of their power series. From this, we can immediately diagonalize $U(t)$ by using the eigenbasis for the component form of $\Omega$. In particular, we find

$$U(t) = A\exp\Big( \begin{bmatrix} -\frac{k}{m} & 0 \\ 0 & -\frac{3k}{m} \end{bmatrix}^{1/2} t\Big) + B\exp\Big( - \begin{bmatrix} -\frac{k}{m} & 0 \\ 0 & -\frac{3k}{m} \end{bmatrix}^{1/2} t\Big)$$
$$= A\exp\Big( \begin{bmatrix} i\sqrt{\frac{k}{m}} & 0 \\ 0 & i\sqrt{\frac{3k}{m}} \end{bmatrix} t\Big) + B\exp\Big( - \begin{bmatrix} i\sqrt{\frac{k}{m}} & 0 \\ 0 & i\sqrt{\frac{3k}{m}} \end{bmatrix} t\Big)$$

$$= A \begin{bmatrix} e^{i\sqrt{k/m}} & 0 \\ 0 & e^{i\sqrt{3k/m}} \end{bmatrix} + B \begin{bmatrix} e^{-i\sqrt{k/m}} & 0 \\ 0 & e^{-i\sqrt{3k/m}} \end{bmatrix}$$

In order for

$$|\dot{x}(0)\rangle = \frac{\mathrm{d}}{\mathrm{d}t} U(t)|x(0)\rangle = 0$$

we must have $A = B$, or

$$U(t) = 2A \begin{bmatrix} \cos\left[\left(\frac{k}{m}\right)^{1/2} t\right] & 0 \\ 0 & \cos\left[\left(\frac{3k}{m}\right)^{1/2} t\right] \end{bmatrix}$$

The condition that $U(0)|x(0)\rangle = |x(0)\rangle$ further imposes $A = \frac{1}{2}$, and so

$$U(t) = \begin{bmatrix} \cos\left[\left(\frac{k}{m}\right)^{1/2} t\right] & 0 \\ 0 & \cos\left[\left(\frac{3k}{m}\right)^{1/2} t\right] \end{bmatrix}$$

which is exactly Eq. (1.8.43).

## 1.9 Functions of Operators and Related Concepts

1.9.1. We know that the series

$$f(x) = \sum_{n=0}^{\infty} x^n$$

may be equated to the function $f(x) = (1-x)^{-1}$ if $|x| < 1$. By going to the eigenbasis, examine when the $q$ number power series

$$f(\Omega) = \sum_{n=0}^{\infty} \Omega^n$$

of a Hermitian operator $\Omega$ may be identified with $(1-\Omega)^{-1}$.

As defined for scalar functions, we know that $f(x)$ converges if and only if $|x| < 1$. Examining the equivalent matrix expression in the eigenbasis yields

$$\begin{aligned} f(\Omega) &= \sum_{n=0}^{\infty} \begin{bmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_m \end{bmatrix}^n \\ &= \sum_{n=0}^{\infty} \begin{bmatrix} \omega_1^n & 0 & \cdots & 0 \\ 0 & \omega_2^n & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_m^n \end{bmatrix} \end{aligned}$$

From this, we can immediately see that $f(\Omega)$ will converge if and only if $\omega_i < 1$ for each $i = 1, \ldots, n$.

1.9.2. If $H$ is a Hermitian operator, show that $U = e^{iH}$ is unitary. (Notice the analogy with $c$ numbers: if $\theta$ is real, $u = e^{i\theta}$ is a number of unit modulus.)

Unitarity of an operator can be shown through the property $U^\dagger U = I$. In this case, we have

$$\begin{aligned} U^\dagger U &= e^{-iH^\dagger} e^{iH} \\ &= e^{-iH} e^{iH} \\ &= I \end{aligned}$$

where in the second line we have used the fact that $H^\dagger = H$.

1.9.3. For the case above, show that $\det U = e^{i\mathrm{Tr}H}$.

In the eigenbasis of $H$, its exponentiation becomes

$$\begin{aligned} e^{iH} &= \exp\left( i \begin{bmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_m \end{bmatrix} \right) \\ &= \begin{bmatrix} e^{i\omega_1} & 0 & \cdots & 0 \\ 0 & e^{i\omega_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{i\omega_n} \end{bmatrix} \end{aligned}$$

and so the determinant of $U$ is

$$\begin{aligned} \det U &= \prod_{j=1}^{n} e^{i\omega_j} \\ &= e^{i\sum_{j=1}^{n} \omega_j} \\ &= e^{i\mathrm{Tr}\, H} \end{aligned}$$

## 1.10 Generalization to Infinite Dimensions

1.10.1. Show that $\delta(ax) = \delta(x)/|a|$. [Consider $\int \delta(ax)\,\mathrm{d}(ax)$. Remember that $\delta(x) = \delta(-x)$.]

First consider scaling the delta function argument by a positive constant $a$. We can define $u = ax$ and $\mathrm{d}u = a\mathrm{d}x$ to rewrite such a scaling as

$$\int_{-\infty}^{\infty} \delta(ax)\,\mathrm{d}x = \int_{-\infty}^{\infty} \frac{\delta(u)}{a}\,\mathrm{d}u$$

Now consider negating $a$. Making the appropriate substitutions yields

$$\int_{-\infty}^{\infty} \delta(-ax)\,\mathrm{d}x = -\int_{\infty}^{-\infty} \frac{\delta(u)}{a}\,\mathrm{d}u = \int_{-\infty}^{\infty} \frac{\delta(u)}{a}\,\mathrm{d}x$$

And so we see that $\delta(ax) = \delta(x)/|a|$.

1.10.2. Show that

$$\delta(f(x)) = \sum_i \frac{\delta(x_i - x)}{|\mathrm{d}f/\mathrm{d}x_i|}$$

where $x_i$ are the zeros of $f(x)$. Hint: Where does $\delta(f(x))$ blow up? Expand $f(x)$ near such points in a Taylor series, keeping the first nonzero term.

Clearly, the integrand of

$$\int_{-\infty}^{\infty} \delta(f(x))\,\mathrm{d}x$$

produces nonzero values only at the zeros of $f(x)$. Denoting these by $x_i$, we may rewrite the above integral as

$$\int_{-\infty}^{\infty} \delta(f(x))\,\mathrm{d}x = \sum_i \int_{x_i-\epsilon}^{x_i+\epsilon} \delta(f(x))\,\mathrm{d}x$$

Expanding $f(x)$ about each $x_i$ (keeping in mind that $f(x_i) = 0$) reveals

$$\begin{aligned}
\sum_i \int_{x_i-\epsilon}^{x_i+\epsilon} \delta(f(x))\,\mathrm{d}x &= \sum_i \int_{x_i-\epsilon}^{x_i+\epsilon} \delta\Big(f(x_i) + \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{x=x_i}(x - x_i) + \cdots\Big)\,\mathrm{d}x \\
&= \int_{x_i-\epsilon}^{x_i+\epsilon} \sum_i \delta\Big(\frac{\mathrm{d}f}{\mathrm{d}x_i}(x - x_i)\Big)\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} \sum_i \frac{\delta(x_i - x)}{|\mathrm{d}f/\mathrm{d}x_i|}\,\mathrm{d}x
\end{aligned}$$

where we have used the abuse of notation

$$\frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{x=x_i} = \frac{\mathrm{d}f}{\mathrm{d}x_i}$$

and made use of the evenness and scaling property of the delta function. Equating integrands shows

$$\delta(f(x)) = \sum_i \frac{\delta(x_i - x)}{|\mathrm{d}f/\mathrm{d}x_i|}.$$

1.10.3. Consider the *theta function* $\theta(x - x')$ which vanishes if $x - x'$ is negative and equals 1 if $x - x'$ is positive. Show that $\delta(x - x') = \mathrm{d}/\mathrm{d}x\,\theta(x - x')$.

Consider inserting $\mathrm{d}/\mathrm{d}x\,\theta(x - x')$ into an integral,

$$\lim_{\epsilon\to 0} \int_{-\infty}^{\infty} \frac{\theta(x - x' + \epsilon) - \theta(x - x')}{\epsilon} f(x)\,\mathrm{d}x$$

Since this is nonzero only between $x = x' - \epsilon$ and $x = x'$, we may rewrite the above as

$$\lim_{\epsilon\to 0} \int_{x'-\epsilon}^{x'} \frac{\theta(x - x' + \epsilon) - \theta(x - x')}{\epsilon} f(x)\,\mathrm{d}x = \lim_{\epsilon\to 0} \int_{x'-\epsilon}^{x'} \frac{1}{\epsilon} f(x)\,\mathrm{d}x$$

Just as Shankar does, we can approximate any sufficiently smooth $f$ about the point $x'$ by $f(x')$ and pull it out of the integral to get

$$f(x')\Big(\lim_{\epsilon\to 0} \int_{x'-\epsilon}^{x'} \frac{1}{\epsilon}\,\mathrm{d}x\Big)$$

The parenthesized term evaluates to 1, as it is the area under a rectangle of width $\epsilon$ and height $1/\epsilon$. Hence,

$$\delta(x - x') = \frac{\mathrm{d}}{\mathrm{d}x}\theta(x - x').$$

1.10.4. A string is displaced as follows at $t = 0$:

$$\begin{aligned} \psi(x, 0) &= \frac{2xh}{L}, & 0 \le x \le \frac{L}{2} \\ &= \frac{2h}{L}(L - x), & \frac{L}{2} \le x \le L \end{aligned}$$

Show that

$$\psi(x, t) = \sum_{m=1}^{\infty} \sin\left(\frac{m\pi x}{L}\right) \cos\omega_m t \cdot \left(\frac{8h}{\pi^2 m^2}\right) \sin\left(\frac{\pi m}{2}\right)$$

We first compute $\langle m|\psi(0)\rangle$,

$$\langle m|\psi(0)\rangle = \left(\frac{2}{L}\right)^{1/2} \int_0^{L/2} \sin\left(\frac{m\pi x}{L}\right) \frac{2xh}{L} \mathrm{d}x + \left(\frac{2}{L}\right)^{1/2} \int_{L/2}^{L} \sin\left(\frac{m\pi x}{L}\right) \frac{2h}{L}(L - x)\mathrm{d}x$$

The first term can be integrated by parts to find

$$\left(-\frac{L}{m\pi}\right) \cos\left(\frac{m\pi x}{L}\right) \frac{2xh}{L}\bigg|_0^{L/2} + \left(\frac{2}{L}\right)^{1/2} \int_0^{L/2} \left(\frac{L}{m\pi}\right) \cos\left(\frac{m\pi x}{L}\right) \frac{2h}{L} \mathrm{d}x$$

The leftmost term evaluates to 0 when $x = 0$, and

$$\left(-\frac{Lh}{m\pi}\right) \cos\left(\frac{m\pi}{2}\right)$$

at the other point. Meanwhile, the rightmost term is a simple integral of a cosine, becoming

$$\left(\frac{2}{L}\right)^{1/2} \left(\frac{2Lh}{m^2\pi^2}\right) \sin\left(\frac{m\pi}{2}\right)$$

Integrating the second term by parts, we see that it is equivalent to

$$\left(-\frac{L}{m\pi}\right) \cos\left(\frac{m\pi x}{L}\right) \frac{2h}{L}(L - x)\bigg|_{L/2}^{L} - \left(\frac{2}{L}\right)^{1/2} \int_0^{L/2} \left(\frac{L}{m\pi}\right) \cos\left(\frac{m\pi x}{L}\right) \frac{2h}{L} \mathrm{d}x$$

The leftmost term evaluates to

$$\left(\frac{Lh}{m\pi}\right) \cos\left(\frac{m\pi}{2}\right)$$

while the rightmost term becomes

$$\left(\frac{2}{L}\right)^{1/2} \left(\frac{2Lh}{m^2\pi^2}\right) \sin\left(\frac{m\pi}{2}\right) - \left(\frac{2}{L}\right)^{1/2} \left(\frac{2Lh}{m^2\pi^2}\right) \sin\left(m\pi\right) = \left(\frac{2}{L}\right)^{1/2} \left(\frac{2Lh}{m^2\pi^2}\right) \sin\left(\frac{m\pi}{2}\right)$$

Adding everything together shows that the boundary terms vanish, leaving us with

$$\langle m|\psi(0)\rangle = \left(\frac{2}{L}\right)^{1/2} \left(\frac{4Lh}{m^2\pi^2}\right) \sin\left(\frac{m\pi}{2}\right)$$

Substituting this into (1.10.59) gives us the answer

$$\begin{aligned}\psi(x,t) &= \sum_{m=1}^{\infty}\left(\frac{2}{L}\right)^{1/2}\sin\left(\frac{m\pi x}{L}\right)\cos\omega_m t\cdot\left(\frac{2}{L}\right)^{1/2}\left(\frac{4Lh}{m^2\pi^2}\right)\sin\left(\frac{m\pi}{2}\right)\\ &= \sum_{m=1}^{\infty}\sin\left(\frac{m\pi x}{L}\right)\cos\omega_m t\cdot\left(\frac{8h}{\pi^2 m^2}\right)\sin\left(\frac{m\pi}{2}\right)\end{aligned}$$

# 2 Review of Classical Mechanics

## 2.1 The Principle of Least Action and Lagrangian Mechanics

2.1.1. Consider the following system, called a *harmonic oscillator*. The block has a mass $m$ and lies on a frictionless surface. The spring has a force constant $k$. Write the Lagrangian and get the equation of motion.

From the diagram, we can immediately write

$$\mathcal{L} = T - V = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2.$$

This gives us a conjugate momentum and generalized force of

$$\frac{\partial\mathcal{L}}{\partial\dot{x}} = m\dot{x} \qquad \frac{\partial\mathcal{L}}{\partial x} = -kx$$

which can be combined to give the equation of motion,

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{x}} = m\ddot{x} = -kx = \frac{\partial\mathcal{L}}{\partial x}$$

2.1.2. Do the same for the coupled-mass problem discussed at the end of Section 1.8. Compare the equations of motion with Eqs. (1.8.24) and (1.8.25).

Returning to Figure 1.5, we can write

$$\begin{aligned}T &= \frac{1}{2}m\dot{x}_1^2 + \frac{1}{2}m\dot{x}_2^2\\ &= \frac{1}{2}m(\dot{x}_1^2 + \dot{x}_2^2)\\ V &= \frac{1}{2}kx_1^2 + \frac{1}{2}kx_2^2 + \frac{1}{2}k(x_2 - x_1)^2\\ &= k(x_1^2 - x_1x_2 + x_2^2)\end{aligned}$$

and hence

$$\mathcal{L} = T - V = \frac{1}{2}m(\dot{x}_1^2 + \dot{x}_2^2) - k(x_1^2 - x_1x_2 + x_2^2)$$

Feeding the above into the Euler-Lagrange equations gives us

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{x}_1} &= \frac{\mathrm{d}}{\mathrm{d}t}\Big(m\dot{x}_1\Big) = m\ddot{x}_1 = -2kx_1 + kx_2 = \frac{\partial\mathcal{L}}{\partial x_1}\\ \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{x}_2} &= \frac{\mathrm{d}}{\mathrm{d}t}\Big(m\dot{x}_2\Big) = m\ddot{x}_2 = x_1 - 2kx_2 = \frac{\partial\mathcal{L}}{\partial x_2}\end{aligned}$$

which is exactly Eqs. (1.8.24) and (1.8.25).

2.1.3. A particle of mass $m$ moves in three dimensions under a potential $V(r,\theta,\phi) = V(r)$. Write its $\mathcal{L}$ and find the equations of motion.

Using a similar geometric argument to Shankar, we see that the distance covered by a particle in time $\Delta t$ is

$$\mathrm{d}S = [(\mathrm{d}r)^2 + (r\sin(\theta)\mathrm{d}\phi)^2 + (r\mathrm{d}\theta)^2]$$

where $\phi$ is the azimuthal angle and $\theta$ is the inclination. This gives us a squared velocity of

$$v^2 = \dot{r}^2 + r^2\sin^2(\theta)\dot{\phi}^2 + r^2\dot{\theta}^2$$

and thus a Lagrangian of

$$\mathcal{L} = T - V = \frac{1}{2}m(\dot{r}^2 + r^2\sin^2(\theta)\dot{\phi}^2 + r^2\dot{\theta}^2) - V(r)$$

The equations of motion for this particle are given by

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{r}} &= \frac{\mathrm{d}}{\mathrm{d}t}\Big(m\dot{r}\Big) = m\ddot{r} = mr\sin^2(\theta)\dot{\phi}^2 + mr\dot{\theta}^2 - \frac{\partial V(r)}{\partial r} = \frac{\partial\mathcal{L}}{\partial r}\\ \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{\phi}} &= \frac{\mathrm{d}}{\mathrm{d}t}\Big(mr^2\sin^2(\theta)\dot{\phi}\Big) = 2mr\dot{r}\sin^2(\theta)\dot{\phi} + 2mr^2\sin(\theta)\cos(\theta)\dot{\theta}\dot{\phi} + mr^2\sin^2(\theta)\ddot{\phi} = 0 = \frac{\partial\mathcal{L}}{\partial\phi}\\ \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{\theta}} &= \frac{\mathrm{d}}{\mathrm{d}t}\Big(mr^2\dot{\theta}\Big) = 2mr\dot{r}\dot{\theta} + mr^2\ddot{\theta} = mr^2\sin(\theta)\cos(\theta)\dot{\phi}^2 = \frac{\partial\mathcal{L}}{\partial\theta}\end{aligned}$$

Simplifying, these become

$$\begin{aligned}m\ddot{r} &= mr(\dot{\phi}^2\sin^2\theta + \dot{\theta}^2) - \frac{\partial V(r)}{\partial r}\\ m\ddot{\phi} &= -2m\dot{\phi}\Big(\frac{\dot{r}}{r} - \dot{\theta}\cot\theta\Big)\\ m\ddot{\theta} &= m\Big(\dot{\phi}^2\sin\theta\cos\theta - 2\frac{\dot{r}}{r}\dot{\theta}\Big)\end{aligned}$$

## 2.3 The Two-Body Problem

2.3.1. Derive Eq. (2.3.6) from (2.3.5) by changing variables.

This is a straightforward exercise of algebra,

$$
\begin{aligned}
\mathcal{L} &= \frac{1}{2}m_1|\dot{\mathbf{r}}_1|^2 + \frac{1}{2}|\dot{\mathbf{r}}_2|^2 - V(\mathbf{r}_1 - \mathbf{r}_2) \\
&= \frac{1}{2}m_1\left|\dot{\mathbf{r}}_{\mathrm{CM}} + \frac{m_2\dot{\mathbf{r}}}{m_1+m_2}\right|^2 + \frac{1}{2}m_2\left|\dot{\mathbf{r}}_{\mathrm{CM}} - \frac{m_1\dot{\mathbf{r}}}{m_1+m_2}\right|^2 - V(\mathbf{r}) \\
&= \frac{1}{2}m_1\Big(|\dot{\mathbf{r}}_{\mathrm{CM}}|^2 + \frac{2m_2\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}_{\mathrm{CM}}}{m_1+m_2} + \frac{m_2^2|\dot{\mathbf{r}}|^2}{(m_1+m_2)^2}\Big) + \frac{1}{2}m_2\Big(|\dot{\mathbf{r}}_{\mathrm{CM}}|^2 - \frac{2m_1\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}_{\mathrm{CM}}}{m_1+m_2} + \frac{m_1^2|\dot{\mathbf{r}}|^2}{(m_1+m_2)^2}\Big) - V(\mathbf{r}) \\
&= \frac{1}{2}(m_1+m_2)|\dot{\mathbf{r}}_{\mathrm{CM}}|^2 + \frac{m_1m_2\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}_{\mathrm{CM}}}{m_1+m_2} - \frac{m_1m_2\dot{\mathbf{r}}\cdot\dot{\mathbf{r}}_{\mathrm{CM}}}{m_1+m_2} + \frac{1}{2}\frac{m_1m_2^2+m_1^2m_2}{(m_1+m_2)^2}|\dot{\mathbf{r}}|^2 - V(r) \\
&= \frac{1}{2}(m_1+m_2)|\dot{\mathbf{r}}_{\mathrm{CM}}|^2 + \frac{1}{2}\frac{m_1m_2(m_1+m_2)}{(m_1+m_2)^2}|\dot{\mathbf{r}}|^2 - V(r) \\
&= \frac{1}{2}(m_1+m_2)|\dot{\mathbf{r}}_{\mathrm{CM}}|^2 + \frac{1}{2}\frac{m_1m_2}{m_1+m_2}|\dot{\mathbf{r}}|^2 - V(r)
\end{aligned}
$$

## 2.5 The Hamiltonian Formalism

2.5.1. Show that if $T = \sum_i\sum_j T_{ij}(q)\dot{q}^i\dot{q}^j$, where $\dot{q}$'s are generalized velocities, $\sum_i p_i\dot{q}^i = 2T$.

Assuming the Lagrangian built from $T$ contains a potential term independent of velocity, the conjugate momentum to $q$ is

$$
\begin{aligned}
p_i &= \frac{\partial L}{\partial \dot{q}^i} \\
&= \frac{\partial}{\partial \dot{q}^i}\Big(\sum_j\sum_k T_{kj}(q)\dot{q}^j\dot{q}^k\Big) \\
&= \sum_j\sum_k T_{kj}(q)\frac{\partial \dot{q}^j}{\partial \dot{q}^i}\dot{q}^k + \sum_j\sum_k T_{kj}(q)\dot{q}^j\frac{\partial \dot{q}^k}{\partial \dot{q}^i} \\
&= \sum_j\sum_k T_{kj}(q)\delta_i^j\dot{q}^k + \sum_j\sum_k T_{kj}(q)\dot{q}^j\delta_i^k \\
&= \sum_k T_{ki}(q)\dot{q}^k + \sum_j T_{ij}(q)\dot{q}^j \\
&= 2\sum_j T_{ij}(q)\dot{q}^j
\end{aligned}
$$

where we have assumed that $T_{ij}$ is symmetric in the last equality. From the above, we see

$$\sum_i p_i\dot{q}^i = 2\sum_i\sum_j T_{ij}(q)\dot{q}^i\dot{q}^j = 2T.$$

2.5.2. Using the conservation of energy, show that the trajectories in phase space for the oscillator are ellipses of the form $(x/a)^2 + (p/b)^2 = 1$, where $a^2 = 2E/k$ and $b^2 = 2mE$.

The Hamiltonian (and thus the energy) for the classical harmonic oscillator is given by

$$\mathcal{H} = \frac{p^2}{2m} + \frac{k}{2}x^2 \equiv E.$$

Since energy is conserved, $\partial\mathcal{H}/\partial t = 0$ and we can divide by $E$ (a constant) to get

$$\left(\frac{p}{\sqrt{2mE}}\right)^2 + \left(\frac{x}{\sqrt{2E/k}}\right)^2 = 1,$$

or, defining $a^2 = 2E/k$ and $b^2 = 2mE$,

$$\left(\frac{x}{a}\right)^2 + \left(\frac{p}{b}\right)^2 = 1.$$

2.5.3. Solve Exercise 2.1.2 using the Hamiltonian formalism.

In this simple case, we can make the replacement $\dot{x}_i^2 \to p_i^2/m^2$ and flip the sign of $V$ in the found $\mathcal{L}$ to arrive at

$$\mathcal{H} = T + V = \frac{p_1^2 + p_2^2}{2m} + k(x_1^2 - x_1x_2 + x_2^2)$$

To obtain the dynamical equations for the system, we compute

$$\frac{\partial\mathcal{H}}{\partial p_i} = \frac{p_i}{m} = \dot{x}_i \quad \text{and} \quad -\frac{\partial\mathcal{H}}{\partial x_i} = kx_j - 2kx_i = \dot{p}_i$$

where $j \neq i$. Taking the time derivative of $\partial\mathcal{H}/\partial p_i$ allows us to substitute the resulting equations into $-\partial\mathcal{H}/\partial x_i$ to obtain

$$\ddot{x}_i = \frac{k}{m}(x_j - 2x_i)$$

which is exactly what we found in Exercise 2.1.2.

2.5.4. Show that $\mathcal{H}$ corresponding to $\mathcal{L}$ in Eq. (2.3.6) is $\mathcal{H} = |\mathbf{p}_{\mathrm{CM}}|^2/2M + |\mathbf{p}|^2/2\mu + V(\mathbf{r})$, where $M$ is the total mass, $\mu$ is the reduced mass, $\mathbf{p}_{\mathrm{CM}}$ and $\mathbf{p}$ are the momenta conjugate to $\mathbf{r}_{\mathrm{CM}}$ and $\mathbf{r}$, respectively.

Starting from the Lagrangian,

$$\begin{aligned}\mathcal{L} &= \frac{1}{2}(m_1 + m_2)|\dot{\mathbf{r}}_{\mathrm{CM}}|^2 + \frac{1}{2}\frac{m_1m_2}{m_1 + m_2}|\dot{\mathbf{r}}|^2 - V(r),\\ &= \frac{M}{2}|\dot{\mathbf{r}}_{\mathrm{CM}}|^2 + \frac{\mu}{2}|\dot{\mathbf{r}}|^2 - V(r),\end{aligned}$$

we can find the conjugate momenta to $\mathbf{r}$ and $\mathbf{r}_{\mathrm{CM}}$ via

$$\begin{aligned}\mathbf{p}_{\mathrm{CM}} &= \frac{\partial\mathcal{L}}{\partial\dot{\mathbf{r}}_{\mathrm{CM}}} = M\dot{\mathbf{r}}_{\mathrm{CM}},\\ \mathbf{p} &= \frac{\partial\mathcal{L}}{\partial\dot{\mathbf{r}}} = \mu\dot{\mathbf{r}}.\end{aligned}$$

Performing the necessary Legendre transform reveals

$$\begin{aligned}
\mathcal{H} &= \mathbf{p}\cdot\dot{\mathbf{r}} + \mathbf{p}_{\text{CM}}\cdot\dot{\mathbf{r}}_{\text{CM}} - \mathcal{L} \\
&= \frac{|\mathbf{p}|^2}{\mu} + \frac{|\mathbf{p}_{\text{CM}}|^2}{M} - \Big(\frac{M}{2}\frac{|\mathbf{p}_{\text{CM}}|^2}{M^2} + \frac{\mu}{2}\frac{|\mathbf{p}|^2}{\mu^2} - V(r)\Big) \\
&= \frac{|\mathbf{p}|^2}{2\mu} + \frac{|\mathbf{p}_{\text{CM}}|^2}{2M} + V(r)
\end{aligned}$$

## 2.7 Cyclic Coordinates, Poisson Brackets, and Canonical Transformations

2.7.1. Show that

$$\begin{aligned}
\{\omega,\lambda\} &= -\{\lambda,\omega\} \\
\{\omega,\lambda+\sigma\} &= \{\omega,\lambda\} + \{\omega,\sigma\} \\
\{\omega,\lambda\sigma\} &= \{\omega,\lambda\}\sigma + \lambda\{\omega,\sigma\}
\end{aligned}$$

Starting from the definition, we see

$$\begin{aligned}
\{\omega,\lambda\} &= \sum_i \Big(\frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i}\Big) \\
&= -\sum_i \Big(\frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i} - \frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i}\Big) \\
&= -\{\lambda,\omega\}
\end{aligned}$$

while the linearity of the partial derivative produces

$$\begin{aligned}
\{\omega,\lambda+\sigma\} &= \sum_i \Big(\frac{\partial\omega}{\partial q_i}\frac{\partial(\lambda+\sigma)}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial(\lambda+\sigma)}{\partial q_i}\Big) \\
&= \sum_i \Big(\frac{\partial\omega}{\partial q_i}\Big[\frac{\partial\lambda}{\partial p_i} + \frac{\partial\sigma}{\partial p_i}\Big] - \frac{\partial\omega}{\partial p_i}\Big[\frac{\partial\lambda}{\partial q_i} + \frac{\partial\sigma}{\partial q_i}\Big]\Big) \\
&= \sum_i \Big(\frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i} + \frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial q_i}\Big) \\
&= \sum_i \Big(\frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i}\Big) + \sum_i \Big(\frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial q_i}\Big) \\
&= \{\omega,\lambda\} + \{\omega,\sigma\}
\end{aligned}$$

and the product rule gives

$$\begin{aligned}
\{\omega,\lambda\sigma\} &= \sum_i \Big(\frac{\partial\omega}{\partial q_i}\frac{\partial(\lambda\sigma)}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial(\lambda\sigma)}{\partial q_i}\Big) \\
&= \sum_i \Big(\frac{\partial\omega}{\partial q_i}\Big[\frac{\partial\lambda}{\partial p_i}\sigma + \lambda\frac{\partial\sigma}{\partial p_i}\Big] - \frac{\partial\omega}{\partial p_i}\Big[\frac{\partial\lambda}{\partial q_i}\sigma + \lambda\frac{\partial\sigma}{\partial q_i}\Big]\Big) \\
&= \sum_i \Big(\frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i}\sigma + \lambda\frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i}\sigma - \lambda\frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial q_i}\Big)
\end{aligned}$$

$$
\begin{aligned}
&= \sum_i \Big(\frac{\partial\omega}{\partial q_i}\frac{\partial\lambda}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\lambda}{\partial q_i}\Big)\sigma + \lambda\sum_i \Big(\frac{\partial\omega}{\partial q_i}\frac{\partial\sigma}{\partial p_i} - \frac{\partial\omega}{\partial p_i}\frac{\partial\sigma}{\partial q_i}\Big) \\
&= \{\omega,\lambda\}\sigma + \lambda\{\omega,\sigma\}
\end{aligned}
$$

2.7.2. (i) Verify Eqs. (2.7.4) and (2.7.5). (ii) Consider a problem in two dimensions given by $\mathcal{H} = p_x^2 + p_y^2 + ax^2 + by^2$. Argue that if $a = b$, $\{l_z, \mathcal{H}\}$ must vanish. Verify by explicit computation.

Eq. (2.7.4) is immediately obvious from the fact that $\partial q_i/\partial q_j = \partial p_i/\partial p_j = \delta_{ij}$, and so $\{q_i, q_j\} = \{p_i, p_j\} = 0$. Furthermore,

$$
\begin{aligned}
\{q_i, p_j\} &= \sum_k \Big(\frac{\partial q_i}{\partial q_k}\frac{\partial p_j}{\partial p_k} - \frac{\partial q_i}{\partial p_k}\frac{\partial p_j}{\partial q_k}\Big) \\
&= \sum_k \delta_{ik}\delta_{jk} \\
&= \delta_{ij}
\end{aligned}
$$

For eq (2.7.5), we see

$$
\begin{aligned}
\{q_i, \mathcal{H}\} &= \sum_j \Big(\frac{\partial q_i}{\partial q_j}\frac{\partial \mathcal{H}}{\partial p_j} - \frac{\partial q_i}{\partial p_j}\frac{\partial \mathcal{H}}{\partial q_j}\Big) \\
&= \sum_j \delta_{ij}\frac{\partial \mathcal{H}}{\partial p_j} \\
&= \frac{\partial \mathcal{H}}{\partial p_i} \\
&= \dot{q}_i
\end{aligned}
$$

and

$$
\begin{aligned}
\{p_i, \mathcal{H}\} &= \sum_j \Big(\frac{\partial p_i}{\partial q_j}\frac{\partial \mathcal{H}}{\partial p_j} - \frac{\partial p_i}{\partial p_j}\frac{\partial \mathcal{H}}{\partial q_j}\Big) \\
&= -\sum_j \delta_{ij}\frac{\partial \mathcal{H}}{\partial q_j} \\
&= -\frac{\partial \mathcal{H}}{\partial q_i} \\
&= \dot{p}_i
\end{aligned}
$$

If $a = b$ in the given Hamiltonian, the potential energy is dependent only on the radial distance from the origin, i.e. the Hamiltonian is circularly symmetric. With no preferred direction in space, we expect $l_z$ to be conserved, or $\{l_z, \mathcal{H}\} = 0$. We can verify this explicitly via by noting that

$$
\begin{aligned}
\frac{\partial l_z}{\partial x} &= \frac{\partial}{\partial x}(xp_y - yp_x) = p_y \\
\frac{\partial l_z}{\partial y} &= \frac{\partial}{\partial y}(xp_y - yp_x) = -p_x \\
\frac{\partial l_z}{\partial p_x} &= \frac{\partial}{\partial p_x}(xp_y - yp_x) = -y
\end{aligned}
$$

$$\frac{\partial l_z}{\partial p_y} = \frac{\partial}{\partial p_y}(xp_y - yp_x) = x$$

and

$$\begin{aligned}
\frac{\partial \mathcal{H}}{\partial x} &= \frac{\partial}{\partial x}(p_x^2 + p_y^2 + ax^2 + by^2) = 2ax \\
\frac{\partial \mathcal{H}}{\partial y} &= \frac{\partial}{\partial y}(p_x^2 + p_y^2 + ax^2 + by^2) = 2by \\
\frac{\partial \mathcal{H}}{\partial p_x} &= \frac{\partial}{\partial p_x}(p_x^2 + p_y^2 + ax^2 + by^2) = 2p_x \\
\frac{\partial \mathcal{H}}{\partial p_y} &= \frac{\partial}{\partial p_y}(p_x^2 + p_y^2 + ax^2 + by^2) = 2p_y
\end{aligned}$$

and so, with $a = b$,

$$\begin{aligned}
\{l_z, \mathcal{H}\} &= \frac{\partial l_z}{\partial x}\frac{\partial \mathcal{H}}{\partial p_x} - \frac{\partial l_z}{\partial p_x}\frac{\partial \mathcal{H}}{\partial x} + \frac{\partial l_z}{\partial y}\frac{\partial \mathcal{H}}{\partial p_y} - \frac{\partial l_z}{\partial p_y}\frac{\partial \mathcal{H}}{\partial y} \\
&= (p_y)(2p_x) - (-y)(2ax) + (-p_x)(2p_y) - (x)(2ay) \\
&= 2p_xp_y - 2p_xp_y + 2axy - 2axy \\
&= 0
\end{aligned}$$

2.7.3. Fill in the missing steps leading to Eq. (2.7.18) starting from Eq. (2.7.14).

If we view $\mathcal{H}$ as a function of $\bar{q}$ and $\bar{p}$, we find

$$\begin{aligned}
\dot{\bar{q}}_j &= \{\bar{q}, \mathcal{H}\} \\
&= \sum_i \Big(\frac{\partial \bar{q}_j}{\partial q_i}\frac{\partial \mathcal{H}}{\partial p_i} - \frac{\partial \bar{q}_j}{\partial p_i}\frac{\partial \mathcal{H}}{\partial q_i}\Big) \\
&= \sum_i \Big(\frac{\partial \bar{q}_j}{\partial q_i}\Big[\sum_k \frac{\partial \mathcal{H}}{\partial \bar{q}_k}\frac{\partial \bar{q}_k}{\partial p_i} + \frac{\partial \mathcal{H}}{\partial \bar{p}_k}\frac{\partial \bar{p}_k}{\partial p_i}\Big] - \frac{\partial \bar{q}_j}{\partial p_i}\Big[\sum_l \frac{\partial \mathcal{H}}{\partial \bar{q}_l}\frac{\partial \bar{q}_l}{\partial q_i} + \frac{\partial \mathcal{H}}{\partial \bar{p}_l}\frac{\partial \bar{p}_l}{\partial q_i}\Big]\Big) \\
&= \sum_i \sum_k \Big(\frac{\partial \bar{q}_j}{\partial q_i}\frac{\partial \mathcal{H}}{\partial \bar{q}_k}\frac{\partial \bar{q}_k}{\partial p_i} + \frac{\partial \bar{q}_j}{\partial q_i}\frac{\partial \mathcal{H}}{\partial \bar{p}_k}\frac{\partial \bar{p}_k}{\partial p_i} - \frac{\partial \bar{q}_j}{\partial p_i}\frac{\partial \mathcal{H}}{\partial \bar{q}_k}\frac{\partial \bar{q}_k}{\partial q_i} - \frac{\partial \bar{q}_j}{\partial p_i}\frac{\partial \mathcal{H}}{\partial \bar{p}_k}\frac{\partial \bar{p}_k}{\partial q_i}\Big) \\
&= \sum_k \Big(\frac{\partial \mathcal{H}}{\partial \bar{q}_k}\Big[\sum_i \frac{\partial \bar{q}_j}{\partial q_i}\frac{\partial \bar{q}_k}{\partial p_i} - \frac{\partial \bar{q}_j}{\partial p_i}\frac{\partial \bar{q}_k}{\partial q_i}\Big] + \frac{\partial \mathcal{H}}{\partial \bar{p}_k}\Big[\sum_i \frac{\partial \bar{q}_j}{\partial q_i}\frac{\partial \bar{p}_k}{\partial p_i} - \frac{\partial \bar{q}_j}{\partial p_i}\frac{\partial \bar{p}_k}{\partial q_i}\Big]\Big) \\
&= \sum_k \Big(\frac{\partial \mathcal{H}}{\partial \bar{q}_k}\{\bar{q}_j, \bar{q}_k\} + \frac{\partial \mathcal{H}}{\partial \bar{p}_k}\{\bar{q}_j, \bar{p}_k\}\Big)
\end{aligned}$$

We can find $\dot{\bar{p}}_j$ by exchanging $\bar{q}_j$ for $\bar{p}_j$ in the result above,

$$\dot{\bar{p}}_j = \Big(\frac{\partial \mathcal{H}}{\partial \bar{q}_k}\{\bar{p}_j, \bar{q}_k\} + \frac{\partial \mathcal{H}}{\partial \bar{p}_k}\{\bar{p}_j, \bar{p}_k\}\Big)$$

In order for these to reduce to the canonical equations,

$$\dot{\bar{q}}_k = \frac{\partial \mathcal{H}}{\partial \bar{p}_k} \qquad \dot{\bar{p}}_k = -\frac{\partial \mathcal{H}}{\partial \bar{q}_k}$$

we must have $\{\bar{q}_j, \bar{q}_k\} = \{\bar{p}_j, \bar{p}_k\} = 0$ and $\{\bar{q}_j, \bar{p}_k\} = -\{\bar{p}_k, \bar{q}_j\} = \delta_{jk}$.

2.7.4. Verify that the change to a rotated frame

$$\begin{aligned}
\bar{x} &= x\cos\theta - y\sin\theta \\
\bar{y} &= x\sin\theta + y\cos\theta \\
\bar{p}_x &= p_x\cos\theta - p_y\sin\theta \\
\bar{p}_y &= p_x\sin\theta + p_y\cos\theta
\end{aligned}$$

is a canonical transformation.

From the above, we immediately see $\{\bar{x},\bar{y}\} = \{\bar{p}_x,\bar{p}_y\} = 0$ and

$$\begin{aligned}
\{\bar{x},\bar{p}_x\} &= \frac{\partial\bar{x}}{\partial x}\frac{\partial\bar{p}_x}{\partial p_x} - \frac{\partial\bar{x}}{\partial p_x}\frac{\partial\bar{p}_x}{\partial x} + \frac{\partial\bar{x}}{\partial y}\frac{\partial\bar{p}_x}{\partial p_y} - \frac{\partial\bar{x}}{\partial p_y}\frac{\partial\bar{p}_x}{\partial y} \\
&= \cos^2\theta + \sin^2\theta \\
&= 1 \\
\{\bar{x},\bar{p}_y\} &= \frac{\partial\bar{x}}{\partial x}\frac{\partial\bar{p}_y}{\partial p_x} - \frac{\partial\bar{x}}{\partial p_x}\frac{\partial\bar{p}_y}{\partial x} + \frac{\partial\bar{x}}{\partial y}\frac{\partial\bar{p}_y}{\partial p_y} - \frac{\partial\bar{x}}{\partial p_y}\frac{\partial\bar{p}_y}{\partial y} \\
&= \cos\theta\sin\theta - \sin\theta\cos\theta \\
&= 0 \\
\{\bar{y},\bar{p}_y\} &= \frac{\partial\bar{y}}{\partial x}\frac{\partial\bar{p}_y}{\partial p_x} - \frac{\partial\bar{y}}{\partial p_x}\frac{\partial\bar{p}_y}{\partial x} + \frac{\partial\bar{y}}{\partial y}\frac{\partial\bar{p}_y}{\partial p_y} - \frac{\partial\bar{y}}{\partial p_y}\frac{\partial\bar{p}_y}{\partial y} \\
&= \sin^2\theta + \cos^2\theta \\
&= 1 \\
\{\bar{y},\bar{p}_x\} &= \frac{\partial\bar{y}}{\partial x}\frac{\partial\bar{p}_x}{\partial p_x} - \frac{\partial\bar{y}}{\partial p_x}\frac{\partial\bar{p}_x}{\partial x} + \frac{\partial\bar{y}}{\partial y}\frac{\partial\bar{p}_x}{\partial p_y} - \frac{\partial\bar{y}}{\partial p_y}\frac{\partial\bar{p}_x}{\partial y} \\
&= \sin\theta\cos\theta - \sin\theta\cos\theta \\
&= 0
\end{aligned}$$

i.e. $\{\bar{q}_j,\bar{q}_k\} = \{\bar{p}_j,\bar{p}_k\} = 0$ and $\{\bar{q}_j,\bar{p}_k\} = -\{\bar{p}_k,\bar{q}_j\} = \delta_{jk}$—the transformation is canonical.

2.7.5. Show that the polar variables $\rho = (x^2+y^2)^{1/2}$, $\phi = \tan^{-1}(y/x)$,

$$p_\rho = \hat{e}_\rho \cdot \mathbf{p} = \frac{xp_x + yp_y}{(x^2+y^2)^{1/2}}, \quad p_\phi = xp_y - yp_x (= l_z)$$

are canonical. ($\hat{e}_\rho$ is the unit vector in the radial direction.)

First we collect the necessary derivatives,

$$\frac{\partial\rho}{\partial x} = \frac{x}{(x^2+y^2)^{1/2}} \qquad \frac{\partial\rho}{\partial y} = \frac{y}{(x^2+y^2)^{1/2}} \qquad \frac{\partial\rho}{\partial p_x} = 0 \qquad \frac{\partial\rho}{\partial p_y} = 0$$

$$\frac{\partial\phi}{\partial x} = -\frac{y}{x^2+y^2} \qquad \frac{\partial\phi}{\partial y} = \frac{x}{x^2+y^2} \qquad \frac{\partial\phi}{\partial p_x} = 0 \qquad \frac{\partial\phi}{\partial p_y} = 0$$

$$\frac{\partial p_\rho}{\partial x} = -\frac{y(p_y x - p_x y)}{(x^2+y^2)^{3/2}} \qquad \frac{\partial p_\rho}{\partial y} = -\frac{x(p_x y - p_y x)}{(x^2+y^2)^{3/2}} \qquad \frac{\partial p_\rho}{\partial p_x} = \frac{x}{(x^2+y^2)^{1/2}} \qquad \frac{\partial p_\rho}{\partial p_y} = \frac{y}{(x^2+y^2)^{1/2}}$$

$$\frac{\partial p_\phi}{\partial x} = p_y \qquad \frac{\partial p_\phi}{\partial y} = -p_x \qquad \frac{\partial p_\phi}{\partial p_x} = -y \qquad \frac{\partial p_\phi}{\partial p_y} = x$$

From these, we can compute the Poisson bracket of all variable combinations. Clearly the Poisson bracket of any coordinate (or conjugate momenta) with itself is 0, so we need only check those that differ:

$$\begin{aligned}
\{\rho, \phi\} &= \frac{\partial \rho}{\partial x}\frac{\partial \phi}{\partial p_x} - \frac{\partial \rho}{\partial p_x}\frac{\partial \phi}{\partial x} + \frac{\partial \rho}{\partial y}\frac{\partial \phi}{\partial p_y} - \frac{\partial \rho}{\partial p_y}\frac{\partial \phi}{\partial y} \\
&= 0 \\
\{p_\rho, p_\phi\} &= \frac{\partial p_\rho}{\partial x}\frac{\partial p_\phi}{\partial p_x} - \frac{\partial p_\rho}{\partial p_x}\frac{\partial p_\phi}{\partial x} + \frac{\partial p_\rho}{\partial y}\frac{\partial p_\phi}{\partial p_y} - \frac{\partial p_\rho}{\partial p_y}\frac{\partial p_\phi}{\partial y} \\
&= \frac{y^2(p_y x - p_x y)}{(x^2+y^2)^{3/2}} - \frac{p_y x}{(x^2+y^2)^{1/2}} - \frac{x^2(p_x y - p_y x)}{(x^2+y^2)^{3/2}} + \frac{p_x y}{(x^2+y^2)^{1/2}} \\
&= \frac{p_y x - p_x y}{(x^2+y^2)^{1/2}} - \frac{p_y x - p_x y}{(x^2+y^2)^{1/2}} \\
&= 0 \\
\{\rho, p_\rho\} &= \frac{\partial \rho}{\partial x}\frac{\partial p_\rho}{\partial p_x} - \frac{\partial \rho}{\partial p_x}\frac{\partial p_\rho}{\partial x} + \frac{\partial \rho}{\partial y}\frac{\partial p_\rho}{\partial p_y} - \frac{\partial \rho}{\partial p_y}\frac{\partial p_\rho}{\partial y} \\
&= \frac{x^2}{x^2+y^2} + \frac{y^2}{x^2+y^2} \\
&= 1 \\
\{\rho, p_\phi\} &= \frac{\partial \rho}{\partial x}\frac{\partial p_\phi}{\partial p_x} - \frac{\partial \rho}{\partial p_x}\frac{\partial p_\phi}{\partial x} + \frac{\partial \rho}{\partial y}\frac{\partial p_\phi}{\partial p_y} - \frac{\partial \rho}{\partial p_y}\frac{\partial p_\phi}{\partial y} \\
&= -xy + xy \\
&= 0 \\
\{\phi, p_\rho\} &= \frac{\partial \phi}{\partial x}\frac{\partial p_\rho}{\partial p_x} - \frac{\partial \phi}{\partial p_x}\frac{\partial p_\rho}{\partial x} + \frac{\partial \phi}{\partial y}\frac{\partial p_\rho}{\partial p_y} - \frac{\partial \phi}{\partial p_y}\frac{\partial p_\rho}{\partial y} \\
&= -\frac{xy}{(x^2+y^2)^{3/2}} + \frac{xy}{(x^2+y^2)^{3/2}} \\
&= 0 \\
\{\phi, p_\phi\} &= \frac{\partial \phi}{\partial x}\frac{\partial p_\phi}{\partial p_x} - \frac{\partial \phi}{\partial p_x}\frac{\partial p_\phi}{\partial x} + \frac{\partial \phi}{\partial y}\frac{\partial p_\phi}{\partial p_y} - \frac{\partial \phi}{\partial p_y}\frac{\partial p_\phi}{\partial y} \\
&= \frac{y^2}{x^2+y^2} + \frac{x^2}{x^2+y^2} \\
&= 1
\end{aligned}$$

2.7.6. Verify that the change from the variables $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{p}_1$, $\mathbf{p}_2$ to $\mathbf{r}_{\text{CM}}$, $\mathbf{p}_{\text{CM}}$, $\mathbf{r}$, and $\mathbf{p}$ is a canonical transformation. (See Exercise 2.5.4).

The new variables are defined by

$$\begin{aligned}
\mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2 \\
\mathbf{p} &= \frac{m_1 m_2}{m_1+m_2}\left(\frac{\mathbf{p}_1}{m_1} - \frac{\mathbf{p}_2}{m_2}\right) \\
\mathbf{r}_{\text{CM}} &= \frac{1}{m_1+m_2}\left(m_1\mathbf{r}_1 + m_2\mathbf{r}_2\right)
\end{aligned}$$

$$\mathbf{p}_{\text{CM}} = \mathbf{p}_1 + \mathbf{p}_2$$

Because these are linear relationships, we can work entirely in the Poisson algebra,

$$\begin{aligned}
\{\mathbf{r}, \mathbf{p}\} &= \frac{m_1 m_2}{m_1 + m_2}\{\mathbf{r}_1 - \mathbf{r}_2, \frac{\mathbf{p}_1}{m_1} - \frac{\mathbf{p}_2}{m_2}\} \\
&= \frac{m_2}{m_1 + m_2}\{\mathbf{r}_1, \mathbf{p}_1\} + \frac{m_1}{m_1 + m_2}\{\mathbf{r}_2, \mathbf{p}_2\} \\
&= \frac{m_2 + m_1}{m_1 + m_2} \\
&= 1 \\
\{\mathbf{r}, \mathbf{p}_{\text{CM}}\} &= \{\mathbf{r}_1 - \mathbf{r}_2, \mathbf{p}_1 + \mathbf{p}_2\} \\
&= \{\mathbf{r}_1, \mathbf{p}_1\} - \{\mathbf{r}_2, \mathbf{p}_2\} \\
&= 1 - 1 \\
&= 0 \\
\{\mathbf{r}_{\text{CM}}, \mathbf{p}\} &= \frac{m_1 m_2}{(m_1 + m_2)^2}\{m_1\mathbf{r}_1 + m_2\mathbf{r}_2, \frac{\mathbf{p}_1}{m_1} - \frac{\mathbf{p}_2}{m_2}\} \\
&= \frac{m_1 m_2}{(m_1 + m_2)^2}(\{\mathbf{r}_1, \mathbf{p}_1\} - \{\mathbf{r}_2, \mathbf{p}_2\}) \\
&= \frac{m_1 m_2}{(m_1 + m_2)^2}(1 - 1) \\
&= 0 \\
\{\mathbf{r}_{\text{CM}}, \mathbf{p}_{\text{CM}}\} &= \frac{1}{m_1 + m_2}\{m_1\mathbf{r}_1 + m_2\mathbf{r}_2, \mathbf{p}_1 + \mathbf{p}_2\} \\
&= \frac{m_1}{m_1 + m_2}\{\mathbf{r}_1, \mathbf{p}_1\} + \frac{m_2}{m_1 + m_2}\{\mathbf{r}_2, \mathbf{p}_2\} \\
&= \frac{m_1 + m_2}{m_1 + m_2} \\
&= 1
\end{aligned}$$

All other combinations are trivially 0, implying that the transformation is canonical.

2.7.7. Verify that

$$\begin{aligned}
\bar{q} &= \ln(q^{-1} \sin p) \\
\bar{p} &= q \cot p
\end{aligned}$$

is a canonical transformation.

Once again collecting derviatives,

$$\begin{aligned}
\frac{\partial \bar{q}}{\partial q} &= -\frac{1}{q} & \frac{\partial \bar{q}}{\partial p} &= \cot p \\
\frac{\partial \bar{p}}{\partial q} &= \cot p & \frac{\partial \bar{p}}{\partial p} &= -q \csc^2 p
\end{aligned}$$

we find

$$\{\bar{q}, \bar{p}\} = \csc^2 p - \cot^2 p$$

$$= 1$$

where this identity can be seen from

$$\cos^2 p + \sin^2 p = 1$$

and so

$$\cot^2 p + 1 = \csc^2 p.$$

As this is the only nontrivial combination we are done: the transformation is canonical.

2.7.8. We would like to derive here Eq. (2.7.9), which gives the transformation of the momenta under a coordinate transformation in configuration space:

$$q_i \to \bar{q}_i(q_1, \ldots, q_n)$$

(1) Argue that if we invert the above equation to get $q = q(\bar{q})$, we can derive the following counterpart of Eq. (2.7.7):

$$\dot{q}_i = \sum_j \frac{\partial q_i}{\partial \bar{q}_j} \dot{\bar{q}}_j$$

(2) Show from the above that

$$\left(\frac{\partial \dot{q}_i}{\partial \dot{\bar{q}}_j}\right)_{\bar{q}} = \frac{\partial q_i}{\partial \bar{q}_j}$$

(3) Now calculate

$$\bar{p}_i = \left[\frac{\partial \mathcal{L}(\bar{q}, \dot{\bar{q}})}{\partial \dot{\bar{q}}_i}\right]_{\bar{q}} = \left[\frac{\partial \mathcal{L}(q, \dot{q})}{\partial \dot{\bar{q}}_i}\right]_{\bar{q}}$$

Use the chain rule and the fact that $q = q(\bar{q})$ and note $q(\bar{q}, \dot{\bar{q}})$ to derive Eq. (2.7.9).

(4) Verify, by calculating the PB in Eq. (2.7.18), that the point transformation is canonical.

The first step is simply applying the chain rule when taking the total time derivative of $q_i = q_i(\bar{q}_1, \ldots \bar{q}_n)$, yielding

$$\dot{q}_i = \sum_k \frac{\partial q_i}{\partial \bar{q}_k} \dot{\bar{q}}_k.$$

Taking the partial derivative of this with respect to a particular $\dot{\bar{q}}_j$ gives

$$\frac{\partial \dot{q}_i}{\partial \dot{\bar{q}}_j} = \sum_k \frac{\partial q_i}{\partial \bar{q}_k} \frac{\partial \dot{\bar{q}}_k}{\partial \dot{\bar{q}}_j} = \sum_k \frac{\partial q_i}{\partial \bar{q}_k} \delta_{kj} = \frac{\partial q_i}{\partial \bar{q}_j},$$

where we have used the fact that $\partial q_i / \partial \bar{q}_k$ is independent of $\dot{\bar{q}}_j$.

Differentiating the Lagrangian with respect to $\dot{\bar{q}}_i$ gives

$$\bar{p}_i = \frac{\partial \mathcal{L}(q, \dot{q})}{\partial \dot{\bar{q}}_i} = \sum_j \frac{\partial \mathcal{L}}{\partial q_j} \frac{\partial q_j}{\partial \dot{\bar{q}}_i} + \frac{\partial \mathcal{L}}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial \dot{\bar{q}}_i} = \sum_j \frac{\partial q_j}{\partial \bar{q}_i} p_j$$

where we have used $q = q(\bar{q})$ and so $\partial q_j / \partial \dot{\bar{q}}_i = 0$.

We skip verification of the invariance of the Poisson bracket, noting the fact that $\bar{p}_i$ defined this way guarantees canonical phase space coordiantes.

2.7.9. Verify Eq. (2.7.19) by direct computation. Use the chain rule to go from $q, p$ derivatives to $\bar{q}, \bar{p}$ derivatives. Collect terms that represent PB of the latter.

Canonical transformations must obey $\dot{\bar{q}}_i = \frac{\partial \mathcal{H}}{\partial \bar{p}}$. Expanded out, this requirement becomes

$$\begin{aligned}
\frac{\mathrm{d}\bar{q}_i}{\mathrm{d}t} &= \sum_j \frac{\partial \bar{q}_i}{\partial q_j}\frac{\partial q_j}{\partial t} + \frac{\partial \bar{q}_i}{\partial p_j}\frac{\partial p_j}{\partial t} \\
&= \sum_j \frac{\partial \bar{q}_i}{\partial q_j}\frac{\partial \mathcal{H}}{\partial p_j} - \frac{\partial \bar{q}_i}{\partial p_j}\frac{\partial \mathcal{H}}{\partial q_j} \\
&= \frac{\partial \mathcal{H}}{\partial \bar{p}_i} \\
&= \sum_j \frac{\partial \mathcal{H}}{\partial q_j}\frac{\partial q_j}{\partial \bar{p}_i} + \frac{\partial \mathcal{H}}{\partial p_j}\frac{\partial p_j}{\partial \bar{p}_i}
\end{aligned}$$

i.e. $\partial q_j/\partial \bar{p}_i = -\partial \bar{q}_i/\partial p_j$ and $\partial p_j/\partial \bar{p}_i = \partial \bar{q}_i/\partial q_j$. Using this last relationship makes this verification especially easy, as

$$\begin{aligned}
\{\omega, \sigma\}_{q,p} &= \sum_i \frac{\partial \omega}{\partial q_i}\frac{\partial \sigma}{\partial p_i} - \frac{\partial \omega}{\partial p_i}\frac{\partial \sigma}{\partial q_i} \\
&= \sum_{i,j,k} \frac{\partial \omega}{\partial \bar{q}_j}\frac{\partial \bar{q}_j}{\partial q_i}\frac{\partial \sigma}{\partial \bar{p}_k}\frac{\partial \bar{p}_k}{\partial p_i} - \frac{\partial \omega}{\partial \bar{p}_k}\frac{\partial \bar{p}_k}{\partial p_i}\frac{\partial \sigma}{\partial \bar{q}_j}\frac{\partial \bar{q}_j}{\partial q_i} \\
&= \sum_{j,k} \left(\frac{\partial \omega}{\partial \bar{q}_j}\frac{\partial \sigma}{\partial \bar{p}_k} - \frac{\partial \omega}{\partial \bar{p}_k}\frac{\partial \sigma}{\partial \bar{q}_j}\right) \sum_i \frac{\partial \bar{q}_j}{\partial q_i}\frac{\partial \bar{p}_k}{\partial p_i} \\
&= \sum_{j,k} \left(\frac{\partial \omega}{\partial \bar{q}_j}\frac{\partial \sigma}{\partial \bar{p}_k} - \frac{\partial \omega}{\partial \bar{p}_k}\frac{\partial \sigma}{\partial \bar{q}_j}\right) \sum_i \frac{\partial p_i}{\partial \bar{p}_j}\frac{\partial \bar{p}_k}{\partial p_i} \\
&= \sum_{j,k} \left(\frac{\partial \omega}{\partial \bar{q}_j}\frac{\partial \sigma}{\partial \bar{p}_k} - \frac{\partial \omega}{\partial \bar{p}_k}\frac{\partial \sigma}{\partial \bar{q}_j}\right) \frac{\partial \bar{p}_k}{\partial p_j} \\
&= \sum_{j,k} \left(\frac{\partial \omega}{\partial \bar{q}_j}\frac{\partial \sigma}{\partial \bar{p}_k} - \frac{\partial \omega}{\partial \bar{p}_k}\frac{\partial \sigma}{\partial \bar{q}_j}\right) \delta_{kj} \\
&= \sum_j \frac{\partial \omega}{\partial \bar{q}_j}\frac{\partial \sigma}{\partial \bar{p}_j} - \frac{\partial \omega}{\partial \bar{p}_j}\frac{\partial \sigma}{\partial \bar{q}_j} \\
&= \{\omega, \sigma\}_{\bar{q},\bar{p}}
\end{aligned}$$

## 2.8 Symmetries and Their Consequences

2.8.1. Show that $p = p_1 + p_2$, the total momentum, is the generator of infinitesimal translations for a two-particle system.

A generic two-particle system has the Hamiltonian

$$\mathcal{H} = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(q_1 - q_2)$$

Consider the generator

$$g(q,p) = p_1 + p_2$$

which has the partial derivatives

$$\frac{\partial g}{\partial q_i} = 0 \quad \text{and} \quad \frac{\partial g}{\partial p_i} = 1 \quad \text{for } i = 1, 2.$$

Under the canonical transformation

$$\begin{aligned}
q_i &\to q_i + \varepsilon \frac{\partial g}{\partial p_i} = q_i + \varepsilon \\
p_i &\to p_i - \varepsilon \frac{\partial g}{\partial q_i} = p_i
\end{aligned}$$

the Hamiltonian is clearly left unchanged. Physically, this transformation can be seen as a spatial translation, offsetting the positions of the particles by an amount $\varepsilon$.

2.8.2. Verify that the infinitesimal transformation generated by any dynamical variables $g$ is a canonical transformation. (Hint: Work, as usual, to first order in $\varepsilon$.)

This process is made easier if we first examine the Poisson bracket of $\{q_i, f\}$ and $\{p_i, f\}$ for an arbitrary well-behaved function $f(q,p)$,

$$\begin{aligned}
\{q_i, f\} &= \sum_k \frac{\partial q_i}{\partial q_k}\frac{\partial f}{\partial p_k} - \frac{\partial q_i}{\partial p_k}\frac{\partial f}{\partial q_k} \\
&= \sum_k \delta_{ik} \frac{\partial f}{\partial p_k} \\
&= \frac{\partial f}{\partial p_i} \\
\{p_i, f\} &= \sum_k \frac{\partial p_i}{\partial q_k}\frac{\partial f}{\partial p_k} - \frac{\partial p_i}{\partial p_k}\frac{\partial f}{\partial q_k} \\
&= -\sum_k \delta_{ik} \frac{\partial f}{\partial q_k} \\
&= -\frac{\partial f}{\partial q_i}
\end{aligned}$$

where we have used the fact that phase space coordinates are independent of one another. Remembering the Jacobi identity, we proceed to check that the given transformation preserves the Poisson bracket. For the position coordinates we have

$$\begin{aligned}
\{\bar{q}_i, \bar{q}_j\} &= \{q_i + \varepsilon \frac{\partial g}{\partial p_i}, q_j + \varepsilon \frac{\partial g}{\partial p_j}\} \\
&= \{q_i, q_j\} + \varepsilon \Big(\{q_i, \frac{\partial g}{\partial p_j}\} + \{\frac{\partial g}{\partial p_i}, q_j\}\Big) + \mathcal{O}(\varepsilon^2) \\
&= \varepsilon \Big(\{q_i, \{q_j, g\}\} + \{\{q_i, g\}, q_j\}\Big) \\
&= \varepsilon \Big(\{q_i, \{q_j, g\}\} + \{q_j, \{g, q_i\}\}\Big) \\
&= -\varepsilon \{g, \{q_i, q_j\}\}
\end{aligned}$$

$$
\begin{aligned}
&= -\varepsilon\{g, 0\} \\
&= 0
\end{aligned}
$$

while the momenta coordinates are

$$
\begin{aligned}
\{\bar{p}_i, \bar{p}_j\} &= \{p_i - \varepsilon\frac{\partial g}{\partial q_i}, p_j - \varepsilon\frac{\partial g}{\partial q_j}\} \\
&= \{p_i, p_j\} - \varepsilon\Big(\{p_i, \frac{\partial g}{\partial q_j}\} + \{\frac{\partial g}{\partial q_i}, p_j\}\Big) + \mathcal{O}(\varepsilon^2) \\
&= -\varepsilon\Big(\{p_i, \{g, p_j\}\} + \{\{g, p_i\}, p_j\}\Big) \\
&= -\varepsilon\Big(\{p_i, \{g, p_j\}\} + \{p_j, \{p_i, g\}\}\Big) \\
&= \varepsilon\{g, \{p_i, p_j\}\} \\
&= \varepsilon\{g, 0\} \\
&= 0
\end{aligned}
$$

Finally, the Poisson bracket of an arbitrary pair of position and momentum coordinates is given by

$$
\begin{aligned}
\{\bar{q}_i, \bar{p}_j\} &= \{q_i + \varepsilon\frac{\partial g}{\partial p_i}, p_j - \varepsilon\frac{\partial g}{\partial q_j}\} \\
&= \{q_i, p_j\} - \varepsilon\Big(\{q_i, \frac{\partial g}{\partial q_j}\} - \{\frac{\partial g}{\partial p_i}, p_j\}\Big) + \mathcal{O}(\varepsilon^2) \\
&= \delta_{ij} - \varepsilon\Big(\{q_i, \{g, p_j\}\} - \{\{q_i, g\}, p_j\}\Big) \\
&= \delta_{ij} - \varepsilon\Big(\{q_i, \{g, p_j\}\} + \{p_j, \{q_i, g\}\}\Big) \\
&= \delta_{ij} + \varepsilon\{g, \{p_j, q_i\}\} \\
&= \delta_{ij} - \varepsilon\{g, \delta_{ji}\} \\
&= \delta_{ij}
\end{aligned}
$$

2.8.3. Consider

$$
\mathcal{H} = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2}m\omega^2(x^2 + y^2)
$$

whose invariance under the rotation of the coordinates *and* momenta leads to the conservation of $l_z$. But $\mathcal{H}$ is also invariant under the rotation of *just the coordinates*. Verify that this is a *noncanonical* transformation. Convince yourself that in this case it is not possible to write $\delta\mathcal{H}$ as $\varepsilon\{\mathcal{H}, g\}$ for any $g$, i.e. that no conservation law follows.

If we transform solely the coordinates as

$$
\begin{aligned}
\bar{x} &= x\cos\theta + y\sin\theta \\
\bar{y} &= -x\sin\theta + y\cos\theta
\end{aligned}
$$

the momenta become

$$
\begin{aligned}
p_x(\bar{x}, \bar{y}) &= m\dot{x} = m(\dot{\bar{x}}\cos\theta - \dot{\bar{y}}\sin\theta) = p_{\bar{x}}\cos\theta - p_{\bar{y}}\sin\theta \\
p_y(\bar{x}, \bar{y}) &= m\dot{y} = m(\dot{\bar{x}}\sin\theta + \dot{\bar{y}}\cos\theta) = p_{\bar{x}}\sin\theta + p_{\bar{y}}\cos\theta
\end{aligned}
$$

where $p_{\bar{x}}$ and $p_{\bar{y}}$ are the canonical momenta conjugate to $x$ and $y$.

The only possible nonzero Poisson brackets are

$$\begin{aligned}
\{\bar{x}, p_x\} &= \{\bar{x}, p_{\bar{x}} \cos\theta - p_{\bar{y}} \sin\theta\} \\
&= \{\bar{x}, p_{\bar{x}}\} \cos\theta - \{\bar{x}, p_{\bar{y}}\} \sin\theta \\
&= \cos\theta \\
\{\bar{x}, p_y\} &= \{\bar{x}, p_{\bar{x}} \sin\theta + p_{\bar{y}} \cos\theta\} \\
&= \{\bar{x}, p_{\bar{x}}\} \sin\theta + \{\bar{x}, p_{\bar{y}}\} \cos\theta \\
&= \sin\theta \\
\{\bar{y}, p_x\} &= \{\bar{y}, p_{\bar{x}} \cos\theta - p_{\bar{y}} \sin\theta\} \\
&= \{\bar{y}, p_{\bar{x}}\} \cos\theta - \{\bar{y}, p_{\bar{y}}\} \sin\theta \\
&= -\sin\theta \\
\{\bar{y}, p_y\} &= \{\bar{y}, p_{\bar{x}} \sin\theta + p_{\bar{y}} \cos\theta\} \\
&= \{\bar{y}, p_{\bar{x}}\} \sin\theta + \{\bar{y}, p_{\bar{y}}\} \cos\theta \\
&= \cos\theta
\end{aligned}$$

Because the Poisson bracket no longer reproduces $\{q_i, p_j\} = \delta_{ij}$, this is a noncanonical coordinate transformation.

We know that $\{\mathcal{H}, g\}$ should capture the time derivative of $g$, which depends on the system's coordinates. Because the new coordinates are noncanonical, their time derivatives are *not* captured by their Poisson bracket with $\mathcal{H}$, and so those functions depending on them lose this property, too.

2.8.4. Consider $\mathcal{H} = \frac{1}{2}p^2 + \frac{1}{2}x^2$, which is invariant under infinitesimal rotations in *phase space* (the $x$-$p$ plane). Find the generator of this transformation (after verifying that it is canonical). (You could have guessed the answer based on Exercise 2.5.2).

A rotation in the $x$-$p$ plane by an angle $\theta$ can be written

$$\begin{aligned}
\bar{x} &= x\cos\theta + p\sin\theta \\
\bar{p} &= -x\sin\theta + p\cos\theta
\end{aligned}$$

which, as $\theta$ becomes infinitesimal, transforms to

$$\begin{aligned}
\bar{x} &= x + \varepsilon p \stackrel{?}{=} x + \varepsilon \frac{\partial g}{\partial p} \\
\bar{p} &= p - \varepsilon x \stackrel{?}{=} p - \varepsilon \frac{\partial g}{\partial x}
\end{aligned}$$

We can simply integrate to find $g$,

$$\begin{aligned}
\frac{\partial g}{\partial p} = p &\implies g(x,p) = \frac{1}{2}p^2 + \mathcal{O}(x) \\
\frac{\partial g}{\partial x} = x &\implies g(x,p) = \frac{1}{2}x^2 + \mathcal{O}(p)
\end{aligned}$$

i.e. $g(x,p) = \mathcal{H}$ up to the addition of a constant factor.

To verify the canonical nature of the transformation, observe

$$\begin{aligned}
\{\bar{x}, \bar{x}\} &= \{x + \varepsilon p, x + \varepsilon p\} \\
&= \{x, x\} + \varepsilon\Big(\{x, p\} + \{p, x\}\Big) + \mathcal{O}(\varepsilon^2) \\
&= 0 \\
\{\bar{x}, \bar{p}\} &= \{x + \varepsilon p, p - \varepsilon x\} \\
&= \{x, p\} - \varepsilon\Big(\{x, x\} - \{p, p\}\Big) + \mathcal{O}(\varepsilon^2) \\
&= 1 \\
\{\bar{p}, \bar{p}\} &= \{p - \varepsilon x, p - \varepsilon x\} \\
&= \{p, p\} - \varepsilon\Big(\{p, x\} + \{x, p\}\Big) + \mathcal{O}(\varepsilon^2) \\
&= 0
\end{aligned}$$

2.8.5. Why is it that a *non*canonical transformation that leaves $\mathcal{H}$ invariant does not map a solution into another? Or, in view of the discussion on consequence II, why is it that an experiment and its transformed version do not give the same result when the transformation that leaves $\mathcal{H}$ invariant is not canonical? It is best to consider an example. Consider the potential given in Exercise 2.8.3. Suppose I release a particle at $(x = a, y = 0)$ with $(p_x = b, p_y = 0)$ and you release one in the transformed state in which $(x = 0, y = a)$ and $(p_x = b, p_y = 0)$, i.e., you rotate the coordinates but not the momenta. This is a noncanonical transformation that leaves $\mathcal{H}$ invariant. Convince yourself that at later times the states of the two particles are no related by the same transformation. Try to understand what goes wrong in the general case.

As detailed on p. 94, the transformation

$$\begin{aligned}
q &\to \bar{q}(q, p) \\
p &\to \bar{p}(q, p)
\end{aligned}$$

sends

$$\begin{aligned}
\dot{\bar{q}}_j &\to \sum_k \frac{\partial \mathcal{H}}{\partial \bar{q}_k}\{\bar{q}_j, \bar{q}_k\} + \frac{\partial \mathcal{H}}{\partial \bar{p}_k}\{\bar{q}_j, \bar{p}_k\} \\
\dot{\bar{p}}_j &\to \sum_k \frac{\partial \mathcal{H}}{\partial \bar{q}_k}\{\bar{p}_j, \bar{q}_k\} + \frac{\partial \mathcal{H}}{\partial \bar{p}_k}\{\bar{p}_j, \bar{p}_k\}
\end{aligned}$$

If the transformation is noncanonical, the Poison brackets will be nontrivial and we have

$$\begin{aligned}
\dot{\bar{q}}_j &\neq \frac{\partial \mathcal{H}}{\partial \bar{p}_j} \\
\dot{\bar{p}}_j &\neq \frac{\partial \mathcal{H}}{\partial \bar{q}_j}
\end{aligned}$$

thus showing that such a transformation does not map one solution of Hamilton's equation to another.

2.8.6. Show that $\partial S_{\mathrm{cl}}/\partial x_f = p(t_f)$.

Consider the classical action with the path parameterized by both $t$ and $x_f$. Its partial derivative with respect to $x_f$ is then

$$\begin{aligned}
\frac{\partial S_{\text{cl}}}{\partial x_f} &= \frac{\partial}{\partial x_f}\int_0^{t_f} \mathcal{L}(x_{\text{cl}}(x_f,t), \dot{x}_{\text{cl}}(x_f,t))\,\mathrm{d}t \\
&= \int_0^{t_f} \frac{\partial \mathcal{L}}{\partial x_{\text{cl}}}\frac{\partial x_{\text{cl}}}{\partial x_f} + \frac{\partial \mathcal{L}}{\partial \dot{x}_{\text{cl}}}\frac{\partial \dot{x}_{\text{cl}}}{\partial x_f}\,\mathrm{d}t \\
&= \int_0^{t_f} \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{x}_{\text{cl}}}\frac{\partial x_{\text{cl}}}{\partial x_f} + \frac{\partial \mathcal{L}}{\partial \dot{x}_{\text{cl}}}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial x_{\text{cl}}}{\partial x_f}\,\mathrm{d}t \\
&= \int_0^{t_f} \frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial \mathcal{L}}{\partial \dot{x}_{\text{cl}}}\frac{\partial x_{\text{cl}}}{\partial x_f}\Big)\mathrm{d}t \\
&= p(t)\frac{\partial x_{\text{cl}}}{\partial x_f}\Big|_0^{t_f} \\
&= p(t_f)
\end{aligned}$$

where $x_{\text{cl}}(0) = x_1$ and $x_{\text{cl}}(t_f) = x_f$, and so $\partial x_{\text{cl}}/\partial x_f|_0^{t_f} = 1 - 0 = 1$.

2.8.7. Consider the harmonic oscillator, for which the general solution is

$$x(t) = A\cos\omega t + B\sin\omega t.$$

Express the energy in terms of $A$ and $B$ and note that it does not depend on time. Now choose $A$ and $B$ such that $x(0) = x_1$ and $x(T) = x_2$. Write down the energy in terms of $x_1$, $x_2$, and $T$. Show that the action for the trajectory connecting $x_1$ and $x_2$ is

$$S_{\text{cl}}(x_1, x_2, T) = \frac{m\omega}{2\sin\omega T}[(x_1^2 + x_2^2)\cos\omega T - 2x_1x_2].$$

Verify that $\partial S_{\text{cl}}/\partial T = -E$.

The kinetic energy of the harmonic oscillator is given by

$$\begin{aligned}
\frac{1}{2}m\dot{x}^2 &= \frac{1}{2}m(-\omega A\sin\omega t + \omega B\cos\omega t)^2 \\
&= \frac{1}{2}m\omega^2(B\cos\omega t - A\sin\omega t)^2 \\
&= \frac{1}{2}m\omega^2\Big(B\frac{e^{i\omega t} + e^{-i\omega t}}{2} - A\frac{e^{i\omega t} - e^{-i\omega t}}{2i}\Big)^2 \\
&= \frac{1}{2}m\omega^2\Big((B + iA)\frac{e^{i\omega t}}{2} + (B - iA)\frac{e^{-i\omega t}}{2}\Big)^2 \\
&= \frac{1}{2}m\omega^2(A^2 + B^2)\Big(\frac{e^{i(\omega t + \tan^{-1}(A/B))} + e^{-i(\omega t + \tan^{-1}(A/B))}}{2}\Big)^2 \\
&= \frac{1}{2}m\omega^2(A^2 + B^2)\cos^2(\omega t + \tan^{-1}(A/B)) \\
&\leq \frac{1}{2}m\omega^2(A^2 + B^2)
\end{aligned}$$

Since the total energy of the harmonic oscillator is equal to the maximum of the kinetic energy, $E = \frac{1}{2}m\omega^2(A^2 + B^2)$.

To satisfy the first initial condition, $A = x_1$. The second is equivalent to

$$x_2 = x_1 \cos \omega T + B \sin \omega T,$$

which, upon solving for $B$, yields

$$B = \frac{x_2 - x_1 \cos \omega T}{\sin \omega T}.$$

Using the above, we can rewrite the energy in terms of $x_1$ and $x_2$,

$$\begin{aligned} E &= \frac{1}{2} m\omega^2 \Big( x_1^2 + \frac{x_2^2 - 2x_1 x_2 \cos \omega T + x_1^2 \cos^2 \omega T}{\sin^2 \omega T} \Big) \\ &= \frac{1}{2} m\omega^2 \Big( \frac{x_1^2 - 2x_1 x_2 \cos \omega T + x_2^2}{\sin^2 \omega T} \Big) \end{aligned}$$

The Lagrangian for the simple harmonic oscillator is given by

$$\mathcal{L} = T - V = \frac{1}{2} m\dot{x}^2 - \frac{1}{2} m\omega^2 x^2$$

or, substituting in the classical path,

$$\begin{aligned} \mathcal{L} &= \frac{1}{2} m(\dot{x}^2 - \omega^2 x^2) \\ &= \frac{1}{2} m\omega^2 (B^2 \cos^2 \omega t + A^2 \sin^2 \omega t - A^2 \cos^2 \omega t - B^2 \sin^2 \omega t - 4AB \cos \omega t \sin \omega t) \\ &= \frac{1}{2} m\omega^2 \Big( (B^2 - A^2) \cos 2\omega t - 2AB \sin 2\omega t \Big) \end{aligned}$$

The action is thus

$$\begin{aligned} S_{\text{cl}} &= \frac{1}{2} m\omega^2 (B^2 - A^2) \int_0^T \cos 2\omega t \, \mathrm{d}t - m\omega^2 AB \int_0^T \sin 2\omega t \, \mathrm{d}t \\ &= \frac{1}{4} m\omega (B^2 - A^2) \sin 2\omega T + \frac{1}{2} m\omega AB (\cos 2\omega T - 1) \end{aligned}$$

where in our calculations of both $\mathcal{L}$ and $S$ we have relied on the following identities

$$\begin{aligned} \sin 2\theta &= 2 \sin \theta \cos \theta \\ \cos 2\theta &= \cos^2 \theta - \sin^2 \theta \\ &= 1 - 2\sin^2 \theta \end{aligned}$$

Using a CAS, $S$ simplifies to the solution,

$$S_{\text{cl}}(x_1, x_2, T) = \frac{m\omega}{2 \sin \omega T} [(x_1^2 + x_2^2) \cos \omega T - 2x_1 x_2].$$

Finally,

$$\begin{aligned} \frac{\partial S_{\text{cl}}}{\partial T} &= \frac{-m\omega^2 \cos \omega T}{2 \sin^2 \omega T} [(x_1^2 + x_2^2) \cos \omega T - 2x_1 x_2] - \frac{m\omega^2}{2} (x_1^2 + x_2^2) \\ &= -\frac{1}{2} m\omega^2 \Big( \frac{x_1^2 - 2x_1 x_2 \cos \omega T + x_2^2}{\sin^2 \omega T} \Big) \\ &= -E \end{aligned}$$

# 4 The Postulates—a General Discussion

## 4.2 Discussion of Postulates I-III

4.2.1. (*Very Important*). Consider the following operators on a Hilbert space $\mathbb{V}^3(C)$:

$$L_x = \frac{1}{2^{1/2}}\begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{bmatrix}, \quad L_y = \frac{1}{2^{1/2}}\begin{bmatrix}0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0\end{bmatrix}, \quad L_z = \begin{bmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{bmatrix}$$

(a) What are the possible values one can obtain if $L_z$ is measured?

(b) Take the state in which $L_z = 1$. In this state what are $\langle L_x\rangle$, $\langle L_x^2\rangle$, and $\Delta L_x$?

(c) Find the normalized eigenstates and the eigenvalues of $L_x$ in the $L_z$ basis.

(d) If the particle is in the state with $L_z = -1$, and $L_x$ is measured, what are the possible outcomes and their probabilities?

(e) Consider the state

$$|\psi\rangle = \begin{bmatrix}1/2\\ 1/2\\ 1/2^{1/2}\end{bmatrix}$$

in the $L_z$ basis. If $L_z^2$ is measured in this state and a result $+1$ is obtained, what is the state after measurement? How probable was this result? If $L_z$ is measured immediately afterwards, what are the outcomes and respective probabilities?

(f) A particle is in a state for which the probabilites are $P(L_z = 1) = 1/4$, $P(L_z = 0) = 1/2$, and $P(L_z = -1) = 1/4$. Convince yourself that the most general, normalized state with this property is

$$|\psi\rangle = \frac{e^{i\delta_1}}{2}|L_z = 1\rangle + \frac{e^{i\delta_2}}{2^{1/2}}|L_z = 0\rangle + \frac{e^{i\delta_3}}{2}|L_z = -1\rangle$$

It was stated earlier on that if $|\psi\rangle$ is a normalized state then the state $e^{i\theta}|\psi\rangle$ is a physically equivalent normalized state. Does this mean that the factors $e^{i\delta_i}$ multiplying the $L_z$ eigenstates are irrelevant? [Calculate for example $P(L_x = 0)$.]

(a) These are the eigenvalues of $L_z$,

$$L_z = 1, 0, \text{ or } -1$$

(b) $L_z = 1$ when the state has the form

$$|\psi\rangle = \begin{bmatrix}1\\ 0\\ 0\end{bmatrix}$$

Using this, we calculate

$$\begin{aligned}\langle L_x\rangle &= \langle\psi|L_x|\psi\rangle\\ &= \frac{1}{2^{1/2}}\begin{bmatrix}1 & 0 & 0\end{bmatrix}\begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{bmatrix}\begin{bmatrix}1\\ 0\\ 0\end{bmatrix}\\ &= \frac{1}{2^{1/2}}\begin{bmatrix}1 & 0 & 0\end{bmatrix}\begin{bmatrix}0\\ 1\\ 0\end{bmatrix}\\ &= 0\end{aligned}$$

$$\begin{aligned}
\langle L_x^2\rangle &= \langle\psi|L_x^2|\psi\rangle \\
&= \frac{1}{2}\begin{bmatrix}1 & 0 & 0\end{bmatrix}\begin{bmatrix}0 & 1 & 0\\1 & 0 & 1\\0 & 1 & 0\end{bmatrix}\begin{bmatrix}0 & 1 & 0\\1 & 0 & 1\\0 & 1 & 0\end{bmatrix}\begin{bmatrix}1\\0\\0\end{bmatrix} \\
&= \frac{1}{2}\begin{bmatrix}0 & 1 & 0\end{bmatrix}\begin{bmatrix}0\\1\\0\end{bmatrix} \\
&= \frac{1}{2} \\
\Delta L_x &= \langle\psi|(L_x - \langle L_x\rangle)^2|\psi\rangle \\
&= \langle\psi|L_x^2 - L_x\langle L_x\rangle - \langle L_x\rangle L_x + \langle L_x\rangle^2|\psi\rangle \\
&= \langle\psi|L_x^2|\psi\rangle - 2\langle L_x\rangle\langle\psi|L_x|\psi\rangle + \langle L_x\rangle^2\langle\psi|\psi\rangle \\
&= \langle L_x^2\rangle - \langle L_x\rangle^2 \\
&= \langle L_x^2\rangle \\
&= \frac{1}{2}
\end{aligned}$$

(c) Noting that we are already in the $L_z$ basis ($L_z$ is diagonal), this amounts to simply finding the eigenvalues and eigenvectors of $L_x$. We do so by examining the characteristic equation,

$$\begin{aligned}
\det(\lambda I - L_x) &= \begin{vmatrix}\lambda & -\frac{1}{2^{1/2}} & 0\\ -\frac{1}{2^{1/2}} & \lambda & -\frac{1}{2^{1/2}}\\ 0 & -\frac{1}{2^{1/2}} & \lambda\end{vmatrix} \\
&= \lambda\Big(\lambda^2 - \frac{1}{2}\Big) + \frac{1}{2^{1/2}}\Big(-\frac{\lambda}{2^{1/2}}\Big) \\
&= \lambda^3 - \frac{\lambda}{2} - \frac{\lambda}{2} \\
&= \lambda(\lambda^2 - 1)
\end{aligned}$$

i.e. the eigenvalues of $L_x$ are

$$L_x = 1, 0, \text{ and } -1$$

The eigenstate $|\lambda_i\rangle$ is found by solving $\ker(\lambda_i I - L_x)$,

$$\begin{aligned}
(I - L_x)|L_x = 1\rangle &= \begin{bmatrix}1 & -\frac{1}{2^{1/2}} & 0\\ -\frac{1}{2^{1/2}} & 1 & -\frac{1}{2^{1/2}}\\ 0 & -\frac{1}{2^{1/2}} & 1\end{bmatrix}|L_x = 1\rangle = 0 \\
-L_x|L_x = 0\rangle &= \begin{bmatrix}0 & -\frac{1}{2^{1/2}} & 0\\ -\frac{1}{2^{1/2}} & 0 & -\frac{1}{2^{1/2}}\\ 0 & -\frac{1}{2^{1/2}} & 0\end{bmatrix}|L_x = 0\rangle = 0 \\
(-I - L_x)|L_x = -1\rangle &= \begin{bmatrix}-1 & -\frac{1}{2^{1/2}} & 0\\ -\frac{1}{2^{1/2}} & -1 & -\frac{1}{2^{1/2}}\\ 0 & -\frac{1}{2^{1/2}} & -1\end{bmatrix}|L_x = -1\rangle = 0
\end{aligned}$$

By inspection, we can write

$$|L_x = 1\rangle \propto \begin{bmatrix}\frac{1}{2^{1/2}}\\ 1\\ \frac{1}{2^{1/2}}\end{bmatrix}$$

$$|L_x = 0\rangle \propto \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

$$|L_x = -1\rangle \propto \begin{bmatrix} -\frac{1}{2^{1/2}} \\ 1 \\ -\frac{1}{2^{1/2}} \end{bmatrix}$$

Normalizing these yields

$$|L_x = 1\rangle = \frac{1}{2}\begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix}$$

$$|L_x = 0\rangle = \frac{1}{2^{1/2}}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

$$|L_x = -1\rangle = \frac{1}{2}\begin{bmatrix} -1 \\ \sqrt{2} \\ -1 \end{bmatrix}$$

(d) $L_z = -1$ when the state has the form

$$|\psi\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

The only possible measurements for $L_x$ are its eigenvalues, 1, 0, and $-1$. We project the state onto the $L_x$ eigenbasis via the projection operator $P_{L_x} = \sum_k |\lambda_k\rangle\langle\lambda_k|$

$$\begin{aligned}
|\psi\rangle &= \sum_k |\lambda_k\rangle\langle\lambda_k|\psi\rangle \\
&= \langle L_x = 1|\psi\rangle|L_x = 1\rangle + \langle L_x = 0|\psi\rangle|L_x = 0\rangle + \langle L_x = -1|\psi\rangle|L_x = -1\rangle \\
&= \frac{1}{2}\begin{bmatrix} 1 & \sqrt{2} & 1 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}|L_x = 1\rangle + \frac{1}{2^{1/2}}\begin{bmatrix} 1 & 0 & -1 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}|L_x = 0\rangle + \frac{1}{2}\begin{bmatrix} -1 & \sqrt{2} & -1 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}|L_x = -1\rangle \\
&= \frac{1}{2}|L_x = 1\rangle - \frac{1}{2^{1/2}}|L_x = 0\rangle - \frac{1}{2}|L_x = -1\rangle
\end{aligned}$$

From this, we can read off the probabilities of the various measurements,

$$\begin{aligned}
P(L_x = 1) &= \left(\frac{1}{2}\right)^2 = \frac{1}{4} \\
P(L_x = 0) &= \left(-\frac{1}{2^{1/2}}\right)^2 = \frac{1}{2} \\
P(L_x = -1) &= \left(-\frac{1}{2}\right)^2 = \frac{1}{4}
\end{aligned}$$

(e) $L_z^2$ will have eigenvalues that are the square of the eigenvalues of $L_z$, i.e.

$$L_z^2 = 1 \text{ or } 0.$$

Since

$$L_z^2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

a measurement of 1 projects the state $|\psi\rangle$ onto the eigenspace associated with this eigenvalue,

$$|1\rangle = \begin{bmatrix}1\\0\\0\end{bmatrix}, \quad |1'\rangle = \begin{bmatrix}0\\0\\1\end{bmatrix},$$

and so the new (normalized) state is

$$|\psi'\rangle = \frac{2}{3^{1/2}}\begin{bmatrix}1/2\\0\\1/2^{1/2}\end{bmatrix}$$

The probability of this result is

$$|\langle 1|\psi\rangle|^2 + |\langle 1'|\psi\rangle|^2 = \frac{1}{4} + \frac{1}{2} = \frac{3}{4}.$$

If we measure $L_z$ in this new state, we find two possibilities: $L_z = -1, 1$ (the $L_z = 0$ state is excluded). The first has the associated state and probability

$$|\psi_{+1}\rangle = \begin{bmatrix}1\\0\\0\end{bmatrix}, \quad P = |\langle +1|\psi'\rangle|^2 = \Big(\frac{2}{3^{1/2}}\cdot\frac{1}{2}\Big)^2 = \frac{1}{3}$$

while the second has the associated state and probability

$$|\psi_{-1}\rangle = \begin{bmatrix}0\\0\\1\end{bmatrix}, \quad P = |\langle -1|\psi'\rangle|^2 = \Big(\frac{2}{3^{1/2}}\cdot\frac{1}{2^{1/2}}\Big)^2 = \frac{2}{3}$$

(f) This is clear from how we measure the probability of a state. If the probability of finding $|\psi\rangle$ in the eigenstate $|\alpha\rangle$ is $p$ and $\langle\alpha|\psi\rangle = \psi_\alpha \in \mathbb{C}$, then

$$\begin{aligned} p &= |\langle\alpha|\psi\rangle|^2 \\ &= \langle\alpha|\psi\rangle\langle\psi|\alpha\rangle \\ &= \psi_\alpha \cdot \bar{\psi}_\alpha \\ &= re^{i\delta}\cdot re^{-i\delta} \\ &= r^2 \end{aligned}$$

where we have written $\psi_\alpha$ in polar form as $re^{i\delta}$. From this, it is clear that the most general form for $\psi_\alpha$ that guarantees $p = |\langle\alpha|\psi\rangle|^2$ is

$$\psi_\alpha = \sqrt{p}\, e^{i\delta}$$

Despite the seeming arbitrariness of $\delta$, it plays a role when performing a measurement with an operator whose eigenstates are different than the currently used eigenstates. To take the given example,

$$\begin{aligned} P(L_x = 0) &= |\langle L_x = 0|\psi\rangle|^2 \\ &= \Big|\frac{1}{2^{1/2}}\Big(\frac{e^{i\delta_1}}{2} - \frac{e^{i\delta_3}}{2}\Big)\Big|^2 \\ &= \frac{1}{8}(e^{i\delta_1} - e^{i\delta_3})(e^{-i\delta_1} - e^{-i\delta_3}) \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{8}(2 - e^{i(\delta_1-\delta_3)} - e^{-i(\delta_1-\delta_3)}) \\
&= \frac{1}{4}(1 - \cos(\delta_1 - \delta_3))
\end{aligned}
$$

From this, we see that it is the *relative* phase values that significantly alter our measurements. This is similar to what we find in electromagnetism: the relative phase of two waves creates measurable effects, while the phase of a single, monochromatic plane wave is undetectable.

4.2.2. Show that for a real wave function $\psi(x)$, the expectation value of momentum $\langle P \rangle = 0$. (Hint: Show that the probabilities for the momenta $\pm p$ are equal.) Generalize this result to the case $\psi = c\psi_r$, where $\psi_r$ is real and $c$ an arbitrary (real or complex) constant. (Recall that $|\psi\rangle$ and $\alpha|\psi\rangle$ are physically equivalent.)

Following the hint, we compute

$$
\begin{aligned}
P(P = +p) &= |\langle p|\psi\rangle|^2 \\
&= \langle \psi|p\rangle\langle p|\psi\rangle \\
&= \Big(\int_{-\infty}^{\infty} \langle\psi|x\rangle\langle x|p\rangle \,\mathrm{d}x\Big)\Big(\int_{-\infty}^{\infty} \langle p|x'\rangle\langle x'|\psi\rangle \,\mathrm{d}x'\Big) \\
&= \Big(\int_{-\infty}^{\infty} \bar{c}\psi_r(x)\frac{e^{ipx/\hbar}}{(2\pi\hbar)^{1/2}} \,\mathrm{d}x\Big)\Big(\int_{-\infty}^{\infty} \frac{e^{-ipx'/\hbar}}{(2\pi\hbar)^{1/2}} c\psi_r(x') \,\mathrm{d}x'\Big) \\
&= \frac{|c|^2}{2\pi\hbar}\Big(\int_{-\infty}^{\infty} \psi_r(x)e^{ipx/\hbar} \,\mathrm{d}x\Big)\Big(\int_{-\infty}^{\infty} \psi_r(x')e^{-ipx'/\hbar} \,\mathrm{d}x'\Big)
\end{aligned}
$$

Since this is invariant under the exchange $p \to -p$, the probability of finding a particle at momentum $p$ is exactly the same as finding that same particle at momentum $-p$. But any probability distribution $f_P(p)$ with this property is even about $p = 0$, and so $pf_P(p)$ is odd and $\langle P \rangle = 0$.

4.2.3. Show that if $\psi(x)$ has mean momentum $\langle P \rangle$, $e^{ip_0x/\hbar}\psi(x)$ has mean momentum $\langle P \rangle + p_0$.

Assuming the state $|\psi'\rangle$ is normalized, we have

$$
\begin{aligned}
\langle \psi'|P|\psi'\rangle &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle\psi'|x\rangle\langle x|P|x'\rangle\langle x'|\psi'\rangle \,\mathrm{d}x\,\mathrm{d}x' \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-ip_0x/\hbar}\bar{\psi}(x)\Big(-i\hbar\delta(x-x')\frac{\mathrm{d}}{\mathrm{d}x'}\Big)e^{ip_0x'/\hbar}\psi(x') \,\mathrm{d}x\,\mathrm{d}x' \\
&= \int_{-\infty}^{\infty} e^{-ip_0x/\hbar}\bar{\psi}(x)\Big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\Big)e^{ip_0x/\hbar}\psi(x) \,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} e^{-ip_0x/\hbar}\bar{\psi}(x)\Big(-i\hbar\cdot\frac{ip_0}{\hbar}\cdot e^{ip_0x/\hbar}\psi(x) - i\hbar\cdot e^{ip_0x/\hbar}\frac{\mathrm{d}}{\mathrm{d}x}\psi(x)\Big) \,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} \bar{\psi}(x)\Big(p_0 - i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\Big)\psi(x) \,\mathrm{d}x \\
&= p_0\int_{-\infty}^{\infty} |\psi(x)|^2 \,\mathrm{d}x + \int_{-\infty}^{\infty} \bar{\psi}(x)\Big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\Big)\psi(x) \,\mathrm{d}x \\
&= p_0 + \langle P \rangle
\end{aligned}
$$

where in the last step we used the fact that $\langle P \rangle$ in the position basis is

$$\langle P \rangle = \int_{-\infty}^{\infty} \bar{\psi}(x)\Big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\Big)\psi(x)\,\mathrm{d}x.$$

Another way to show this relation is to recall that position space and momentum space are dual in the Fourier sense, and so a multiplication by $e^{ip_0x}$ (or $e^{ipx_0}$) in one space becomes addition by $p_0$ (or $x_0$) in the other.

# 5 Simple Problems in One Dimension

## 5.1 The Free Particle

5.1.1. Show that Eq. (5.1.9) may be rewritten as an integral over $E$ and a sum over the $\pm$ index as

$$U(t) = \sum_{\alpha=\pm}\int_0^{\infty}\Big[\frac{m}{(2mE)^{1/2}}\Big]|E,\alpha\rangle\langle E,\alpha|e^{-iEt/\hbar}\,\mathrm{d}E$$

Using Eqs. (5.1.6) and (5.1.7), we can replace $p$ in Eq. (5.1.9) with $E_-$ and $E_+$ over the negative and positive parts of the real line. Doing so gives

$$\begin{aligned}
U(t) &= \int_{-\infty}^{\infty}|p\rangle\langle p|e^{-ip^2t/2m\hbar}\,\mathrm{d}p \\
&= \int_{-\infty}^{0}|p\rangle\langle p|e^{-ip^2t/2m\hbar}\,\mathrm{d}p + \int_{0}^{\infty}|p\rangle\langle p|e^{-ip^2t/2m\hbar}\,\mathrm{d}p \\
&= \int_{\infty}^{0}|E,-\rangle\langle E,-|e^{-i(2mE)t/2m\hbar}\Big(-\frac{1}{2}\cdot 2m\cdot(2mE)^{-1/2}\Big)\,\mathrm{d}E \\
&\quad + \int_{0}^{\infty}|E,+\rangle\langle E,+|e^{-i(2mE)t/2m\hbar}\Big(\frac{1}{2}\cdot 2m\cdot(2mE)^{-1/2}\Big)\,\mathrm{d}E \\
&= \int_0^{\infty}\Big[\frac{m}{(2mE)^{1/2}}\Big]|E,-\rangle\langle E,-|e^{-iEt/\hbar}\,\mathrm{d}E \\
&\quad + \int_0^{\infty}\Big[\frac{m}{(2mE)^{1/2}}\Big]|E,+\rangle\langle E,-|e^{-iEt/\hbar}\,\mathrm{d}E \\
&= \sum_{\alpha=\pm}\int_0^{\infty}\Big[\frac{m}{(2mE)^{1/2}}\Big]|E,\alpha\rangle\langle E,\alpha|e^{-iEt/\hbar}\,\mathrm{d}E
\end{aligned}$$

where we have used the fact that $\lim_{p\to\pm\infty} E = \infty$.

5.1.2. By solving the eigenvalue equation (5.1.3) in the $X$ basis, regain Eq. (5.1.8), i.e., show that the general solution of energy $E$ is

$$\psi_E(x) = \beta\frac{\exp[i(2mE)^{1/2}x/\hbar]}{(2\pi\hbar)^{1/2}} + \gamma\frac{\exp[-i(2mE)^{1/2}x/\hbar]}{(2\pi\hbar)^{1/2}}$$

[The factor $(2\pi\hbar)^{-1/2}$ is arbitrary and may be absorbed into $\beta$ and $\gamma$.] Though $\psi_E(x)$ will satisfy the equation even if $E < 0$, are these functions in the Hilbert space?

In the $X$ basis, Eq. (5.1.3) becomes

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_E(x) = E\psi_E(x)$$

This is the well known differential equation of a harmonic oscillator, spanned by

$$\psi_E(x) = A\exp(i(2mE)^{1/2}x/\hbar) + B\exp(-i(2mE)^{1/2}x/\hbar)$$

We can replace $A$ and $B$ by $\beta/(2\pi\hbar)^{1/2}$ and $\gamma/(2\pi\hbar)^{1/2}$ to arrive at the given form of the general solution.

If $E < 0$, Eq. (5.1.3) does not describe a harmonic oscillator, but a real exponential. This is non-normalizable, and so the associated $\psi_E(x)$ is not within Hilbert space.

5.1.3. (*Another Way to Do the Gaussian Problem*). We have seen that there exists another formula for $U(t)$, namely, $U(t) = e^{iHt/\hbar}$. For a free particle this becomes

$$U(t) = \exp\left[\frac{i}{\hbar}\left(\frac{\hbar^2 t}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\hbar t}{2m}\right)^n\frac{\mathrm{d}^{2n}}{\mathrm{d}x^{2n}}$$

Consider the initial state in Eq. (5.1.14) with $p_0 = 0$, and set $\Delta = 1$, $t' = 0$:

$$\psi(x,0) = \frac{e^{-x^2/2}}{(\pi)^{1/4}}$$

Find $\psi(x,t)$ using Eq. (5.1.18) above and compare with Eq. (5.1.15).

Hints: (1) Write $\psi(x,0)$ as a power series:

$$\psi(x,0) = (\pi)^{-1/4}\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{n!(2)^n}$$

(2) Find the action of a few terms

$$1, \qquad \left(\frac{i\hbar t}{2m}\right)\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \qquad \frac{1}{2!}\left(\frac{i\hbar t}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)^2$$

etc., on this power series.

(3) Collect terms with the same power of $x$.

(4) Look for the following series expansion in the coefficient of $x^{2n}$:

$$\left(1+\frac{it\hbar}{m}\right)^{-n-1/2} = 1-(n+1/2)\left(\frac{i\hbar t}{m}\right)+\frac{(n+1/2)(n+3/2)}{2!}\left(\frac{it\hbar}{m}\right)^2+\cdots$$

(5) Juggle around till you get the answer.

Labeling the terms of the power series of $U(t)$ by $U(t) = U_0(t) + U_1(t) + U_2(t) + \cdots$, we find

$$U_0(t)\psi(x,0) = \frac{1}{(\pi)^{1/4}}\sum_{n=0}^{\infty}\frac{(-1)^n x^{2n}}{n!(2)^n}$$

$$
\begin{aligned}
U_1(t)\psi(x,0) &= \frac{1}{(\pi)^{1/4}}\Big(\frac{i\hbar t}{2m}\Big)\sum_{n=0}^{\infty}(2n)(2n-1)\frac{(-1)^n x^{2(n-1)}}{n!(2)^n} \\
&= \frac{1}{(\pi)^{1/4}}\Big(\frac{i\hbar t}{2m}\Big)\sum_{k=-1}^{\infty}(2k+2)(2k+1)\frac{(-1)^{k+1}x^{2k}}{(k+1)!(2)^{k+1}} \\
&= \frac{1}{(\pi)^{1/4}}\Big(\frac{i\hbar t}{m}\Big)\sum_{k=0}^{\infty}(k+1)(k+\tfrac{1}{2})\frac{(-1)^{k+1}x^{2k}}{(k+1)!(2)^k} \\
&= \frac{1}{(\pi)^{1/4}}\sum_{k=0}^{\infty}-(k+\tfrac{1}{2})\Big(\frac{i\hbar t}{m}\Big)\frac{(-1)^k x^{2k}}{k!(2)^k} \\
U_2(t)\psi(x,0) &= \frac{1}{2!}\frac{1}{(\pi)^{1/4}}\Big(\frac{i\hbar t}{2m}\Big)^2\sum_{n=0}^{\infty}(2n)(2n-1)(2n-2)(2n-3)\frac{(-1)^n x^{2(n-2)}}{n!(2)^n} \\
&= \frac{1}{2!}\frac{1}{(\pi)^{1/4}}\Big(\frac{i\hbar t}{2m}\Big)^2\sum_{k=-2}^{\infty}(2k+4)(2k+3)(2k+2)(2k+1)\frac{(-1)^{k+2}x^{2k}}{(k+2)!(2)^{k+2}} \\
&= \frac{1}{2!}\frac{1}{(\pi)^{1/4}}\Big(\frac{i\hbar t}{m}\Big)^2\sum_{k=0}^{\infty}(k+2)(k+\tfrac{3}{2})(k+1)(k+\tfrac{1}{2})\frac{(-1)^k x^{2k}}{(k+2)!(2)^k} \\
&= \frac{1}{2!}\frac{1}{(\pi)^{1/4}}\sum_{k=0}^{\infty}(k+\tfrac{3}{2})(k+\tfrac{1}{2})\Big(\frac{i\hbar t}{m}\Big)^2\frac{(-1)^k x^{2k}}{k!(2)^k} \\
&\;\;\vdots
\end{aligned}
$$

If we collect those terms that have similar powers of $x$, we find

$$
\begin{aligned}
U(t)\psi(x,0) &= \frac{1}{(\pi)^{1/4}}\sum_{n=0}^{\infty}\Big(1-(n+\tfrac{1}{2})\Big(\frac{i\hbar t}{m}\Big)+(n+\tfrac{3}{2})(n+\tfrac{1}{2})\Big(\frac{i\hbar t}{m}\Big)^2+\cdots\Big)\frac{(-1)^n x^{2n}}{n!(2)^n} \\
&= \frac{1}{(\pi)^{1/4}}\sum_{n=0}^{\infty}\Big(1+\frac{i\hbar t}{m}\Big)^{-n-1/2}\frac{(-1)^n x^{2n}}{n!(2)^n} \\
&= \Big[\pi^{1/2}\Big(1+\frac{i\hbar t}{m}\Big)\Big]^{-1/2}\sum_{n=0}^{\infty}\frac{1}{n!}\Big[\frac{-x^2}{2(1+i\hbar t/m)}\Big]^n \\
&= \Big[\pi^{1/2}\Big(1+\frac{i\hbar t}{m}\Big)\Big]^{-1/2}\cdot\exp\Big[\frac{-x^2}{2(1+i\hbar t/m)}\Big]
\end{aligned}
$$

This is the solution for a Gaussian wavepacket in free space with a mean momentum of $p_0 = 0$ and uncertainty in position of $\Delta = 1$.

5.1.4. *A Famous Counterexample.* Consider the wave function

$$
\begin{aligned}
\psi(x,0) &= \sin\Big(\frac{\pi x}{L}\Big), && |x| \le L/2 \\
&= 0, && |x| > L/2
\end{aligned}
$$

It is clear that when this function is differentiated any number of times we get another function confined to the interval $|x| \le L/2$. Consequently the action of

$$
U(t) = \exp\Big[\frac{i}{\hbar}\Big(\frac{\hbar^2 t}{2m}\Big)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Big]
$$

on this function is to give a function confined to $|x| \leq L/2$. What about the spreading of the wave packet?

[Answer: Consider the derivatives at the boundary. We have here an example where the (exponential) operator power series doesn't converge. Notice that the convergence of an operator power series depends not just on the operator but also on the operand. So there is no paradox: if the function dies abruptly as above, so that there seems to be a paradox, the derivatives are singular at the boundary, while if it falls of continuously, the function will definitely leak out given enough time, no matter how rapid the falloff.]

As the answer points out, the power series of $U(t)\psi(x,0)$ does not converge, and so we cannot use the propagator to determine the time evolution of this system.

## 5.2 The Particle in a Box

5.2.1. A particle is in the ground state of a box of length $L$. Suddenly the box expands (symmetrically) to twice its size, leaving the wave function undisturbed. Show that the probability of finding the particle in the ground state of the new box is $(8/3\pi)^2$.

Our particle is in the initial state

$$\psi_{1,L} \propto \cos\left(\frac{\pi x}{L}\right)$$

Upon expansion of the box, the wave function is unaffected except up to a multiplicative factor. Normalizing the integral of its squared magnitude over $-L \leq x \leq L$ gives

$$\psi_{2L} = \langle x|\psi_{2L}\rangle = \left(\frac{2}{2L}\right)^{1/2} \cos\left(\frac{\pi x}{L}\right)$$

To find the probability amplitude that the particle can be found in the ground state of this new box, we compute

$$\begin{aligned}
\langle\psi_{1,2L}|\psi_{2L}\rangle &= \int_{-\infty}^{\infty} \langle\psi_{1,2L}|x\rangle\langle x|\psi_{2L}\rangle \,\mathrm{d}x \\
&= \int_{-L}^{L} \left(\frac{2}{2L}\right)^{1/2} \cos\left(\frac{\pi x}{2L}\right)\left(\frac{2}{2L}\right)^{1/2} \cos\left(\frac{\pi x}{L}\right) \mathrm{d}x \\
&= \frac{1}{L}\int_{-L}^{L} \frac{(e^{i\pi x/2L} + e^{-i\pi x/2L})}{2}\frac{(e^{i2\pi x/2L} + e^{-i2\pi x/2L})}{2}\,\mathrm{d}x \\
&= \frac{1}{L}\int_{-L}^{L} \frac{e^{i3\pi x/2L} + e^{-i3\pi x/2L}}{2} + \frac{e^{i\pi x/2L} + e^{-i\pi x/2L}}{2}\,\mathrm{d}x \\
&= \frac{1}{L}\int_{-L}^{L} \cos\left(\frac{3\pi x}{2L}\right) + \cos\left(\frac{\pi x}{2L}\right) \mathrm{d}x \\
&= \frac{1}{L}\left[\frac{2L}{3\pi}\sin\left(\frac{3\pi x}{2L}\right)\Big|_{-L}^{L} + \frac{2L}{\pi}\sin\left(\frac{\pi x}{2L}\right)\Big|_{-L}^{L}\right] \\
&= \frac{2}{3\pi}(-1-(1)) + \frac{2}{\pi}(1-(-1)) \\
&= -\frac{4}{3\pi} + \frac{4}{\pi} \\
&= \frac{8}{3\pi}
\end{aligned}$$

Squaring this quantity gives the probability for finding the particle in the ground state of the new box, $(8/3\pi)^2$.

5.2.2. (a) Show that for any normalized $|\psi\rangle$, $\langle\psi|H|\psi\rangle \geq E_0$, where $E_0$ is the lowest-energy eigenvalue. (Hint: Expand $|\psi\rangle$ in the eigenbasis of $H$.)

(b) Prove the following theorem: Every attractive potential in one dimension has at least one bound state. Hint: Since $V$ is attractive, if we define $V(\infty) = 0$, it follows that $V(x) = -|V(x)|$ for all $x$. To show that there exists a bound state with $E < 0$, consider

$$\psi_\alpha(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

and calculate

$$E(\alpha) = \langle\psi_\alpha|H|\psi_\alpha\rangle, \qquad H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - |V(x)|$$

Show that $E(\alpha)$ can be made negative by a suitable choice of $\alpha$. The desired result follows from the application of the theorem proved above.

(a) If $|\psi\rangle$ is normalized, then

$$\begin{aligned}\langle\psi|\psi\rangle &= (\langle E_0|A_0^* + \langle E_1|A_1^* + \langle E_2|A_2^* + \cdots)(A_0|E_0\rangle + A_1|E_1\rangle + A_2|E_2\rangle + \cdots) \\ &= |A_0|^2 + |A_1|^2 + |A_2|^2 + \cdots \\ &= 1\end{aligned}$$

Applying the Hamitlonian operator to $|\psi\rangle$ before applying its bra vector gives

$$\langle\psi|H|\psi\rangle = E_0|A_0|^2 + E_1|A_1|^2 + E_2|A_2|^2 + \cdots$$

This computation gives the expectation value of the energy, with each $|A_i|^2$ acting as a value from a probability mass function. This cannot be smaller than the lowest possible energy state $E_0$, thus $\langle\psi|H|\psi\rangle \geq E_0$.

(b) Working in the position basis, we find

$$\begin{aligned}E(\alpha) &= \int_{-\infty}^{\infty} \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}\Big(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - |V(x)|\Big)\left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}\,\mathrm{d}x \\ &= \left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{\infty} e^{-\alpha x^2/2}\Big(-\frac{\hbar^2}{2m}(\alpha^2x^2 - \alpha) - |V(x)|\Big)e^{-\alpha x^2/2}\,\mathrm{d}x \\ &= \left(\frac{\alpha}{\pi}\right)^{1/2}\Big[\frac{-\hbar^2\alpha^2}{2m}\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2}\,\mathrm{d}x + \alpha\int_{-\infty}^{\infty} e^{-\alpha x^2}\,\mathrm{d}x - \int_{-\infty}^{\infty}|V(x)|e^{-\alpha x^2}\,\mathrm{d}x\Big] \\ &= \left(\frac{\alpha}{\pi}\right)^{1/2}\Big[\frac{-\hbar^2\alpha^2}{2m}\frac{1}{2\alpha}\left(\frac{\pi}{\alpha}\right)^{1/2} + \alpha\left(\frac{\pi}{\alpha}\right)^{1/2} - \int_{-\infty}^{\infty}|V(x)|e^{-\alpha x^2}\,\mathrm{d}x\Big]\end{aligned}$$

In order for this to evaluate to $E(\alpha) < 0$, we must have

$$\alpha < \frac{1}{\pi}\frac{1}{(1-\hbar^2/4m)^2}\Big(\int_{-\infty}^{\infty}|V(x)|e^{-\alpha x^2}\,\mathrm{d}x\Big)^2$$

i.e. the wave function must be suitably spread over position space. Maximal uncertainty in position space gives minimal uncertainty in momentum space, and since a bound state will have $\langle P\rangle = 0$, this small uncertainty in momentum space allows a lower energy ground state.

5.2.3. Consider $V(x) = -aV_0\delta(x)$. Show that it admits a bound state of energy $E = -ma^2V_0^2/2\hbar^2$. Are there any other bound states? Hint: Solve Schrödinger's equation outside the potential for $E < 0$, and keep only the solution that has the right behavior at infinity and is continuous at $x = 0$. Draw the wave function and see how there is a cusp, or a discontinuous change of slope at $x = 0$. Calculate the change in slope and equate it to

$$\int_{-\varepsilon}^{\varepsilon} \left(\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}\right) \mathrm{d}x$$

(where $\varepsilon$ is infinitesimal) determined from Schrödinger's equation.

Outside the potential the particle is free, and thus the wave function has the general solution

$$\psi(x) = A\exp(i(2mE)^{1/2}x/\hbar) + B\exp(-i(2mE)^{1/2}x/\hbar)$$

When $E < 0$ a factor of $i$ is introduced into the arguments, changing the above into

$$\psi(x) = A\exp(-(2mE)^{1/2}x/\hbar) + B\exp((2mE)^{1/2}x/\hbar)$$

In order for this function be normalizable, we must have $A = 0$ when $x < 0$ and $B = 0$ when $x > 0$. At $x = 0$, $A = B$ to enforce continuity.

$$\psi(x) = \begin{cases} A\exp((2mE)^{1/2}x/\hbar), & x < 0 \\ A\exp(-(2mE)^{1/2}x/\hbar), & x > 0 \end{cases}$$

We can normalize this via

$$2A^2\int_0^\infty \exp(-2(2mE)^{1/2}x/\hbar)\,\mathrm{d}x = \frac{-2A^2\hbar}{2(2mE)^{1/2}}\exp(-2(2mE)^{1/2}x/\hbar)\Big|_0^\infty = \frac{A^2\hbar}{(2mE)^{1/2}}$$

and thus $A = (2mE/\hbar^2)^{1/4}$, or

$$\psi(x) = \begin{cases} (\frac{2mE}{\hbar^2})^{1/4}\exp(\frac{(2mE)^{1/2}}{\hbar}x), & x < 0 \\ (\frac{2mE}{\hbar^2})^{1/4}\exp(-\frac{(2mE)^{1/2}}{\hbar}x), & x > 0 \end{cases}$$

The change in slope from $x < 0$ to $x > 0$ is given by

$$\psi'(0^+) - \psi'(0^-) = -\left(\frac{8m^3E^3}{\hbar^6}\right)^{1/4} - \left(\frac{8m^3E^3}{\hbar^6}\right)^{1/4} = -\left(\frac{128m^3E^3}{\hbar^6}\right)^{1/4}$$

From the Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - aV_0\delta(x)\psi(x) = E\psi(x)$$

we can isolate the second derivative term via

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{2mE}{\hbar^2}\psi(x) - \frac{2maV_0}{\hbar^2}\delta(x)\psi(x)$$

The first of these terms will go to 0 as $\varepsilon \to 0$, and so

$$\int_{-\varepsilon}^{\varepsilon}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}\,\mathrm{d}x = -\frac{2maV_0}{\hbar^2}\psi(0) = -\frac{2maV_0}{\hbar^2}\left(\frac{2mE}{\hbar^2}\right)^{1/4} = -\left(\frac{32m^5a^4V_0^4E}{\hbar^{10}}\right)$$

Equating this with the found change in slope gives the requirement that

$$E^2 = \frac{m^2a^4V_0^4}{4\hbar^4}.$$

Enforcing $E < 0$ gives

$$E = -\frac{ma^2V_0^2}{2\hbar^2}.$$

5.2.4. Consider a particle of mass $m$ in the state $|n\rangle$ of a box of length $L$. Find the force $F = -\partial E/\partial L$ encountered when the walls are slowly pushed in, assuming the particle remains in the $n$th state of the box as its size changes. Consider a classical particle of energy $E_n$ in this box. Find its velocity, the frequency of collision on a given wall, the momentum transfer per collision, and hence the average force. Compare it to $-\partial E/\partial L$ computed above.

With the energy given by

$$E_n = \frac{\hbar^2\pi^2n^2}{2mL^2},$$

the force is

$$F = -\frac{\partial E}{\partial L} = \frac{\hbar^2\pi^2n^2}{mL^3}$$

In the classical case, a particle of energy $E_n$ will have a velocity of

$$v = \left(\frac{2E_n}{m}\right)^{1/2} = \frac{\hbar\pi n}{mL}$$

The time between successive collisions on the same wall is

$$T = \frac{2L}{v} = \frac{2mL^2}{\hbar\pi n}$$

and so the collision frequency is $f = \hbar\pi n/(2mL^2)$. Upon colliding with the wall, the particle feels a change in momentum of $\Delta p_p = -2mv$, and so the wall feels a transfer of momentum of

$$\Delta p_w = 2mv = \frac{2\hbar\pi n}{L}.$$

The change in momentum over time (i.e. force) is given by $f\Delta p_w$,

$$F = f\Delta p_w = \frac{\hbar^2\pi^2n^2}{mL^3}$$

This is the same as the force we found quantum mechanically!

5.2.5. If the box extends from $x = 0$ to $L$ (instead of $-L/2$ to $L/2$) show that $\psi_n(x) = (2/L)^{1/2}\sin(n\pi x/L)$, $n = 1, 2, \ldots, \infty$ and $E_n = \hbar^2\pi^2n^2/2mL^2$.

Just as before, $\psi(x)$ must be 0 in the region of infinite potential, so we need only solve for the case where $0 \leq x \leq L$. The Schrödinger equation in this region is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = E\psi(x)$$

which has the general solution

$$\psi(x) = A\cos((2mE)^{1/2}x/\hbar) + B\sin((2mE)^{1/2}x/\hbar)$$

If $\psi(0) = 0$, we must have $A = 0$. To enforce $\psi(L) = 0$, we must have

$$\frac{(2mE)^{1/2}}{\hbar}L = n\pi$$

or

$$E = \frac{\hbar^2\pi^2n^2}{2mL^2}$$

$B$ can then be set by normalizing $\psi(x)$,

$$B^2 \int_0^L \sin^2((2mE)^{1/2}x/\hbar)\,\mathrm{d}x = B^2 \int_0^L \frac{1}{2} - \frac{1}{2}\cos(2(2mE)^{1/2}x/\hbar)\,\mathrm{d}x = B^2 \frac{L}{2}$$

i.e. $B = (2/L)^{1/2}$. Since $n = 0$ would give us a trivial solution (it would imply there is no particle) $n < 0$ gives the same set of solutions as $n > 0$ (due to the wave function's indifference to an overall phase factor), we have found

$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right),$$
$$E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}$$

5.2.6. *Square Well Potential.* Consider a particle in a square well potential:

$$V(x) = \begin{cases} 0, & |x| \leq a \\ V_0, & |x| \geq a \end{cases}$$

Since when $V_0 \to \infty$, we have a box, let us guess what the lowering of the walls does to the states. First of all, all the bound states (which alone we are interested in), will have $E \leq V_0$. Second, the wave functions of the low-lying levels will look like those of the particle in a box, with the obvious difference that $\psi$ will not vanish at the walls but instead spill out with an exponential tail. The eigenfunctions will still be even, odd, even, etc.

(1) Show that the even solutions have energies that satisfy the transcendental equation

$$k \tan ka = \kappa$$

while the odd ones will have energies that satisfy

$$k \cot ka = -\kappa$$

where $k$ and $i\kappa$ are the real and complex wave numbers inside and outside the well, respectively. Note that $k$ and $\kappa$ are related by

$$k^2 + \kappa^2 = 2mV_0/\hbar^2$$

Verify that as $V_0$ tends to $\infty$, we regain the levels in the box.

(2) Equations (5.2.23) and (5.2.24) must be solved graphically. In the ($\alpha = ka, \beta = \kappa a$) plane, imagine a circle that obeys Eq. (5.2.25). The bound states are then given by the intersection of the curve $\alpha \tan \alpha = \beta$ or $\alpha \cot \alpha = -\beta$ with the circle. (Remember $\alpha$ and $\beta$ are positive.)

(3) Show that there is always one even solution and that there is no odd solution unless $V_0 \geq \hbar^2\pi^2/8ma^2$. What is $E$ when $V_0$ just meets this requirement? Note that the general result from Exercise 5.2.2b holds.

Where $|x| \leq a$, Schrödinger's equation becomes

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi(x)$$

which has the general solution

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

where we have defined $k = (2mE)^{1/2}/\hbar$. Outside of the well, the equation becomes

$$\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = (V_0 - E)\psi(x)$$

Since both sides are positive, the solutions here are exponentials, i.e.

$$\psi(x) = Ce^{-\kappa x} + De^{\kappa x}$$

where we have defined $\kappa = [2m(V_0 - E)]^{1/2}/\hbar$. To be a physically valid solution, we must have $\lim_{x\to\pm\infty}\psi(x) = 0$, and so $C = 0$ when $x < a$ and $D = 0$ when $x > a$. That is, our preliminary wave function has the form

$$\psi(x) = \begin{cases} De^{\kappa x}, & x < -a \\ A\sin(kx) + B\cos(kx), & |x| \le a \\ Ce^{-\kappa x}, & x > a \end{cases}$$

Enforcing continuity of $\psi(x)$ and $\psi'(x)$ at $x = \pm a$ gives the restrictions

$$\begin{aligned} De^{-\kappa a} &= -A\sin(ka) + B\cos(ka) \\ \kappa De^{-\kappa a} &= kA\cos(ka) + kB\sin(ka) \\ Ce^{-\kappa a} &= A\sin(ka) + B\cos(ka) \\ -\kappa Ce^{-\kappa a} &= kA\cos(ka) - kB\sin(ka) \end{aligned}$$

Odd solutions are those in which $B = 0$, in which case we can divide Eq. 2 by Eq. 1 (or Eq. 4 by Eq. 3) to find

$$-\kappa = k\cot(ka)$$

Doing the same with even solutions (those in which $A = 0$) gives the restriction

$$\kappa = k\tan(ka)$$

Of course, as $V_0 \to \infty$, $\kappa \to \infty$ and so the wave function in regimes where $|x| > a$ falls to 0, just as we found for the infinite square well.

As the problem statement suggests, we can find valid values of $k$ and $\kappa$ by treating $\kappa$ as the vertical axis of our plane, $k$ as the horizontal axis, plotting

$$\begin{aligned} \kappa &= k\tan(ka) \\ \kappa &= -k\cot(ka) \\ k^2 + \kappa^2 &= \frac{2mV_0}{\hbar^2} \end{aligned}$$

and looking for intersections of the first two equations with the last one in the first quadrant (since both $k$ and $\kappa$ must be positive). Since $k\tan(ka)$ goes through the origin of the plane, it will always intersect the circle at least once, and so there will always be a bound state that is an even solution.

The first intersection of the circle with the odd solution requirement occurs at the the latter's first zero, $-k\cot(ka) = 0$. This happens when $ka = \pi/2$ and $\kappa = 0$, or

$$\frac{\pi^2}{4a^2} = \frac{2mV_0}{\hbar^2}$$

Rearranging to isolate $V_0$ gives

$$V_0 = \frac{\hbar^2\pi^2}{8ma^2}$$

Since this is a lower bound (a higher potential will permit more bound states), we can write

$$V_0 \geq \frac{\hbar^2 \pi^2}{8ma^2}.$$

When this is an equality, $\kappa = 0$ and so $E = V_0$.

## 5.3 The Continuity Equation for Probability

5.3.1. Consider the case where $V = V_r - iV_i$, where the imaginary part $V_i$ is a constant. Is the Hamiltonian Hermitian? Go through the derivation of the continuity equation and show that the total probability for finding the particle decreases exponentially as $e^{-2V_i t/\hbar}$. Such complex potentials are used to describe processes in which particles are absorbed by a sink.

In this case, the Hamiltonian (in the position basis) is given by

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + (V_r - iV_i)$$

This is not Hermitian, as $H^\dagger$ will have a $+iV_i$ term. Now, consider the Schrödinger equation and its conjugate

$$\begin{aligned} i\hbar\frac{\partial \psi}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2\psi + V_r\psi - iV_i\psi \\ -i\hbar\frac{\partial \psi^*}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2\psi^* + V_r\psi^* + iV_i\psi^* \end{aligned}$$

Multiplying the top equation by $\psi^*$ and the bottom one by $\psi$ and subtracting gives

$$i\hbar\psi^*\frac{\partial \psi}{\partial t} + i\hbar\psi\frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\psi^*\nabla^2\psi + \frac{\hbar^2}{2m}\psi\nabla^2\psi^* + V_r\psi^*\psi - V_r\psi\psi^* - iV_i\psi^*\psi - iV_i\psi\psi^*$$

which can be simplified to

$$i\hbar\frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\hbar^2}{2m}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*) - i2V_i\psi^*\psi$$

or

$$\frac{\partial P}{\partial t} = -\nabla \cdot \mathbf{j} - \frac{2V_i P}{\hbar}$$

where $P = \psi^*\psi$ and $\mathbf{j} = (\frac{\hbar}{2mi})(\psi^*\nabla\psi - \psi\nabla\psi^*)$. We can move all terms with $P$ to the left side to find

$$\frac{\partial P}{\partial t} + \frac{2V_i P}{\hbar} = -\nabla \cdot \mathbf{j}$$

The homogeneous solution solution to this differential equation is

$$P \propto e^{-2V_i t/\hbar}$$

which shows that the probability decreases on its own with an influx of probability current, i.e. there is a particle sink.

5.3.2. Convince yourself that if $\psi = c\tilde{\psi}$, where $c$ is constant (real or complex) and $\tilde{\psi}$ is real, the corresponding $\mathbf{j}$ vanishes.

In the given case, the probability current is

$$\begin{aligned}\mathbf{j} &= \frac{\hbar}{2mi}(c^*\tilde{\psi}\nabla c\tilde{\psi} - c\tilde{\psi}\nabla c^*\tilde{\psi}) \\ &= \frac{\hbar}{2mi}(|c|^2\tilde{\psi}\nabla\tilde{\psi} - |c|^2\tilde{\psi}\nabla\tilde{\psi}) \\ &= \mathbf{0}\end{aligned}$$

which follows from the fact that $c$ commutes with $\nabla$.

5.3.3. Consider

$$\psi_{\mathbf{p}} = \left(\frac{1}{2\pi\hbar}\right)^{3/2} e^{i(\mathbf{p}\cdot\mathbf{r})/\hbar}$$

Find $\mathbf{j}$ and $P$ and compare the relation between them to the electromagnetic equation $\mathbf{j} = \rho\mathbf{v}$, $\mathbf{v}$ being the velocity. Since $\rho$ and $\mathbf{j}$ are constant, note that the continuity Eq. (5.3.7) is trivially satisfied.

The probability $P$ is given by

$$P = \psi_{\mathbf{p}}^*\psi_{\mathbf{p}} = \left(\frac{1}{2\pi\hbar}\right)^{3/2} e^{-i(\mathbf{p}\cdot\mathbf{r})/\hbar}\left(\frac{1}{2\pi\hbar}\right)^{3/2} e^{i(\mathbf{p}\cdot\mathbf{r})/\hbar} = \frac{1}{8\pi^3\hbar^3}$$

The gradient of $\psi_{\mathbf{p}}$ is

$$\nabla\psi_{\mathbf{p}} = \frac{i}{\hbar}\left(\frac{1}{2\pi\hbar}\right)^{3/2} e^{i(\mathbf{p}\cdot\mathbf{r})/\hbar}\mathbf{p} = \frac{i\psi_{\mathbf{p}}}{\hbar}\mathbf{p}$$

and so the probability current $\mathbf{j}$ is given by

$$\begin{aligned}\mathbf{j} &= \frac{\hbar}{2mi}(\psi_{\mathbf{p}}^*\nabla\psi_{\mathbf{p}} - \psi_{\mathbf{p}}\nabla\psi_{\mathbf{p}}^*) \\ &= \frac{\hbar}{2mi}\left(\psi_{\mathbf{p}}^*\frac{i\psi_{\mathbf{p}}}{\hbar}\mathbf{p} + \psi_{\mathbf{p}}\frac{i\psi_{\mathbf{p}}^*}{\hbar}\mathbf{p}\right) \\ &= P\frac{\mathbf{p}}{m}\end{aligned}$$

This is of the same form as the electromagnetic equation $\mathbf{j} = \rho\mathbf{v}$.

5.3.4. Consider $\psi = Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$ in one dimension. Show that $j = (|A|^2 - |B|^2)p/m$. The absence of cross terms between the right- and left-moving pieces in $\psi$ allows us to associate the two parts of $j$ with corresponding parts of $\psi$.

In one dimension,

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = \frac{ip}{\hbar}Ae^{ipx/\hbar} - \frac{ip}{\hbar}Be^{-ipx/\hbar}$$

and so

$$\begin{aligned}\psi^*\frac{\mathrm{d}\psi}{\mathrm{d}x} &= \frac{ip}{\hbar}(A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar})(Ae^{ipx/\hbar} - Be^{-ipx/\hbar}) \\ &= \frac{ip}{\hbar}(|A|^2 - A^*Be^{-i2px/\hbar} + B^*Ae^{i2px/\hbar} - |B|^2)\end{aligned}$$

The probability current is then

$$j = \frac{\hbar}{2mi}\left(\psi^*\frac{\mathrm{d}\psi}{\mathrm{d}x} - \psi\frac{\mathrm{d}\psi^*}{\mathrm{d}x}\right)$$

$$
\begin{aligned}
&= \frac{p}{2m}\Big(2|A|^2 - 2|B|^2 - A^*Be^{-i2px/\hbar} + B^*Ae^{i2px/\hbar} - AB^*e^{i2px/\hbar} + BA^*e^{-i2px/\hbar}\Big) \\
&= \frac{p}{m}(|A|^2 - |B|^2)
\end{aligned}
$$

## 5.4 The Single-Step Potential: A Problem in Scattering

5.4.1. (*Quite Hard*). Evaluate the third piece in Eq. (5.4.16) and compare the resulting $T$ with Eq. (5.4.21). [Hint: Expand the factor $(k_1^2 - 2mV_0/\hbar^2)^{1/2}$ near $k_1 = k_0$, keeping just the first derivative in the Taylor series.]

...

5.4.2. (a) Calculate $R$ and $T$ for scattering off a potential $V(x) = V_0 a\delta(x)$. (b) Do the same for the case $V = 0$ for $|x| > a$ and $V = V_0$ for $|x| < a$. Assume that the energy is positive but less than $V_0$.

(a) In both the positive and negative parts of the real line, the wave function will have the free space solution

$$
\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ Ce^{ikx}, & x > 0 \end{cases}
$$

where $k$ is the same in both areas owing to their lack of potential and $D$ is suppressed (since there are no waves incident from the right). By continuity,

$$
\psi(0^-) = \psi(0^+) \implies A + B = C
$$

Since the potential is infinitely large, we expect a discontinuity in the wave function's derivative at $x = 0$. This discontinuity is given by

$$
\psi'(0^+) - \psi'(0^-) = ikC - ik(A - B) = ik(C + B - A)
$$

Furthermore, since Schrödinger's equation for this potential (written in terms of $k$ instead of $E$) is given by

$$
\frac{\hbar^2 k^2}{2m}\psi(x) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + V_0 a\delta(x)\psi(x)
$$

we have

$$
\begin{aligned}
\psi'(0^+) - \psi'(0-) &= \lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}\mathrm{d}x \\
&= \lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon}\Big(\frac{2m}{\hbar^2}V_0 a\delta(x) - k^2\Big)\psi(x)\mathrm{d}x \\
&= \frac{2m}{\hbar^2}V_0 a\psi(0) \\
&= \frac{2m}{\hbar^2}V_0 a(A + B)
\end{aligned}
$$

Removing $C$ from the first discontinuity equation and comparing gives the condition

$$
i2kB = \frac{2m}{\hbar^2}V_0 a(A + B)
$$

or

$$\frac{B}{A} = \frac{2maV_0}{i2\hbar^2 k + 2maV_0}$$

Removing the common factor of two and taking the squared modulus of this gives us

$$R = \frac{(maV_0)^2}{\hbar^4 k^2 + (maV_0)^2}$$

in which case we have

$$T = \frac{\hbar^4 k^2}{\hbar^4 k^2 + (maV_0)^2}$$

We see that larger energies have a greater chance of being transmitted, as expected.

(b) The general solution to the wave function in such a space is given by

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < -a \\ Ce^{\kappa x} + De^{-\kappa x}, & |x| < a \\ Fe^{ikx} + Ge^{-ikx}, & x > a \end{cases}$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}$$
$$\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

Setting $G = 0$ (i.e. there are no particles incident from the right) and imposing continuity of $\psi(x)$ and $\psi'(x)$ gives the system of equations

$$\begin{aligned} Ae^{-ika} + Be^{ika} &= Ce^{-\kappa a} + De^{\kappa a} \\ ik(Ae^{-ika} - Be^{ika}) &= \kappa(Ce^{-\kappa a} - De^{\kappa a}) \\ Ce^{\kappa a} + De^{-\kappa a} &= Fe^{ika} \\ \kappa(Ce^{\kappa a} - De^{-\kappa a}) &= ikFe^{ika} \end{aligned}$$

By adding and subtracting the last two of these equations, we can solve for $C$ and $D$ in terms of $F$,

$$\begin{aligned} C &= \frac{F}{2}e^{-\kappa a}e^{ika}\Big(1 + \frac{ik}{\kappa}\Big) \\ D &= \frac{F}{2}e^{\kappa a}e^{ika}\Big(1 - \frac{ik}{\kappa}\Big) \end{aligned}$$

By adding the first two of these equations, we can solve $A$ in terms of $C$ and $D$, then substitute in our found expressions for $C$ and $D$ to get

$$\begin{aligned} A &= \frac{C}{2}e^{-\kappa a}e^{ika}\Big(1 + \frac{\kappa}{ik}\Big) + \frac{D}{2}e^{\kappa a}e^{ika}\Big(1 - \frac{\kappa}{ik}\Big) \\ &= \frac{F}{4}e^{-2\kappa a}e^{i2ka}\Big(1 + \frac{ik}{\kappa}\Big)\Big(1 + \frac{\kappa}{ik}\Big) + \frac{F}{4}e^{2\kappa a}e^{i2ka}\Big(1 - \frac{ik}{\kappa}\Big)\Big(1 - \frac{\kappa}{ik}\Big) \\ &= \frac{F}{4}e^{i2ka}\Big\{e^{-2\kappa a}\Big(2 - i\Big[\frac{\kappa}{k} - \frac{k}{\kappa}\Big]\Big) + e^{2\kappa a}\Big(2 + i\Big[\frac{\kappa}{k} - \frac{k}{\kappa}\Big]\Big)\Big\} \\ &= \frac{F}{4}e^{i2ka}\Big\{2(e^{2\kappa a} + e^{-2\kappa a}) + i\Big[\frac{\kappa^2 - k^2}{\kappa k}\Big](e^{2\kappa a} - e^{-2\kappa a})\Big\} \\ &= Fe^{i2ka}\Big(\cosh(2\kappa a) + i\Big[\frac{\kappa^2 - k^2}{2\kappa k}\Big]\sinh(2\kappa a)\Big) \end{aligned}$$

$$= Fe^{i2ka}\Big(\cosh(2\kappa a) + i\Big[\frac{V_0 - 2E}{(4E(V_0 - E))^{1/2}}\Big]\sinh(2\kappa a)\Big)$$

Defining

$$\alpha = \frac{V_0 - 2E}{(4E(V_0 - E))^{1/2}}$$

we find a transmission coefficient of

$$T = \frac{|F|^2}{|A|^2} = [\cosh^2(2\kappa a) + \alpha^2 \sinh^2(2\kappa a)]^{-1}$$

in which case we have $R = 1 - T$. From this, we see that transmission of an incident particle drops exponentially as we increase the width of the potential barrier.

5.4.3. Consider a particle subject to a constant force $f$ in one dimension. Solve for the propagator in momentum space and get

$$U(p, t; p', 0) = \delta(p - p' - ft)e^{i(p'^3 - p^3)/6m\hbar f}$$

Transform back to coordinate space and obtain

$$U(x, t; x', 0) = \Big(\frac{m}{2\pi\hbar i t}\Big)^{1/2} \exp\Big\{\frac{i}{\hbar}\Big[\frac{m(x - x')^2}{2t} + \frac{1}{2}ft(x + x') - \frac{f^2 t^3}{24m}\Big]\Big\}$$

[Hint: Normalize $\psi_E(p)$ such that $\langle E|E'\rangle = \delta(E - E')$. Note that $E$ is not restricted to be positive.]

Since force is related to potential via

$$F = -\frac{\mathrm{d}V}{\mathrm{d}x},$$

we can encode a constant force $f$ via $V = -fx$. In momentum space (where $\hat{P} = p$ and $\hat{X} = i\hbar\frac{\mathrm{d}}{\mathrm{d}p}$), the time-independent Schrödinger equation is then

$$E\psi(p) = \frac{p^2}{2m}\psi(p) - i\hbar f \frac{\mathrm{d}\psi(p)}{\mathrm{d}p}$$

Dividing both sides by $\psi(p)$ and isolating the derivative terms yields

$$\begin{aligned}
\frac{1}{\psi(p)}\frac{\mathrm{d}\psi(p)}{\mathrm{d}p} &= \frac{iE}{\hbar f} - \frac{ip^2}{2m\hbar f} \\
\int \frac{1}{\psi(p)}\frac{\mathrm{d}\psi(p)}{\mathrm{d}p}\mathrm{d}p &= \int \frac{iE}{\hbar f}\mathrm{d}p - \int \frac{ip^2}{2m\hbar f}\mathrm{d}p \\
\ln(\psi(p)) &= \frac{iEp}{\hbar f} - \frac{ip^3}{6m\hbar f} \\
\psi(p) &= Ae^{iEp/\hbar f}e^{-ip^3/6m\hbar f}
\end{aligned}$$

where, as a reminder, $\psi(p) = \langle p|E\rangle$. To normalize this state, we use

$$\begin{aligned}
\langle E|E'\rangle &= \int_{-\infty}^{\infty} \langle E|p\rangle\langle p|E'\rangle\,\mathrm{d}p \\
&= A^2 \int_{-\infty}^{\infty} e^{ip(E' - E)/\hbar f}\,\mathrm{d}p
\end{aligned}$$

$$
\begin{aligned}
&= A^2\hbar f\int_{-\infty}^{\infty} e^{ip'(E'-E)}\mathrm{d}p' \\
&= \delta(E-E')
\end{aligned}
$$

where we have made the substitution $p = p/\hbar f$. From this we see

$$
A = \frac{1}{(2\pi\hbar f)^{1/2}}
$$

The propagator in momentum space is then given by

$$
\begin{aligned}
\langle p|e^{-i\hat{H}t/\hbar}|p'\rangle &= \int_{-\infty}^{\infty}\langle p|E\rangle\langle E|e^{-i\hat{H}t/\hbar}|p'\rangle\,\mathrm{d}E \\
&= \int_{-\infty}^{\infty}\langle p|E\rangle\langle E|p'\rangle e^{-iEt/\hbar}\,\mathrm{d}E \\
&= \frac{1}{2\pi\hbar f}\int_{-\infty}^{\infty} e^{iE(p-p')/\hbar f}e^{-i(p^3-p'^3)/6m\hbar f}e^{-iEt/\hbar}\,\mathrm{d}E \\
&= e^{-i(p^3-p'^3)/6m\hbar f}\cdot\frac{1}{2\pi\hbar f}\int_{-\infty}^{\infty} e^{iE(p-p'-ft)/\hbar f}\,\mathrm{d}E \\
&= \delta(p-p'-ft)e^{i(p'^3-p^3)/6m\hbar f}
\end{aligned}
$$

To find the position space variant of this, we examine

$$
\begin{aligned}
\langle x|e^{-i\hat{H}t/\hbar}|x'\rangle &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\langle x|p\rangle\langle p|e^{-i\hat{H}t/\hbar}|p'\rangle\langle p'|x'\rangle\,\mathrm{d}p\,\mathrm{d}p' \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{ixp/\hbar}\delta(p-p'-ft)e^{i(p'^3-p^3)/6m\hbar f}e^{-ix'p'/\hbar}\,\mathrm{d}p\,\mathrm{d}p' \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ixp/\hbar}e^{i\left((p-ft)^3-p^3\right)/6m\hbar f}e^{-ix'(p-ft)/\hbar}\,\mathrm{d}p \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\exp\Big(\frac{i}{6m\hbar f}(-3p^2ft+3pf^2t^2-f^3t^3)+\frac{ixp}{\hbar}-\frac{ix'p}{\hbar}+\frac{iftx'}{\hbar}\Big)\mathrm{d}p \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\exp\Big(-\frac{i}{\hbar}\frac{t}{2m}p^2+\frac{i}{\hbar}\Big[\frac{ft^2}{2m}+x-x'\Big]p+\frac{i}{\hbar}\Big[ftx'-\frac{f^2t^3}{6m}\Big]\Big)\mathrm{d}p \\
&= \frac{1}{2\pi\hbar}\Big(\frac{2\pi\hbar m}{it}\Big)^{1/2}\exp\Bigg(\frac{-\frac{1}{\hbar^2}\Big(\frac{ft^2}{2m}+x-x'\Big)^2}{\frac{4it}{2m\hbar}}\Bigg)\exp\Big(\frac{i}{\hbar}\Big[ftx'-\frac{f^2t^3}{6m}\Big]\Big) \\
&= \Big(\frac{m}{2\pi\hbar it}\Big)^{1/2}\exp\Big(\frac{i}{\hbar}\Big[\frac{f^2t^3}{8m}+\frac{ft}{2}(x-x')+\frac{m}{2t}(x-x')^2\Big]\Big)\exp\Big(\frac{i}{\hbar}\Big[\frac{ft}{2}(2x')-\frac{f^2t^3}{6m}\Big]\Big) \\
&= \Big(\frac{m}{2\pi\hbar it}\Big)^{1/2}\exp\Big(\frac{i}{\hbar}\Big[\frac{m(x-x')^2}{2t}+\frac{1}{2}ft(x+x')-\frac{f^2t^3}{24m}\Big]\Big)
\end{aligned}
$$

# 7 The Harmonic Oscillator

## 7.3 Quantization of the Oscillator (Coordinate Basis)

7.3.1. Consider the question why we tried a power-series solution for Eq. (7.3.11) but not Eq. (7.3.8). By feeding in a series into the latter, verify that a three-term recursion relation between $C_{n+2}$, $C_n$, and $C_{n-2}$

obtains, from which the solution does not follow so readily. The problem is that $\psi''$ has two powers of $y$ less than $2\epsilon y$, while the $-y^2$ piece has two more powers of $y$. In Eq. (7.3.11) on the other hand, of the three pieces $u''$, $-2yu'$, and $(2\epsilon - 1)u$, the last two have the same powers of $y$.

The differential equation in terms of $\psi$ is given by

$$\psi'' + (2\varepsilon - y^2)\psi = 0$$

Substituting in

$$\psi = \sum_{n=0}^{\infty} C_n y^n$$

yields

$$\begin{aligned}
\psi'' + (2\varepsilon - y^2)\psi &= \sum_{n=0}^{\infty} C_n n(n-1) y^{n-2} + (2\varepsilon - y^2) \sum_{n=0}^{\infty} C_n y^n \\
&= \sum_{m=-2}^{\infty} C_{m+2}(m+2)(m+1) y^m + \sum_{n=0}^{\infty} 2\varepsilon C_n y^n - \sum_{n=0}^{\infty} C_n y^{n+2} \\
&= \sum_{n=0}^{\infty} y^n [C_{n+2}(n+2)(n+1) + 2\varepsilon C_n] - \sum_{m=2}^{\infty} C_{m-2} y^m
\end{aligned}$$

That is, the relationship

$$C_{n+2}(n+2)(n+1) + 2\varepsilon C_n = 0$$

holds for $n = 0$ and $n = 1$, after which we find

$$C_{n+2}(n+2)(n+1) + 2\varepsilon C_n - C_{n-2} = 0$$

This is a three term recursion relation and is much more difficult to work with.

7.3.2. Verify that $H_3(y)$ and $H_4(y)$ obey the recursion relation, Eq. (7.3.15).

We know that

$$\begin{aligned}
H_3(y) &= -12(y - \tfrac{2}{3}y^3) = -12y + 8y^3 = C_1 y + C_3 y^3 \\
H_4(y) &= 12(1 - 4y^2 + \tfrac{4}{3}y^4) = 12 - 48y^2 + 16y^4 = C_0 + C_2 y^2 + C_4 y^4
\end{aligned}$$

By Eq. (7.3.15), we know

$$C_{n+2} = C_n \frac{2(n-m)}{(n+2)(n+1)}$$

where $m$ denotes the energy level. For $H_3(y)$ with $C_1 = -12$, we have

$$C_3 = (-12)\frac{2(1-3)}{(1+2)(1+1)} = (-12)\left(\frac{-2}{3}\right) = 8$$

while for $H_4(y)$ with $C_1 = 12$, we have

$$C_2 = 12\frac{2(0-4)}{(0+2)(0+1)} = 12(-4) = -48$$

$$C_4 = (-48)\frac{2(2-4)}{(2+2)(2+1)} = (-48)\Big(-\frac{1}{3}\Big) = 16$$

7.3.3. If $\psi(x)$ is even and $\phi(x)$ is odd under $x \to -x$, show that

$$\int_{-\infty}^{\infty} \psi(x)\phi(x)\,\mathrm{d}x = 0$$

Use this to show that $\psi_2(x)$ and $\psi_1(x)$ are orthogonal. Using the values of Gaussian integrals in Appendix A.2 verify that $\psi_2(x)$ and $\psi_0(x)$ are orthogonal.

If $\psi(x)$ is even and $\phi(x)$ is odd, then

$$\begin{aligned}\int_{-\infty}^{\infty} \psi(x)\phi(x)\,\mathrm{d}x &= \int_{\infty}^{-\infty} \psi(-x)\phi(-x)(-\mathrm{d}x)\\ &= \int_{\infty}^{-\infty} \psi(x)(-\phi(x))(-\mathrm{d}x)\\ &= -\int_{-\infty}^{\infty} \psi(x)\phi(x)\,\mathrm{d}x\end{aligned}$$

which is only possible is the integral evaluates to 0.

Whether a given harmonic oscillator wave function is even or add depends on the behavior of its associate Hermite polynomial. These are

$$\begin{aligned}H_1(y) &= 2y\\ H_2(y) &= -2(1-2y^2)\end{aligned}$$

in the case of $\psi_1(y)$ and $\psi_2(y)$. Since $H_2(y)$ is even and $H_1(y)$ is odd,

$$\int_{-\infty}^{\infty} \psi_1(x)\psi_2(x)\,\mathrm{d}x = 0.$$

The first two wave functions are given by

$$\begin{aligned}\psi_0(x) &= \Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4} \exp\Big(-\frac{m\omega x^2}{2\hbar}\Big)\\ \psi_1(x) &= \Big(\frac{m\omega}{4\pi\hbar}\Big)^{1/4} \exp\Big(-\frac{m\omega x^2}{2\hbar}\Big)2\Big(\frac{m\omega}{\hbar}\Big)^{1/2} x\\ &= \Big(\frac{4m^3\omega^3}{\pi\hbar^3}\Big)^{1/4} x \exp\Big(-\frac{m\omega x^2}{2\hbar}\Big)\end{aligned}$$

Integrating these against one another yields

$$\int_{-\infty}^{\infty} \psi_0(x)\psi_1(x)\,\mathrm{d}x = \frac{m\omega}{\hbar}\Big(\frac{2}{\pi}\Big)^{1/2} \int_{-\infty}^{\infty} x \exp\Big(-\frac{m\omega x^2}{\hbar}\Big)\,\mathrm{d}x = 0$$

where the 0 follows because $x$ is odd and $\exp(-m\omega x^2/\hbar)$ is even.

7.3.4. Using Eqs. (7.3.23)-(7.3.25), show that

$$\langle n'|x|n\rangle = \Big(\frac{\hbar}{2m\omega}\Big)^{1/2}[\delta_{n',n+1}(n+1)^{1/2} + \delta_{n',n-1}n^{1/2}]$$
$$\langle n'|P|n\rangle = \Big(\frac{m\omega\hbar}{2}\Big)^{1/2} i[\delta_{n',n+1}(n+1)^{1/2} - \delta_{n',n-1}n^{1/2}]$$

Plowing straight ahead, we find

$$\begin{aligned}
\langle n'|x|n\rangle &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle n'|x'\rangle\langle x'|x|x\rangle\langle x|n\rangle \,\mathrm{d}x'\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} x\langle n'|x'\rangle\delta(x'-x)\langle x|n\rangle \,\mathrm{d}x'\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} x\,\psi^*_{n'}(x)\,\psi_n(x)\,\mathrm{d}x \\
&= A_{n'}A_n \int_{-\infty}^{\infty} \exp\big(-\tfrac{m\omega x^2}{\hbar}\big) x H_{n'}\Big[\big(\tfrac{m\omega}{\hbar}\big)^{1/2}x\Big] H_n\Big[\big(\tfrac{m\omega}{\hbar}\big)^{1/2}x\Big]\,\mathrm{d}x \\
&= A_{n'}A_n\big(\tfrac{\hbar}{m\omega}\big)\int_{-\infty}^{\infty} yH_n(y)H_{n'}(y)e^{-y^2}\,\mathrm{d}y
\end{aligned}$$

using Eq. (7.3.25), we can replace with $yH_n(y) = \frac{1}{2}H_{n+1}(y) + nH_{n-1}(y)$ to find

$$\begin{aligned}
\langle n'|x|n\rangle &= A_{n'}A_n\big(\tfrac{\hbar}{m\omega}\big)\int_{-\infty}^{\infty}\big(\tfrac{1}{2}H_{n+1}(y) + nH_{n-1}(y)\big)H_{n'}(y)e^{-y^2}\,\mathrm{d}y \\
&= A_{n'}A_n\big(\tfrac{\hbar}{m\omega}\big)\Big[\tfrac{1}{2}\int_{-\infty}^{\infty} H_{n+1}(y)H_{n'}(y)e^{-y^2}\,\mathrm{d}y + n\int_{-\infty}^{\infty} H_{n-1}(y)H_{n'}(y)e^{-y^2}\,\mathrm{d}y\Big] \\
&= \big(\tfrac{m\omega}{\hbar}\big)^{1/2}\big(\tfrac{1}{2^{2n}(n!)^2}\big)^{1/4}\big(\tfrac{1}{2^{2n'}(n'!)^2}\big)^{1/4}\big(\tfrac{\hbar}{m\omega}\big)\big[\tfrac{1}{2}\delta_{n',n+1}(2^{n+1}(n+1)!) + n\delta_{n',n-1}(2^{n-1}(n-1)!)\big]
\end{aligned}$$

From here, let's examine each term one at a time. The term on the left can be simplified as

$$\begin{aligned}
\tfrac{1}{2}\big(\tfrac{\hbar}{m\omega}\big)^{1/2}\big(\tfrac{1}{2^{n+n'}(n!)(n'!)}\big)^{1/2}\delta_{n',n+1}(2^{n+1}(n+1)!) &= \big(\tfrac{\hbar}{m\omega}\big)^{1/2}\big(\tfrac{1}{2^{2n+1}(n!)(n+1)!}\big)^{1/2}\delta_{n',n+1}(2^{n}(n+1)!) \\
&= \big(\tfrac{\hbar}{m\omega}\big)^{1/2}\tfrac{1}{2^n(n!)}\big(\tfrac{1}{2(n+1)}\big)^{1/2}\delta_{n',n+1}(2^{n}(n+1)!) \\
&= \big(\tfrac{\hbar}{m\omega}\big)^{1/2}\big(\tfrac{1}{2(n+1)}\big)^{1/2}\delta_{n',n+1}(n+1) \\
&= \big(\tfrac{\hbar}{2m\omega}\big)^{1/2}\delta_{n',n+1}(n+1)^{1/2}
\end{aligned}$$

while the term on the right becomes

$$\begin{aligned}
n\big(\tfrac{\hbar}{m\omega}\big)^{1/2}\big(\tfrac{1}{2^{n+n'}(n!)(n'!)}\big)^{1/2}\delta_{n',n-1}(2^{n-1}(n-1)!) &= n\big(\tfrac{\hbar}{m\omega}\big)^{1/2}\big(\tfrac{1}{2^{2n-1}(n!)(n-1)!}\big)^{1/2}\delta_{n',n-1}(2^{n-1}(n-1)!) \\
&= n\big(\tfrac{\hbar}{m\omega}\big)^{1/2}\tfrac{1}{2^n(n-1)!}\big(\tfrac{1}{2^{-1}n}\big)^{1/2}\delta_{n',n-1}(2^{n-1}(n-1)!) \\
&= \big(\tfrac{\hbar}{2m\omega}\big)^{1/2}\delta_{n',n-1}n^{1/2}
\end{aligned}$$

and so we have

$$\langle x'|x|n\rangle = \big(\tfrac{\hbar}{2m\omega}\big)^{1/2}[\delta_{n',n+1}(n+1)^{1/2} + \delta_{n',n-1}n^{1/2}]$$

We can perform a similar simplification to the second expression, starting with

$$\langle n'|P|n\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\langle n'|x'\rangle\langle x'|-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}|x\rangle\langle x|n\rangle\,\mathrm{d}x'\,\mathrm{d}x$$

$$
\begin{aligned}
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi_{n'}^*(x')\delta(x-x')\Big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\Big)\psi_n(x)\,\mathrm{d}x'\,\mathrm{d}x \\
&= -i\hbar\int_{-\infty}^{\infty} \psi_{n'}^*(x)\frac{\mathrm{d}\psi_n(x)}{\mathrm{d}x}\,\mathrm{d}x \\
&= -i\hbar A_{n'}A_n\int_{-\infty}^{\infty} \exp\big(-\tfrac{m\omega x^2}{2\hbar}\big)H_{n'}\big[\big(\tfrac{m\omega}{\hbar}\big)^{1/2}x\big]\frac{\mathrm{d}}{\mathrm{d}x}\Big(\exp\big(-\tfrac{m\omega x^2}{2\hbar}\big)H_n\big[\big(\tfrac{m\omega}{\hbar}\big)^{1/2}x\big]\Big)\mathrm{d}x \\
&= -i\hbar A_{n'}A_n\int_{-\infty}^{\infty} \exp\big(-\tfrac{y^2}{2}\big)H_{n'}(y)\frac{\mathrm{d}}{\mathrm{d}y}\Big(\exp\big(-\tfrac{y^2}{2}\big)H_n(y)\Big)\mathrm{d}y \\
&= i\hbar A_{n'}A_n\int_{-\infty}^{\infty} y\exp\big(-y^2\big)H_{n'}(y)H_n(y) - \exp(-y^2)H_{n'}(y)H_n'(y)\mathrm{d}y
\end{aligned}
$$

and then using $H_n'(y) = 2nH_{n-1}(y)$ and $yH_n(y) = \frac{1}{2}H_{n+1}(y) + nH_{n-1}(y)$ to get

$$
\begin{aligned}
&i\hbar A_{n'}A_n\int_{-\infty}^{\infty} \exp(-y^2)\Big(\tfrac{1}{2}H_{n+1}(y) + nH_{n-1}(y) - 2nH_{n-1}(y)\Big)H_{n'}(y)\mathrm{d}y \\
&= i\hbar A_{n'}A_n\Big[\tfrac{1}{2}\int_{-\infty}^{\infty} H_{n+1}(y)H_{n'}(y)e^{-y^2}\mathrm{d}y - n\int_{-\infty}^{\infty} H_{n-1}(y)H_{n'}(y)e^{-y^2}\mathrm{d}y\Big]
\end{aligned}
$$

From here, we can use our previous results to immediately write

$$
\langle n'|P|n\rangle = \big(\tfrac{m\omega\hbar}{2}\big)^{1/2} i[\delta_{n',n+1}(n+1)^{1/2} - \delta_{n',n-1}n^{1/2}]
$$

since the found expression is simply a scaled, alternating version of the first expression.

7.3.5. Using the symmetry arguments from Exercise 7.3.3 show that $\langle n|X|n\rangle = \langle n|P|n\rangle = 0$ and thus that $\langle X^2\rangle = (\Delta X)^2$ and $\langle P^2\rangle = (\Delta P)^2$ in these states. Show that $\langle 1|X^2|1\rangle = 3\hbar/2m\omega$ and $\langle 1|P^2|1\rangle = \frac{3}{2}m\omega\hbar$. Show that $\psi_0(x)$ saturates the uncertainty bound $\Delta X \cdot \Delta P \geq \hbar/2$.

In general, for an operator $L$ in the position basis, we have

$$
\langle n|L|n\rangle = \int_{-\infty}^{\infty} \psi_n^*(x)L\psi_n(x)\,\mathrm{d}x
$$

When $L = X$, this becomes

$$
\langle n|X|n\rangle = \int_{-\infty}^{\infty} \psi_n^*(x)X\psi_n(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} \overbrace{x}^{\text{odd}}\underbrace{|\psi_n(x)|^2}_{\text{even}}\,\mathrm{d}x = 0
$$

When $L = P$, we have

$$
\langle n|P|n\rangle = \int_{-\infty}^{\infty} \psi_n^*(x)\Big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\Big)\psi_n(x)\,\mathrm{d}x = -i2\hbar n\int_{-\infty}^{\infty} \psi_n^*(x)\psi_{n-1}(x)\,\mathrm{d}x = 0
$$

where the last equality follows from the fact that the wave functions alternate between even and odd solutions as $n$ changes by 1. These results show that $\langle X\rangle = \langle P\rangle = 0$. Since

$$
(\Delta X)^2 = \langle X^2\rangle - \langle X\rangle^2
$$

and

$$
(\Delta P)^2 = \langle P^2\rangle - \langle P\rangle^2,
$$

this implies $\langle X^2 \rangle = (\Delta X)^2$ and $\langle P^2 \rangle = (\Delta P)^2$. To calculate $\langle 1|X^2|1\rangle$, we compute

$$\begin{aligned}\int_{-\infty}^{\infty} \psi_1^*(x) x^2 \psi_1(x)\,\mathrm{d}x &= 4\Big(\frac{m\omega}{4\pi\hbar}\Big)^{1/2}\Big(\frac{m\omega}{\hbar}\Big)\int_{-\infty}^{\infty} x^4 \exp\Big(-\frac{m\omega x^2}{\hbar}\Big)\,\mathrm{d}x \\ &= \frac{2}{(\pi)^{1/2}}\Big(\frac{m\omega}{\hbar}\Big)^{3/2}\cdot\Big[(\pi)^{1/2}\cdot\frac{3}{4}\Big(\frac{m\omega}{\hbar}\Big)^{-5/2}\Big] \\ &= \frac{3\hbar}{2m\omega}\end{aligned}$$

where we have used the fact that $H_1(y) = 2y$ and $I_4(\alpha) = (3/4)(\pi/\alpha^5)^{1/2}$. Similarly, we have

$$\begin{aligned}-\hbar^2\int_{-\infty}^{\infty}\psi_1^*(x)\psi_1''(x)\,\mathrm{d}x &= -4\hbar^2\Big(\frac{m\omega}{4\pi\hbar}\Big)^{1/2}\Big(\frac{m\omega}{\hbar}\Big)\int_{-\infty}^{\infty} x\exp\Big(-\frac{m\omega x^2}{2\hbar}\Big)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Big[x\exp\Big(-\frac{m\omega x^2}{2\hbar}\Big)\Big]\mathrm{d}x \\ &= -\frac{2m\omega}{(\pi)^{1/2}}\Big(\frac{m\omega}{\hbar}\Big)^{3/2}\int_{-\infty}^{\infty} x^2\exp\Big(-\frac{m\omega x^2}{\hbar}\Big)(m\omega x^2 - 3\hbar)\mathrm{d}x \\ &= -\frac{2m\omega}{(\pi)^{1/2}}\Big(\frac{m\omega}{\hbar}\Big)^{3/2}\Big(m\omega(\pi)^{1/2}\cdot\frac{3}{4}\Big(\frac{m\omega}{\hbar}\Big)^{-5/2} - 3\hbar\Big(\frac{m\omega}{\hbar}\Big)^{-3/2}\frac{(\pi)^{1/2}}{2}\Big) \\ &= -2\frac{(m\omega)^{5/2}}{(\hbar)^{3/2}}\Big(\frac{3}{4}\frac{(\hbar)^{5/2}}{(m\omega)^{3/2}} - \frac{3}{2}\frac{(\hbar)^{5/2}}{(m\omega)^{3/2}}\Big) \\ &= \frac{3m\omega\hbar}{2}\end{aligned}$$

Finally, we calculate the uncertainties in position and momentum for the ground state of the harmonic oscillator,

$$\begin{aligned}(\Delta X)^2 &= \Big(\frac{m\omega}{\pi\hbar}\Big)^{1/2}\int_{-\infty}^{\infty} x^2\exp\Big(-\frac{m\omega x^2}{\hbar}\Big)\mathrm{d}x \\ &= \Big(\frac{m\omega}{\pi\hbar}\Big)^{1/2}\frac{(\pi)^{1/2}}{2}\Big(\frac{m\omega}{\hbar}\Big)^{-3/2} \\ &= \frac{\hbar}{2m\omega} \\ (\Delta P)^2 &= -\hbar^2\Big(\frac{m\omega}{\pi\hbar}\Big)^{1/2}\int_{-\infty}^{\infty}\exp\Big(-\frac{m\omega x^2}{2\hbar}\Big)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Big[\exp\Big(-\frac{m\omega x^2}{2\hbar}\Big)\Big]\mathrm{d}x \\ &= -\hbar^2\Big(\frac{m\omega}{\pi\hbar}\Big)^{1/2}\frac{m\omega}{\hbar}\int_{-\infty}^{\infty}\exp\Big(-\frac{m\omega x^2}{\hbar}\Big)\Big(\frac{m\omega}{\hbar}x^2 - 1\Big)\mathrm{d}x \\ &= -\hbar^2\Big(\frac{m\omega}{\pi\hbar}\Big)^{1/2}\frac{m\omega}{\hbar}\Big(\frac{m\omega}{2\hbar}\Big(\frac{\pi}{(m\omega/\hbar)^3}\Big)^{1/2} - \Big(\frac{\pi}{m\omega/\hbar}\Big)^{1/2}\Big) \\ &= -\hbar^2\Big(\frac{m\omega}{\hbar}\Big)^{3/2}\Big[\frac{1}{2}\Big(\frac{\hbar}{m\omega}\Big)^{1/2} - \Big(\frac{\hbar}{m\omega}\Big)^{1/2}\Big] \\ &= \frac{m\omega\hbar}{2}\end{aligned}$$

which gives

$$(\Delta X)\cdot(\Delta P) = \Big(\frac{\hbar}{2m\omega}\Big)^{1/2}\Big(\frac{m\omega\hbar}{2}\Big)^{1/2} = \frac{\hbar}{2}$$

7.3.6. Consider a particle in a potential

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2x^2, & x > 0 \\ \infty, & x \le 0 \end{cases}$$

What are the boundary conditions on the wave functions now? Find the eigenvalues and eigenfunctions.

This is a very similar problem to the harmonic oscillator, and we may freely make the assumption that

$$\psi(y) = u(y)e^{-y^2/2}$$

However, unlike the previous case, we now look for a function $u(y)$ that approaches 0 as $y$ approaches 0. This is accomplished when $C_0 = 0$, see Eq. (7.3.16).

Another way to look at the problem is that the wave function in the region $y \ge 0$ should look like its counterpart in the original harmonic oscillator potential, except we should have $\psi(0) = 0$. This only occurs with those odd solutions to the original harmonic oscillator potential, i.e. our wave functions will look like

$$\psi_{2n+1}(x) = \begin{cases} 0, & x \le 0 \\ A_n \exp\left(-\frac{m\omega x^2}{2\hbar}\right) H_{2n+1}\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x\right], & x > 0 \end{cases}$$

To find $A_n$, we normalize this as

$$\begin{aligned} A_n^2 \int_{-\infty}^{\infty} \Theta(x) \exp\left(-\tfrac{m\omega x^2}{\hbar}\right)\left(H_{2n+1}\left[\left(\tfrac{m\omega}{\hbar}\right)^{1/2} x\right]\right)^2 \mathrm{d}x &= A_n^2 \tfrac{1}{2}\left(\tfrac{m\omega}{\hbar}\right)^{1/2} \int_{-\infty}^{\infty} e^{-y^2}\left(H_{2n+1}(y)\right)^2 \mathrm{d}y \\ &= A_n^2 \tfrac{1}{2}\left(\tfrac{m\omega}{\hbar}\right)^{1/2} (\pi^{1/2} 2^{2n+1} (2n+1)!) \\ &= A_n^2 \left(\tfrac{\pi m\omega \cdot 2^{4n}[(2n+1)!]^2}{\hbar}\right)^{1/2} \\ &= 1 \end{aligned}$$

i.e.

$$A_n = \left(\frac{\hbar}{\pi m\omega 2^{4n}[(2n+1)!]^2}\right)$$

7.3.7. *The Oscillator in Momentum Space.* By setting up an eigenvalue equation for the oscillator in the $P$ basis and comparing it to Eq. (7.3.2), show that the momentum space eigenfunctions may be obtained from the ones in coordinate space through the substitution $x \to p$, $m\omega \to 1/m\omega$. Thus, for example,

$$\psi_0(p) = \left(\frac{1}{m\pi\hbar\omega}\right)^{1/4} e^{-p^2/2m\hbar\omega}$$

There are several other pairs, such as $\Delta X$ and $\Delta P$ in the state $|n\rangle$, which are related by the substitution $m\omega \to 1/m\omega$. You may wish to watch out for them. (Refer back to Exercise 7.3.5).

In the $P$ basis, the time-independent Schrödinger equation becomes

$$\frac{p^2}{2m}\psi_E(p) - \frac{1}{2}m\omega^2\hbar^2\frac{\mathrm{d}^2\psi_E(p)}{\mathrm{d}p^2} = E\psi_E(p)$$

or, collecting terms,

$$\frac{\mathrm{d}^2\psi_E(p)}{\mathrm{d}p^2} + \frac{2}{m\omega^2\hbar^2}\left(E - \frac{p^2}{2m}\right)\psi_E(p) = 0$$

Introducing the dimensionless parameter $y$ related to $p$ via $p = by$, we find

$$\frac{\mathrm{d}^2\psi_E(y)}{\mathrm{d}y^2} + \frac{2Eb^2}{m\omega^2\hbar^2}\psi_E(y) - \frac{b^4}{m^2\omega^2\hbar^2}y^2\psi_E(y) = 0$$

which can be simplified nicely through the choice $b = (m\omega\hbar)^{1/2}$. Further defining

$$\varepsilon = \frac{Eb^2}{m\omega^2\hbar^2} = \frac{E}{\hbar\omega},$$

we arrive at

$$\frac{\mathrm{d}^2\psi_E(y)}{\mathrm{d}y^2} + (2\varepsilon - y^2)\psi_E(y) = 0.$$

This is exactly the same as Eq (7.3.8) and so has the same solution. Instead of substituting

$$y = \left(\frac{m\omega}{\hbar}\right)^{1/2} x,$$

we simply substitute

$$y = \left(\frac{1}{m\omega\hbar}\right)^{1/2} p,$$

which is equivalent to the substitutions $x \to p$, $m\omega \to 1/m\omega$ in the problem statement.

## 7.4 The Oscillator in the Energy Basis

7.4.1. Compute the matrix elements of $X$ and $P$ in the $|n\rangle$ basis and compare with the result from Exercise 7.3.4.

Given

$$\begin{aligned} X &= \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a + a^\dagger) \\ P &= i\left(\frac{m\omega\hbar}{2}\right)^{1/2}(a^\dagger - a) \end{aligned}$$

we have

$$\begin{aligned} \langle n'|X|n\rangle &= \left(\frac{\hbar}{2m\omega}\right)^{1/2}\Big[\langle n'|a|n\rangle + \langle n'|a^\dagger|n\rangle\Big] \\ &= \left(\frac{\hbar}{2m\omega}\right)^{1/2}\Big[n^{1/2}\langle n'|n-1\rangle + (n+1)^{1/2}\langle n'|n+1\rangle\Big] \\ &= \left(\frac{\hbar}{2m\omega}\right)^{1/2}\Big[\delta_{n',n-1}n^{1/2} + \delta_{n',n+1}(n+1)^{1/2}\Big] \\ \langle n'|P|n\rangle &= i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\Big[\langle n'|a^\dagger|n\rangle - \langle n'|a|n\rangle\Big] \\ &= i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\Big[(n+1)^{1/2}\langle n'|n+1\rangle - n^{1/2}\langle n'|n-1\rangle\Big] \\ &= i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\Big[\delta_{n',n+1}(n+1)^{1/2} - \delta_{n',n-1}n^{1/2}\Big] \end{aligned}$$

We have found the same results as those in Exercise 7.3.4 with significantly less computation!

7.4.2. Find $\langle X\rangle$, $\langle P\rangle$, $\langle X^2\rangle$, $\langle P^2\rangle$, $\Delta X\cdot\Delta P$ in the state $|n\rangle$.

From the previous exercise, we know that $\langle X\rangle = \langle P\rangle = 0$. The other values are computed as

$$\begin{aligned}
\langle n|X^2|n\rangle &= \frac{\hbar}{2m\omega}\langle n|(a+a^\dagger)^2|n\rangle \\
&= \frac{\hbar}{2m\omega}\langle n|aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger|n\rangle \\
&= \frac{\hbar}{2m\omega}\Big[\langle n|aa^\dagger|n\rangle + \langle n|a^\dagger a|n\rangle\Big] \\
&= \frac{\hbar}{2m\omega}\Big[(n+1)^{1/2}\langle n|a|n+1\rangle + n^{1/2}\langle n|a^\dagger|n-1\rangle\Big] \\
&= \frac{\hbar}{2m\omega}\Big[(n+1)\delta_{n,n} + n\delta_{n,n}\Big] \\
&= \frac{\hbar}{2m\omega}(2n+1)
\end{aligned}$$

and

$$\begin{aligned}
\langle n|P^2|n\rangle &= -\frac{m\omega\hbar}{2}\langle n|(a^\dagger - a)^2|n\rangle \\
&= -\frac{m\omega\hbar}{2}\langle n|a^\dagger a^\dagger - a^\dagger a - aa^\dagger + aa|n\rangle \\
&= \frac{m\omega\hbar}{2}\Big[\langle n|a^\dagger a|n\rangle + \langle n|aa^\dagger|n\rangle\Big] \\
&= \frac{m\omega\hbar}{2}(2n+1)
\end{aligned}$$

Combining our results gives us an uncertainty of

$$\begin{aligned}
\Delta X\cdot\Delta P &= \sqrt{\langle X^2\rangle - \langle X\rangle^2}\cdot\sqrt{\langle P^2\rangle - \langle P\rangle^2} \\
&= \sqrt{\langle X^2\rangle\langle P^2\rangle} \\
&= \sqrt{\frac{\hbar^2}{4}(2n+1)^2} \\
&= \frac{\hbar}{2}(2n+1)
\end{aligned}$$

7.4.3. (*Virial Theorem*). The virial theorem in classical mechanics states that for a particle bound by a potential $V(r) = ar^k$, the average (over the orbit) kinetic and potential energies are related by

$$\bar{T} = c(k)\bar{V}$$

when $c(k)$ depends only on $k$. Show that $c(k) = k/2$ by considering a circular orbit. Using the results from the previous exercise show that for the oscillator ($k = 2$)

$$\langle T\rangle = \langle V\rangle$$

in the quantum state $|n\rangle$.

When a particle undergoes a circular orbit, it experiences a centripetal force equal in magnitude to to

$$|\mathbf{F}| = |-\nabla V| = \frac{mv^2}{r}$$

For the given potential, its gradient is

$$\begin{aligned}
\frac{\partial V}{\partial x_i} &= akr^{k-1}\frac{\partial r}{\partial x_i} \\
&= akr^{k-1}\frac{\partial}{\partial x_i}\Big(\sum_i x_i^2\Big)^{1/2} \\
&= akr^{k-1}\frac{1}{2}\Big(\sum_i x_i^2\Big)^{-1/2}(2x_i) \\
&= akr^{k-2}x_i
\end{aligned}$$

which has a magnitude of

$$|-\nabla V| = akr^{k-2}\sqrt{\sum_i x_i^2} = akr^{k-1}$$

Equating this with our centripetal force allows us to solve for $v^2$ as

$$v^2 = \frac{akr^k}{m}$$

which gives a kinetic energy of

$$T = \frac{1}{2}mv^2 = \frac{akr^k}{2}$$

Since $r$ is constant over a circular orbit, $\bar{T} = T$ and $\bar{V} = V$, in which case it is clear that

$$\bar{T} = \frac{k}{2}\bar{V}$$

In the case of our quantum harmonic oscillator,

$$\begin{aligned}
\langle T\rangle &= \frac{1}{2m}\langle n|P^2|n\rangle \\
&= \frac{\hbar\omega}{2}(n+\tfrac{1}{2}) \\
\langle V\rangle &= \frac{1}{2}m\omega^2\langle n|X^2|n\rangle \\
&= \frac{\hbar\omega}{2}(n+\tfrac{1}{2})
\end{aligned}$$

So the virial theorem holds in the case of the quantum harmonic oscillator.

7.4.4. Show that $\langle n|X^4|n\rangle = (\hbar/2m\omega)^2[3+6n(n+1)]$.

Since we are sandwiching our operator between the same state, only those terms that contain two $a$s and two $a^\dagger$s will survive (all others will have terms like $\langle n|n-2\rangle = \delta_{n,n-2} = 0$). So we have

$$\langle n|X^4|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^2\langle n|a^\dagger a^\dagger aa + a^\dagger aa^\dagger a + aa^\dagger a^\dagger a + a^\dagger aaa^\dagger + aa^\dagger aa^\dagger + aaa^\dagger a^\dagger|n\rangle$$

$$
\begin{aligned}
&= \left(\frac{\hbar}{2m\omega}\right)^2 \Big[n(n-1) + n^2 + n(n+1) + (n+1)n + (n+1)^2 + (n+2)(n+1)\Big] \\
&= \left(\frac{\hbar}{2m\omega}\right)^2 \Big[n^2 - n + n^2 + n^2 + n + n^2 + n + n^2 + 2n + 1 + n^2 + 3n + 2\Big] \\
&= \left(\frac{\hbar}{2m\omega}\right) \big[3 + 6n(n+1)\big]
\end{aligned}
$$

7.4.5. At $t = 0$ a particle starts out in $|\psi(0)\rangle = 1/2^{1/2}(|0\rangle + |1\rangle)$. (1) Find $|\psi(t)\rangle$; (2) find $\langle X(0)\rangle = \langle\psi(0)|X|\psi(0)\rangle$, $\langle P(0)\rangle$, $\langle X(t)\rangle$, $\langle P(t)\rangle$; (3) find $\langle \dot{X}(t)\rangle$ and $\langle \dot{P}(t)\rangle$ using Ehrenfest's theorem and solve for $\langle X(t)\rangle$ and $\langle P(t)\rangle$ and compare with part (2).

From Chapter 4, we know that we can find the time-varying state by appending time evolution operators to each energy eigenstate contributing to the state,

$$
|\psi(t)\rangle = \frac{1}{2^{1/2}}\Big(e^{-iE_0t/\hbar}|0\rangle + e^{-iE_1t/\hbar}|1\rangle\Big) = \frac{1}{2^{1/2}}\Big(e^{-i\omega t/2}|0\rangle + e^{-i3\omega t/2}|1\rangle\Big)
$$

Working with $|\psi(t)\rangle$, we find

$$
\begin{aligned}
\langle\psi(t)|X|\psi(t)\rangle &= \frac{1}{2}\left(\frac{\hbar}{2m\omega}\right)^{1/2}\Big(e^{i\omega t/2}\langle 0| + e^{i3\omega t/2}\langle 1|\Big)\Big(a + a^\dagger\Big)\Big(e^{-i\omega t/2}|0\rangle + e^{-i3\omega t/2}|1\rangle\Big) \\
&= \frac{1}{2}\left(\frac{\hbar}{2m\omega}\right)^{1/2}\Big(e^{i\omega t/2}\langle 0| + e^{i3\omega t/2}\langle 1|\Big)\Big(e^{-i3\omega t/2}|0\rangle + e^{-i\omega t/2}|1\rangle + 2^{1/2}e^{-i3\omega t/2}|2\rangle\Big) \\
&= \frac{1}{2}\left(\frac{\hbar}{2m\omega}\right)^{1/2}\Big(e^{-i\omega t}\langle 0|0\rangle + e^{i\omega t}\langle 1|1\rangle\Big) \\
&= \left(\frac{\hbar}{2m\omega}\right)^{1/2}\cos(\omega t) \\
\langle\psi(t)|P|\psi(t)\rangle &= i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\Big(e^{i\omega t/2}\langle 0| + e^{i3\omega t/2}\langle 1|\Big)\Big(a^\dagger - a\Big)\Big(e^{-i\omega t/2}|0\rangle + e^{-i3\omega t/2}|1\rangle\Big) \\
&= i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\Big(e^{i\omega t/2}\langle 0| + e^{i3\omega t/2}\langle 1|\Big)\Big(e^{-i\omega t/2}|1\rangle + 2^{1/2}e^{-i3\omega t/2}|2\rangle - e^{-i3\omega t/2}|0\rangle\Big) \\
&= i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\Big(-e^{-i\omega t}\langle 0|0\rangle + e^{i\omega t/2}\langle 1|1\rangle\Big) \\
&= -\left(\frac{m\omega\hbar}{2}\right)^{1/2}\sin(\omega t)
\end{aligned}
$$

which immediately implies $\langle X(0)\rangle = (\hbar/2m\omega)^{1/2}$ and $\langle P(0)\rangle = 0$.

Using Ehrenfest's theorem gives

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle &= -\frac{i}{\hbar}\langle\psi|[X, H]|\psi\rangle \\
&= -\frac{i}{\hbar}\langle\psi|[X, \tfrac{1}{2m}P^2 + \tfrac{1}{2}m\omega^2X^2]|\psi\rangle \\
&= -\frac{i}{2m\hbar}\langle\psi|[X, P^2]|\psi\rangle \\
&= -\frac{i}{2m\hbar}\langle\psi|XPP - PXP - PPX + PXP|\psi\rangle \\
&= -\frac{i}{2m\hbar}\langle\psi|[X, P]P + P[X, P]|\psi\rangle
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{1}{2m}\langle\psi|2P|\psi\rangle \\
&= \frac{1}{m}\langle P\rangle
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle &= -\frac{i}{\hbar}\langle\psi|[P,H]|\psi\rangle \\
&= -\frac{i}{\hbar}\langle\psi|[P,\tfrac{1}{2m}P^2+\tfrac{1}{2}m\omega^2X^2]|\psi\rangle \\
&= -\frac{im\omega^2}{2\hbar}\langle\psi|[P,X^2]|\psi\rangle \\
&= -\frac{im\omega^2}{2\hbar}\langle\psi|[P,X]X+X[P,X]|\psi\rangle \\
&= -\frac{m\omega^2}{2}\langle\psi|2X|\psi\rangle \\
&= -m\omega^2\langle X\rangle
\end{aligned}
$$

Differentiating each of these equations again and substituting in the above gives

$$
\begin{aligned}
\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle X\rangle &= -\omega^2\langle X\rangle \\
\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle P\rangle &= -\omega^2\langle X\rangle
\end{aligned}
$$

which each have the solution

$$
\begin{aligned}
\langle X\rangle &= C_1\cos(\omega t)+C_2\sin(\omega t) \\
\langle P\rangle &= C_3\cos(\omega t)+C_4\sin(\omega t)
\end{aligned}
$$

This reduces to the solution we found at the beginning when

$$
\begin{aligned}
C_1 &= \left(\frac{\hbar}{2m\omega}\right)^{1/2} \\
C_2 &= 0 \\
C_3 &= 0 \\
C_4 &= -\left(\frac{m\omega\hbar}{2}\right)^{1/2}
\end{aligned}
$$

7.4.6. Show that $\langle a(t)\rangle = e^{-i\omega t}\langle a(0)\rangle$ and that $\langle a^\dagger(t)\rangle = e^{i\omega t}\langle a^\dagger(0)\rangle$.

We know that an arbitrary state can be written as

$$
|\psi(t)\rangle = \sum_{n=0}^{\infty} A_n e^{-iE_nt/\hbar}|n\rangle
$$

in which case

$$
\langle a(t)\rangle = \langle\psi(t)|a|\psi(t)\rangle
$$

$$
\begin{aligned}
&= \Big( \sum_{n=0}^{\infty} A_n e^{iE_n t/\hbar} \langle n| \Big) a \Big( \sum_{n=0}^{\infty} A_n e^{-iE_n t/\hbar} |n\rangle \Big) \\
&= \Big( \sum_{n=0}^{\infty} A_n e^{iE_n t/\hbar} \langle n| \Big) \Big( \sum_{n=0}^{\infty} n^{1/2} A_{n+1} e^{-iE_{n+1} t/\hbar} |n\rangle \Big) \\
&= \sum_{n=0}^{\infty} n^{1/2} A_n A_{n+1} e^{-i(E_{n+1}-E_n)t/\hbar} \\
&= \sum_{n=0}^{\infty} n^{1/2} A_n A_{n+1} e^{-i\omega t} \\
&= e^{-i\omega t} \langle a(0) \rangle
\end{aligned}
$$

It is clear that the same pattern holds for $a^\dagger$, with

$$
\begin{aligned}
\langle a^\dagger(t) \rangle &= \Big( \sum_{n=0}^{\infty} A_n e^{iE_n t/\hbar} \langle n| \Big) a^\dagger \Big( \sum_{n=0}^{\infty} A_n e^{-iE_n t/\hbar} |n\rangle \Big) \\
&= \Big( \sum_{n=0}^{\infty} A_n e^{iE_n t/\hbar} \langle n| \Big) \Big( \sum_{n=0}^{\infty} (n+1)^{1/2} A_n e^{-iE_n t/\hbar} |n+1\rangle \Big) \\
&= \sum_{n=0}^{\infty} (n+1)^{1/2} A_{n+1} A_n e^{-i(E_n - E_{n+1})t/\hbar} \\
&= \sum_{n=0}^{\infty} (n+1)^{1/2} A_{n+1} A_n e^{i\omega t} \\
&= e^{i\omega t} \langle a^\dagger(0) \rangle
\end{aligned}
$$

7.4.7. Verify Eq. (7.4.40) for the case

$$
\begin{aligned}
&(1)\ \Omega = X, \quad \Lambda = X^2 + P^2 \\
&(2)\ \Omega = X^2, \quad \Lambda = P^2
\end{aligned}
$$

The second case illustrates the ordering ambiguity.

Classically, we have

$$
\begin{aligned}
\{x, x^2 + p^2\} &= \frac{\partial}{\partial x}(x) \frac{\partial}{\partial p}(x^2 + p^2) - \frac{\partial}{\partial p}(x) \frac{\partial}{\partial x}(x^2 + p^2) \\
&= 1 \cdot (2p) - 0 \cdot (2x) \\
&= 2p \\
\{x^2, p^2\} &= \frac{\partial}{\partial x}(x^2) \frac{\partial}{\partial p}(p^2) - \frac{\partial}{\partial p}(x^2) \frac{\partial}{\partial x}(p^2) \\
&= (2x) \cdot (2p) - 0 \cdot 0 \\
&= 4xp
\end{aligned}
$$

while quantum mechanically we have

$$
[X, X^2 + P^2] = [X, X^2] + [X, P^2]
$$

$$
\begin{aligned}
&= 0 + [X,P]P + P[X,P] \\
&= i\hbar P + P i\hbar \\
&= i\hbar \cdot 2P \\
[X^2, P^2] &= [X^2, P]P + P[X^2, P] \\
&= X[X,P]P + [X,P]XP + PX[X,P] + P[X,P]X \\
&= i\hbar XP + i\hbar XP + i\hbar PX + i\hbar PX \\
&= i\hbar \cdot 2XP + i\hbar \cdot 2PX
\end{aligned}
$$

We see that Eq. (7.4.40) relating the commutator to the Poisson bracket through $i\hbar$ holds, though $[X^2, P^2]$ is a symmetrized version of $\{x^2, p^2\}$.

7.4.8. Consider the three angular momentum variables in classical mechanics:

$$
\begin{aligned}
l_x &= yp_z - zp_y \\
l_y &= zp_x - xp_z \\
l_z &= xp_y - yp_x
\end{aligned}
$$

(1) Construct $L_x$, $L_y$, and $L_z$, the quantum counterparts, and note that there are no ordering ambiguities.

(2) Verify that $\{l_x, l_y\} = l_z$ [see Eq. (2.7.3) for the definition of the PB].

(3) Verify that $[L_x, L_y] = i\hbar L_z$.

The quantum mechanical angular momentum operators are given by

$$
\begin{aligned}
L_x &= YP_z - ZP_y \\
L_y &= ZP_x - XP_z \\
L_z &= XP_y - YP_x
\end{aligned}
$$

These have no ordering ambiguities because the momentum operator in each term is independent from the coordinate in the same term.

The Poisson bracket of $l_x$ and $l_y$ is

$$
\begin{aligned}
\{l_x, l_y\} &= \sum_i \frac{\partial}{\partial x_i}(yp_z - zp_y)\frac{\partial}{\partial p_i}(zp_x - xp_z) - \frac{\partial}{\partial p_i}(yp_z - zp_y)\frac{\partial}{\partial x_i}(zp_x - xp_z) \\
&= \big[0 \cdot z - 0 \cdot (-p_z)\big] + \big[p_z \cdot 0 - (-z) \cdot 0\big] + \big[(-p_y) \cdot (-x) - y \cdot p_x\big] \\
&= xp_y - yp_x \\
&= l_z
\end{aligned}
$$

The analogous commutator is

$$
\begin{aligned}
[L_x, L_y] &= [YP_z - ZP_y, ZP_x - XP_z] \\
&= [YP_z, ZP_x] - [YP_z, XP_z] - [ZP_y, ZP_x] + [ZP_y, XP_z] \\
&= Y[P_z, Z]P_x + [Y,Z]P_zP_x + ZY[P_z, P_x] + Z[Y, P_x]P_z - 0 - 0 \\
&\quad + Z[P_y, X]P_z + [Z,X]P_yP_z + XZ[P_y, P_z] + X[Z, P_z]P_y \\
&= -i\hbar YP_x + 0 + 0 + 0 + 0 + 0 + 0 + i\hbar XP_y \\
&= i\hbar(XP_y - YP_x) \\
&= i\hbar L_z
\end{aligned}
$$

7.4.9. (*Important*). Consider the unconventional (but fully acceptable) operator choice

$$\begin{aligned} X &\to x \\ P &\to -i\hbar\frac{\mathrm{d}}{\mathrm{d}x} + f(x) \end{aligned}$$

in the $X$ basis.

(1) Verify that the canonical commutation relation is satisfied.

(2) It is possible to interpret the change in the operator assignment as a result of a unitary change of the $X$ basis:

$$|x\rangle \to |\tilde{x}\rangle = e^{ig(X)/\hbar}|x\rangle = e^{ig(x)/\hbar}|x\rangle$$

where

$$g(x) = \int^x f(x')\mathrm{d}x'$$

First verify that

$$\langle\tilde{x}|X|\tilde{x}'\rangle = x\delta(x - x')$$

i.e.

$$X \xrightarrow[\text{new } X \text{ basis}]{} x$$

Next verify that

$$\langle\tilde{x}|P|\tilde{x}'\rangle = \left[-i\hbar\frac{\mathrm{d}}{\mathrm{d}x} + f(x)\right]\delta(x - x')$$

i.e.

$$P \xrightarrow[\text{new } X \text{ basis}]{} -i\hbar\frac{\mathrm{d}}{\mathrm{d}x} + f(x)$$

This exercise teaches us that the "X basis" is not unique; given a basis $|x\rangle$, we can get another $|\tilde{x}\rangle$, by multiplying by a phase factor which changes neither the norm nor the orthogonality. The matrix elements fo $P$ change with $f$, the standard choice corresponding to $f = 0$. Since the presence of $f$ is related to a change of basis, the invariance of the physics under a change in $f$ (from zero to nonzero) follows. What is novel here is that we are changing from one $X$ basis to another $X$ basis rather than to some other $\Omega$ basis. Another lesson to remember is that two different differential operator $\omega(x, -i\hbar\mathrm{d}/\mathrm{d}x)$ and $\omega(x, -i\hbar\mathrm{d}/\mathrm{d}x + f)$ can have the same eigenvalues and a one-to-one correspondence between their eigenfunctions, since they both represent the same abstract operator $\Omega(X, P)$.

The commutation relation can be obtained by applying the operators to a wave function,

$$\begin{aligned} XP\psi(x) &= x\Big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x} + f(x)\Big)\psi(x) \\ &= -i\hbar x\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) + xf(x)\psi(x) \\ PX\psi(x) &= \Big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x} + f(x)\Big)x\psi(x) \\ &= -i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\big(x\psi(x)\big) + xf(x)\psi(x) \\ &= -i\hbar\psi(x) - i\hbar x\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) + xf(x)\psi(x) \\ [X, P]\psi(x) &= XP\psi(x) - PX\psi(x) \\ &= i\hbar\psi(x) \end{aligned}$$

so $[X, P] = i\hbar$. When we perform the suggested unitary transformation on the state vectors, we find

$$\begin{aligned}\langle \tilde{x}|X|\tilde{x}'\rangle &= \langle x|e^{-ig(x)/\hbar} X e^{ig(x')/\hbar}|x'\rangle \\ &= e^{-i(g(x)-g'(x))/\hbar}\langle x|X|x'\rangle \\ &= e^{-i(g(x)-g'(x))/\hbar} x'\langle x|x'\rangle \\ &= e^{-i(g(x)-g'(x))/\hbar} x'\delta(x-x') \\ &= x\delta(x-x')\end{aligned}$$

and

$$\begin{aligned}\langle \tilde{x}|P|\tilde{x}'\rangle &= \langle x|e^{-ig(x)/\hbar}\Big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x'}\Big)e^{ig(x')/\hbar}|x'\rangle \\ &= \langle x|e^{-ig(x)/\hbar}\Big(-i\hbar e^{ig(x')/\hbar}\cdot\frac{i}{\hbar}\frac{\mathrm{d}}{\mathrm{d}x'}g(x') - i\hbar e^{ig(x')/\hbar}\frac{\mathrm{d}}{\mathrm{d}x'}\Big)|x'\rangle \\ &= e^{-i(g(x)-g(x'))/\hbar}\langle x|\Big(f(x') - i\hbar\frac{\mathrm{d}}{\mathrm{d}x'}\Big)|x'\rangle \\ &= e^{-i(g(x)-g(x'))/\hbar}\Big(f(x')\langle x|x'\rangle - i\hbar\langle x|\frac{\mathrm{d}}{\mathrm{d}x'}|x'\rangle\Big) \\ &= e^{-i(g(x)-g(x'))/\hbar}\Big(f(x')\delta(x-x') - i\hbar\Big[\frac{\mathrm{d}}{\mathrm{d}x'}\langle x|x'\rangle - \Big(\frac{\mathrm{d}}{\mathrm{d}x'}\langle x|\Big)|x'\rangle\Big]\Big) \\ &= e^{-i(g(x)-g(x'))/\hbar}\Big(f(x') - i\hbar\frac{\mathrm{d}}{\mathrm{d}x'}\Big)\delta(x-x') \\ &= \Big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x} + f(x)\Big)\delta(x-x')\end{aligned}$$

7.4.10. Recall that we always quantize a system by promoting the Cartesian coordinate $x_1, \ldots, x_N$; and momenta $p_1, \ldots, p_n$ to operators obeying the canonical commutation rules. If non-Cartesian coordinates seem more natural in some cases, such as the eigenvalue problem of a Hamiltonian with spherical symmetry, we first set up the differential equation in Cartesian coordinates and *then* change to spherical coordinates (Section 4.2). In Section 4.2 it was pointed out that if $\mathcal{H}$ is written in terms of non-Cartesian but canonical coordinates $q_1 \ldots q_N$; $p_1 \ldots p_N$; $\mathcal{H}(q_i \to q_i, p_i \to -i\hbar\partial/\partial q_i)$ does not generate the correct Hamiltonian $H$, even though the operator assignment satisfies the canonical commutation rules. In this section we revisit the problem in order to explain some of the subtleties arising in the direct quantization of non-Cartesian coordinates without the use of Cartesian coordinates in intermediate stages.

(1) Consider a particle in two dimensions with

$$\mathcal{H} = \frac{p_x^2 + p_y^2}{2m} + a(x^2+y^2)^{1/2}$$

which leads to

$$H = \frac{-\hbar^2}{2m}\Big(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial}{\partial\phi^2}\Big) + a\rho$$

Since $\rho$ and $\phi$ are not mixed up as $x$ and $y$ are [in the $(x^2+y^2)^{1/2}$ term] the polar version can be more readily solved.

The question we address is the following: why not *start* with $\mathcal{H}$ expressed in terms of polar coordinates and the conjugate momenta

$$p_\rho = \mathbf{e}_\rho \cdot \mathbf{p} = \frac{xp_x + yp_y}{(x^2+y^2)^{1/2}}$$

(where $\mathbf{e}_\rho$ is the unit vector in the radial direction), and

$$p_\phi = xp_y - yp_x \quad \text{(the angular momentum, also called } l_z\text{)}$$

i.e.

$$\mathcal{H} = \frac{p_\rho^2}{2m} + \frac{p_\phi^2}{2m\rho^2} + a\rho \quad \text{(verify this)}$$

and directly promote all classical variables $\rho$, $p_\rho$, $\phi$, and $p_\phi$ to quantum operators obeying the canonical commutations rules? Let's do it and see what happens. If we choose operators

$$P_\rho \to -i\hbar\frac{\partial}{\partial\rho}$$
$$P_\phi \to -i\hbar\frac{\partial}{\partial\phi}$$

that obey the commutation rules, we end up with

$$H \xrightarrow[\text{coordinate basis}]{} \frac{-\hbar^2}{2m}\Big(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\Big) + a\rho$$

which disagrees with Eq. (7.4.41). Now this in itself is not serious, for as seen in the last exercise the same physics may be hidden in two different equations. In the present case this isn't true: as we will see, the Hamiltonians in Eqs. (7.4.41) and (7.4.42) do not have the same eigenvalues. We know Eq. (7.4.41) is the correct one, since the quantization procedure in terms of Cartesian coordinates has empirical support. What do we do now?

(2) A way out is suggested by the fact that although the choice $P_\rho \to -i\hbar\partial/\partial\rho$ leads to the correct commutation rule, it is not Hermitian! Verify that

$$\begin{aligned}\langle\psi_1|P_\rho|\psi_2\rangle &= \int_0^\infty\int_0^{2\pi}\psi_1^*\Big(-i\hbar\frac{\partial\psi_2}{\partial\rho}\Big)\rho\,\mathrm{d}\rho\,\mathrm{d}\phi \\ &\neq \int_0^\infty\int_0^{2\pi}\Big(-i\hbar\frac{\partial\psi_1}{\partial\rho}\Big)^*\psi_2\rho\,\mathrm{d}\rho\,\mathrm{d}\phi \\ &= \langle\mathbf{P}_\rho\psi_1|\psi_2\rangle\end{aligned}$$

(You may assume $\rho\psi_1^*\psi_2 \to 0$ as $\rho \to 0$ or $\infty$. The problem comes from the fact that $\rho\,\mathrm{d}\rho\,\mathrm{d}\phi$ and not $\mathrm{d}\rho\,\mathrm{d}\phi$ is the measure for integration.)

Show, however, that

$$P_\rho \to -i\hbar\Big(\frac{\partial}{\partial\rho} + \frac{1}{2\rho}\Big)$$

is indeed Hermitian and also satisfies the canonical commutation rule. The angular momentum $P_\rho \to -i\hbar\partial/\partial\phi$ is Hermitian, as it stands, on single-valued functions: $\psi(\rho,\phi) = \psi(\rho,\phi+2\pi)$.

(3) In the Cartesian case we saw that adding an arbitrary $f(x)$ to $-i\hbar\partial/\partial x$ didn't have any physical effect, whereas there the addition of a function of $\rho$ to $-i\hbar\partial/\partial\rho$ seems important. Why? [Is $f(x)$ completely arbitrary? Mustn't it be real? Why? Is the same true for the $-i\hbar/2\rho$ piece?]

(4) Feed in the new momentum operator $P_\rho$ and show that

$$H \xrightarrow[\text{coordinate basis}]{} -\hbar^2 2m\Big(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{1}{4\rho^2} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\Big) + a\rho$$

which still disagrees with Eq. (7.4.41). We have satisfied the commutation rules, chosen Hermitian operators, and yet do not get the right quantum Hamiltonian. The key to the mystery lies in the fact that $\mathcal{H}$ doesn't determine $H$ uniquely since terms of order $\hbar$ (or higher) may be present in $H$ but absent in $\mathcal{H}$. While this ambiguity is present even in the Cartesian case, it is resolved by symmetrization in all interesting cases. With non-Cartesian coordinates the ambiguity is more severe. There *are* ways of constructing $H$ given $\mathcal{H}$ (the path integral formulation suggests one) such that the substitution $P_\rho \to -i\hbar(\partial/\partial\rho + 1/2\rho)$ leads to Eq. (7.4.41). In the present case the quantum Hamiltonian corresponding to

$$\mathcal{H} = \frac{p_\rho^2}{2m} + \frac{p_\phi^2}{2m\rho^2} + a\rho$$

is given by

$$H \xrightarrow[\text{coordinate basis}]{} \mathcal{H}\Big(\rho \to \rho, p_\rho \to -i\hbar\Big[\frac{\partial}{\partial\rho} + \frac{1}{2\rho}\Big]; \phi \to \phi, p_\phi \to -i\hbar\frac{\partial}{\partial\phi}\Big) - \frac{\hbar^2}{8m\rho^2}$$

Notice the additional term is indeed of nonzero order in $\hbar$.

Our Cartesian Hamiltonian is given by

$$\mathcal{H} = \frac{p_x^2 + p_y^2}{2m} + a(x^2+y^2)^{1/2} = \frac{p_x^2 + p_y^2}{2m} + a\rho$$

We are given that

$$\begin{aligned} p_\rho\rho &= xp_x + yp_y \\ p_\phi &= xp_y - yp_x \end{aligned}$$

from which we can find

$$\begin{aligned} p_x &= \frac{p_\rho\rho - yp_y}{x} \\ &= \frac{p_\rho\rho - y\frac{p_\phi + yp_x}{x}}{x} \\ &= \frac{xp_\rho\rho - yp_\phi - y^2p_x}{x^2} \\ &= \frac{xp_\rho\rho - yp_\phi}{x^2+y^2} \\ &= \frac{xp_\rho\rho - yp_\phi}{\rho^2} \end{aligned}$$

and

$$\begin{aligned} p_y &= \frac{p_\rho\rho - xp_x}{y} \\ &= \frac{p_\rho\rho - x\frac{xp_y - p_\phi}{y}}{y} \\ &= \frac{yp_\rho\rho - x^2p_y + xp_\phi}{y^2} \\ &= \frac{yp_\rho\rho + xp_\phi}{x^2+y^2} \\ &= \frac{yp_\rho\rho + xp_\phi}{\rho^2} \end{aligned}$$

Substituting this into our original Hamiltonian gives

$$\mathcal{H} = \frac{1}{2m}\Big(\frac{xp_\rho\rho - yp_\phi}{\rho^2}\Big)^2 + \frac{1}{2m}\Big(\frac{yp_\rho\rho + xp_\phi}{\rho^2}\Big)^2 + a\rho$$

$$
\begin{aligned}
&= \frac{1}{2m}\frac{x^2p_\rho^2\rho^2 - 2xyp_\rho p_\phi\rho + y^2p_\phi^2}{\rho^4} + \frac{1}{2m}\frac{y^2p_\rho^2\rho^2 + 2xyp_\rho p_\phi\rho + x^2p_\phi^2}{\rho^4} + a\rho \\
&= \frac{1}{2m}\frac{x^2+y^2}{\rho^4}p_\rho^2\rho^2 + \frac{1}{2m}\frac{x^2+y^2}{\rho^4}p_\phi^2 + a\rho \\
&= \frac{p_\rho^2}{2m} + \frac{p_\phi^2}{2m\rho^2} + a\rho
\end{aligned}
$$

Given $\rho\psi_1^*\psi_2 \to 0$ as $\rho \to 0$, we can perform integration by parts on $\langle\psi_1|P_\rho|\psi_2\rangle$ to get

$$
\begin{aligned}
\langle\psi_1|P_\rho|\psi_2\rangle &= \int_0^\infty\int_0^{2\pi} \psi_1^*\Big(-i\hbar\frac{\partial\psi_2}{\partial\rho}\Big)\rho\,\mathrm{d}\rho\,\mathrm{d}\phi \\
&= \int_0^\infty\int_0^{2\pi} \Big(i\hbar\frac{\partial(\psi_1^*\rho)}{\partial\rho}\Big)\psi_2\,\mathrm{d}\rho\,\mathrm{d}\phi \\
&= \int_0^\infty\int_0^{2\pi} \Big(i\hbar\frac{\partial\psi_1^*}{\partial\rho}\Big)\psi_2\rho\,\mathrm{d}\rho\,\mathrm{d}\phi + \int_0^\infty\int_0^{2\pi} i\hbar\psi_1^*\psi_2\,\mathrm{d}\rho\,\mathrm{d}\phi \\
&= \int_0^\infty\int_0^{2\pi} \Big(-i\hbar\frac{\partial\psi_1}{\partial\rho}\Big)^*\psi_2\rho\,\mathrm{d}\rho\,\mathrm{d}\phi + \int_0^\infty\int_0^{2\pi} i\hbar\psi_1^*\psi_2\,\mathrm{d}\rho\,\mathrm{d}\phi \\
&\neq \int_0^\infty\int_0^{2\pi} \Big(-i\hbar\frac{\partial\psi_1}{\partial\rho}\Big)^*\psi_2\,\rho\,\mathrm{d}\rho\,\mathrm{d}\phi
\end{aligned}
$$

If we use the suggested new operator, we can build off our results above to find that

$$
\begin{aligned}
\langle\psi_1|P_\rho|\psi_2\rangle &= \int_0^\infty\int_0^{2\pi} \psi_1^*\Big(-i\hbar\Big[\frac{\partial\psi_2}{\partial\rho} + \frac{\psi_2}{2\rho}\Big]\Big)\rho\,\mathrm{d}\rho\,\mathrm{d}\phi \\
&= \int_0^\infty\int_0^{2\pi} \psi_1^*\Big(-i\hbar\frac{\partial\psi_2}{\partial\rho}\Big)\rho\,\mathrm{d}\rho\,\mathrm{d}\phi - \frac{1}{2}\int_0^\infty\int_0^{2\pi} i\hbar\psi_1^*\psi_2\,\mathrm{d}\rho\,\mathrm{d}\phi \\
&= \int_0^\infty\int_0^{2\pi} \Big(-i\hbar\frac{\partial\psi_1}{\partial\rho}\Big)^*\psi_2\rho\,\mathrm{d}\rho\,\mathrm{d}\phi + \frac{1}{2}\int_0^\infty\int_0^{2\pi} i\hbar\psi_1^*\psi_2\,\mathrm{d}\rho\,\mathrm{d}\phi \\
&= \int_0^\infty\int_0^{2\pi} \Big(-i\hbar\Big[\frac{\partial\psi_1}{\partial\rho} + \frac{\psi_1}{2\rho}\Big]\Big)^*\psi_2\rho\,\mathrm{d}\rho\,\mathrm{d}\phi
\end{aligned}
$$

i.e. $P_\rho$ is now Hermitian. To check that it gives rise to the canonical commutation relation, we compute

$$
\begin{aligned}
[\rho, P_\rho]\psi(\rho,\phi) &= (\rho P_\rho - P_\rho\rho)\psi(\rho,\phi) \\
&= -i\hbar\rho\frac{\partial\psi(\rho,\phi)}{\partial\rho} - \frac{i\hbar}{2}\psi(\rho,\phi) + i\hbar\frac{\partial\big(\rho\psi(\rho,\phi)\big)}{\partial\rho} + \frac{i\hbar}{2}\psi(\rho,\phi) \\
&= -i\hbar\rho\frac{\partial\psi(\rho,\phi)}{\partial\rho} + i\hbar\rho\frac{\partial\psi(\rho,\phi)}{\partial\rho} + i\hbar\psi(\rho,\phi) \\
&= i\hbar\psi(\rho,\phi)
\end{aligned}
$$

which shows that $[\rho, P_\rho] = i\hbar$.

There are a few ways to view the difficulties of using this basis: for one, the integration measure is changed, introducing the problem we explored in step (2). For another, the $f(x)$ function considered in the previous exercise was restricted to be real so that the new basis could be seen as a unitary transformation of the previous one—this is not so in the current case, as polar / cylindrical / spherical coordinates are not related to Cartesian coordinates through a simple unitary transformation.

If we feed our new momentum operator into $\mathcal{H}$, we obtain

$$\begin{aligned}
H &= \frac{1}{2m}P_\rho^2 + \frac{1}{2m\rho^2}P_\phi^2 + a\rho \\
&= \frac{1}{2m}\Big(-i\hbar\frac{\partial}{\partial\rho} - i\hbar\frac{1}{2\rho}\Big)^2 + \frac{1}{2m\rho^2}\Big(-i\hbar\frac{\partial}{\partial\phi}\Big)^2 + a\rho \\
&= -\frac{\hbar^2}{2m}\Big(\frac{\partial^2}{\partial\rho^2} - \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{4\rho^2}\Big) - \frac{\hbar^2}{2m\rho^2}\frac{\partial^2}{\partial\phi^2} + a\rho \\
&= -\frac{\hbar^2}{2m}\Big(\frac{\partial^2}{\partial\rho^2} - \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{4\rho^2} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\Big) + a\rho
\end{aligned}$$

## 7.5 Passage from the Energy Basis to the $X$ Basis

7.5.1. Project Eq. (7.5.1) on the $P$ basis and obtain $\psi_0(p)$.

From earlier in the chapter, we know that

$$a = \Big(\frac{m\omega}{2\hbar}\Big)^{1/2} X + i\Big(\frac{1}{2m\omega\hbar}\Big)^{1/2} P$$

which, in the $P$ basis, becomes

$$a = i\Big(\frac{m\omega\hbar}{2}\Big)^{1/2}\frac{\mathrm{d}}{\mathrm{d}p} + i\Big(\frac{1}{2m\omega\hbar}\Big)^{1/2} p$$

Using the choice of

$$y = (m\omega\hbar)^{-1/2} p$$

from an earlier exercise, this simplifies to

$$a = \frac{i}{2^{1/2}}\Big(\frac{\mathrm{d}}{\mathrm{d}y} + y\Big)$$

and so Eq. (7.5.1) becomes

$$\Big(\frac{\mathrm{d}}{\mathrm{d}y} + y\Big)\psi_0(y) = 0$$

which has the solution

$$\psi_0(y) = A_0 e^{-y^2/2}$$

or

$$\psi_0(p) = A_0 e^{-p^2/2m\omega\hbar}$$

We can normalize this by recognizing that

$$\int_{-\infty}^{\infty} \psi_0^2(p)\,\mathrm{d}p = A_0^2(\pi m\omega\hbar)^{1/2} = 1$$

i.e.

$$\psi_0(p) = \Big(\frac{1}{\pi m\omega\hbar}\Big)^{1/4}\exp\Big(-\frac{p^2}{2m\omega\hbar}\Big)$$

7.5.2. Project the relation

$$a|n\rangle = n^{1/2}|n-1\rangle$$

on the $X$ basis and derive the recursion relation

$$H_n'(y) = 2nH_{n-1}(y)$$

using Eq. (7.3.22).

In the $X$ basis, the above equation becomes

$$\frac{1}{2^{1/2}}\Big(y+\frac{\mathrm{d}}{\mathrm{d}y}\Big)\Big(\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2}\Big)^{1/4} e^{-y^2/2}H_n(y) = n^{1/2}\Big(\frac{m\omega}{\pi\hbar 2^{2n-2}([n-1]!)^2}\Big)^{1/4} e^{-y^2/2}H_{n-1}(y)$$

Canceling common terms and collecting what remains gives

$$\Big(y+\frac{\mathrm{d}}{\mathrm{d}y}\Big)e^{-y^2/2}H_n(y) = 2ne^{-y^2/2}H_{n-1}(y)$$

Applying the parenthesized operator to the lefthand side gives

$$\begin{aligned}2ne^{-y^2/2}H_{n-1}(y) &= ye^{-y^2/2}H_n(y) - ye^{-y^2/2}H_n(y) + e^{-y^2/2}H_n'(y)\\ &= e^{-y^2/2}H_n'(y)\end{aligned}$$

i.e. $H_n'(y) = 2nH_{n-1}(y)$.

7.5.3. Starting with

$$a + a^\dagger = 2^{1/2}y$$

and

$$(a+a^\dagger)|n\rangle = n^{1/2}|n-1\rangle + (n+1)^{1/2}|n+1\rangle$$

and Eq. (7.3.22), derive the relation

$$H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y)$$

To reduce clutter, we precancel all common factors (including $e^{-y^2/2}$), giving a (simplified) projection of

$$2^{1/2}y\Big(\frac{1}{(n!)^2}\Big)^{1/4}H_n(y) = n^{1/2}\Big(\frac{1}{2^{-2}([n-1]!)^2}\Big)^{1/4}H_{n-1}(y) + (n+1)^{1/2}\Big(\frac{1}{2^2([n+1]!)^2}\Big)^{1/4}H_{n+1}(y)$$

Canceling the additional overlapping factorial reduces this to

$$2^{1/2}yn^{-1/2}H_n(y) = n^{1/2}2^{1/2}H_{n-1}(y) + (n+1)^{1/2}2^{-1/2}(n+1)^{-1/2}n^{-1/2}H_{n+1}(y)$$

Isolating $H_{n+1}(y)$ gives us the desired relation

$$H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y)$$

7.5.4. *Thermodynamics of Oscillators.* The Boltzmann formula

$$P(i) = e^{-\beta E(i)}/Z$$

where

$$Z = \sum_i e^{-\beta E(i)}$$

gives the probability of finding a system in a state $i$ with energy $E(i)$, when it is in thermal equilibrium with a reservoir of absolute temperature $T = 1/\beta k$, $k = 1.4 \times 10^{-16}$ ergs/K; being Boltzmann's constant. (The "probability" referred to above is in relation to a classical ensemble of similar systems and has nothing to do with quantum mechanics.)

(1) Show that the thermal average of the system's energy is

$$\bar{E} = \sum_i E(i)P(i) = \frac{-\partial}{\partial\beta} \ln Z$$

(2) Let the system be a classical oscillator. The index $i$ is now continuous and corresponds to the variables $x$ and $p$ describing the state of the oscillator, i.e.

$$i \to x, p$$

and

$$\sum_i \to \iint \mathrm{d}x\, \mathrm{d}p$$

and

$$E(i) \to E(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

Show that

$$Z_{\text{cl}} = \left(\frac{2\pi}{\beta m\omega^2}\right)^{1/2}\left(\frac{2\pi m}{\beta}\right)^{1/2} = \frac{2\pi}{\omega\beta}$$

and that

$$\bar{E}_{\text{cl}} = \frac{1}{\beta} = kT$$

Note that $E_{\text{cl}}$ is independent of $m$ and $\omega$.

(3) For the quantum oscillator the quantum number $n$ plays the role of the index $i$. Show that

$$Z_{\text{qu}} = e^{-\beta\hbar\omega/2}(1 - e^{-\beta\hbar\omega})^{-1}$$

and

$$\bar{E}_{\text{qu}} = \hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega} - 1}\right)$$

(4) It is intuitively clear that as the temperature $T$ increases (and $\beta = 1/kT$ decreases) the oscillator will get more and more excited and eventually (from the correspondence principle)

$$\bar{E}_{\text{qu}} \xrightarrow[T\to\infty]{} \bar{E}_{\text{cl}}$$

Verify that this is indeed true and show that "large $T$" means $T \gg \hbar\omega/k$.

(5) Consider a crystal with $N_0$ atoms, which, for small oscillations, is equivalent to $3N_0$ decoupled oscillators. The mean thermal energy of the crystal $\bar{E}_{\text{crystal}}$ is $\bar{E}_{\text{cl}}$ or $\bar{E}_{\text{qu}}$ summed over all the normal modes. Show that if the oscillators are treated classically, the specific heat per atom is

$$C_{\text{cl}}(T) = \frac{1}{N_0}\frac{\partial \bar{E}_{\text{crystal}}}{\partial T} = 3k$$

which is independent of $T$ and the parameters of the oscillators and hence the same for all crystals. This agrees with experiment at high temperatures but not as $T \to 0$. Empirically,

$$\begin{aligned} C(T) &\to 3k \quad (T \text{ large}) \\ &\to 0 \quad (T \to 0) \end{aligned}$$

Following Einstein, treat the oscillators quantum mechanically, assuming for simplicity that they all have the same frequency $\omega$. Show that

$$C_{\text{qu}}(T) = 3k\Big(\frac{\theta_E}{T}\Big)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2}$$

where $\theta_E = \hbar\omega/k$ is called the *Einstein temperature* and varies from crystal to crystal. Show that

$$\begin{aligned} C_{\text{qu}}(T) &\xrightarrow[T \gg \theta_E]{} 3k \\ C_{\text{qu}}(T) &\xrightarrow[T \ll \theta_E]{} 3k\Big(\frac{\theta_E}{T}\Big)^2 e^{-\theta_E/T} \end{aligned}$$

Although $C_{\text{qu}}(T) \to 0$ as $T \to 0$, the exponential falloff disagrees with the observed $C(t) \to_{T\to 0} T^3$ behavior. This discrepancy arises from assuming that the frequencies of all normal modes are equal, which is of course not generally true. [Recall that in the case of two coupled masses we get $\omega_I = (k/m)^{1/2}$ and $\omega_{II} = (3k/m)^{1/2}$.] This discrepancy was eliminated by Debye.

But Einstein's simple picture by itself is remarkably successful (see Fig. 7.3).

By the definition of the expected value, the thermal average is

$$\begin{aligned} \bar{E} &= \sum_i E(i)P(i) \\ &= \frac{1}{Z}\sum_i E(i)e^{-\beta E(i)} \end{aligned}$$

This can be written more compactly as

$$\begin{aligned} -\frac{\partial}{\partial\beta}\ln Z &= -\frac{1}{Z}\frac{\partial Z}{\partial\beta} \\ &= -\frac{1}{Z}\sum_i \frac{\partial}{\partial\beta}e^{-\beta E(i)} \\ &= -\frac{1}{Z}\sum_i \big(-E(i)\big)e^{-\beta E(i)} \\ &= \frac{1}{Z}\sum_i E(i)e^{-\beta E(i)} \\ &= \bar{E} \end{aligned}$$

Moving from a sum to an integral gives

$$\begin{aligned} Z_{\text{cl}} &= \iint \exp\Big(-\frac{\beta}{2m}p^2 - \frac{\beta m\omega^2}{2}x^2\Big)\mathrm{d}x\,\mathrm{d}p \\ &= \int \exp\Big(-\frac{\beta}{2m}p^2\Big)\mathrm{d}p \int \exp\Big(-\frac{\beta m\omega^2}{2}x^2\Big)\mathrm{d}x \\ &= \Big(\frac{\pi}{\beta/2m}\Big)^{1/2}\Big(\frac{\pi}{\beta m\omega^2/2}\Big)^{1/2} \end{aligned}$$

$$= \frac{2\pi}{\omega\beta}$$

which corresponds to an average thermal energy of

$$\begin{aligned}
\bar{E}_{\text{cl}} &= -\frac{\partial}{\partial\beta}\ln Z_{\text{cl}} \\
&= -\frac{\omega\beta}{2\pi}\frac{\partial}{\partial\beta}\Big(\frac{2\pi}{\omega\beta}\Big) \\
&= -\frac{\omega\beta}{2\pi}\Big(-\frac{2\pi}{\omega\beta^2}\Big) \\
&= \frac{1}{\beta}
\end{aligned}$$

For the quantum oscillator, the partition function is given by

$$\begin{aligned}
Z_{\text{qu}} &= \sum_n e^{-\beta E_n} \\
&= \sum_n \exp\Big(-\beta(n+\tfrac{1}{2})\hbar\omega\Big) \\
&= e^{-\beta\hbar\omega/2}\sum_n \left(e^{-\beta\hbar\omega}\right)^n \\
&= \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}
\end{aligned}$$

which corresponds to an average thermal energy of

$$\begin{aligned}
\bar{E}_{\text{qu}} &= -\frac{\partial}{\partial\beta}\ln Z_{\text{qu}} \\
&= -\frac{1-e^{-\beta\hbar\omega}}{e^{-\beta\hbar\omega/2}}\frac{\partial}{\partial\beta}\Big(\frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}\Big) \\
&= -\frac{1-e^{-\beta\hbar\omega}}{e^{-\beta\hbar\omega/2}}\Big(\frac{-\hbar\omega e^{-\beta\hbar\omega/2}}{2(1-e^{-\beta\hbar\omega})} - \frac{e^{-\beta\hbar\omega/2}}{(1-e^{-\beta\hbar\omega})^2}(-e^{-\beta\hbar\omega})(-\hbar\omega)\Big) \\
&= -\frac{1-e^{-\beta\hbar\omega}}{e^{-\beta\hbar\omega/2}}\Big(\frac{-\hbar\omega e^{-\beta\hbar\omega/2}(1-e^{-\beta\hbar\omega})}{2(1-e^{-\beta\hbar\omega})^2} - \frac{\hbar\omega e^{-3\beta\hbar\omega/2}}{(1-e^{-\beta\hbar\omega})^2}\Big) \\
&= \frac{1}{1-e^{-\beta\hbar\omega}}\Big(\frac{1}{2}\hbar\omega(1-e^{-\beta\hbar\omega}) + \hbar\omega e^{-\beta\hbar\omega}\Big) \\
&= \hbar\omega\Big(\frac{1}{2} + \frac{e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}\Big) \\
&= \hbar\omega\Big(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega}-1}\Big)
\end{aligned}$$

As $T$ increases (equivalently, as $\beta$ decreases), the argument of the exponential becomes small and we can Taylor expand this term about 0, giving

$$\begin{aligned}
\lim_{T\to\infty}\bar{E}_{\text{qu}} &= \hbar\omega\Big(\frac{1}{2} + \frac{1}{1+\frac{\hbar\omega}{kT}-1}\Big) \\
&= \frac{\hbar\omega}{2} + kT \\
&\approx kT
\end{aligned}$$

$$= \bar{E}_{\text{cl}}$$

Of course, this approximation is only valid when the argument to the exponential is much less than 1, or

$$\frac{\hbar\omega}{kT} \ll 1 \implies T \gg \frac{\hbar\omega}{k}$$

If we treat a crystal as a system of $3N_0$ decoupled oscillators, the (classical) average thermal energy will be given by

$$\bar{E}_{\text{crystal}} = 3N_0 kT$$

The specific heat per atom is the change in thermal energy with temperature normalized by the number of atoms, or

$$C_{\text{cl}}(T) = \frac{1}{N_0}\frac{\partial \bar{E}_{\text{crystal}}}{\partial T} = 3k$$

If we perform the same calculation quantum mechanically, we find instead that

$$\begin{aligned} C_{\text{qu}}(T) &= \frac{1}{N_0}\frac{\partial}{\partial T}\Big(3N_0\hbar\omega\Big[\frac{1}{2} + \frac{1}{e^{\theta_E/T} - 1}\Big]\Big) \\ &= -3\hbar\omega\frac{1}{(e^{\theta_E/T} - 1)^2}(e^{\theta_E/T})\Big(-\frac{\theta_E}{T^2}\Big) \\ &= 3k\Big(\frac{\theta_E}{T}\Big)^2\frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2} \end{aligned}$$

# 8 The Path Integral Formulation of Quantum Theory

## 8.6 Potentials of the Form $V = a + bx + cx^2 + d\dot{x} + ex\dot{x}$

8.6.1. Verify that

$$U(x,t;x',0) = A(t)\exp(iS_{\text{cl}}/\hbar), A(t) = \Big(\frac{m}{2\pi\hbar it}\Big)^{1/2}$$

agrees with the exact result, Eq. (5.4.31), for $V(x) = -fx$. Hint: Start with $x_{\text{cl}}(t'') = x_0 + v_0 t'' + \frac{1}{2}(f/m)t''^2$ and find the constants $x_0$ and $v_0$ from the requirement that $x_{\text{cl}}(0) = x'$ and $x_{\text{cl}}(t) = x$.

The given propagator agrees with the previously found propagator if

$$S_{\text{cl}} = \frac{m(x-x')^2}{2t} + \frac{1}{2}ft(x+x') - \frac{f^2t^3}{24m}$$

The Lagrangian is

$$\mathcal{L}(x,\dot{x}) = \frac{1}{2}m\dot{x}^2 + fx$$

which can be rewritten as

$$\begin{aligned} \mathcal{L}(t') &= \frac{1}{2}m\Big(v_0 + \frac{f}{m}t'\Big)^2 + f\Big(x_0 + v_0t' + \frac{1}{2}\frac{f}{m}t'^2\Big) \\ &= \frac{1}{2}mv_0^2 + fv_0t' + \frac{1}{2}\frac{f^2}{m}t'^2 + fx_0 + fv_0t' + \frac{1}{2}\frac{f^2}{m}t'^2 \\ &= \frac{1}{2}mv_0^2 + fx_0 + 2fv_0t' + \frac{f^2}{m}t'^2 \end{aligned}$$

We can integrate this to find

$$\begin{aligned} S_{\text{cl}} = \int_0^t \mathcal{L}(t')\mathrm{d}t' &= \int_0^t \frac{1}{2}mv_0^2 + fx_0 + 2fv_0t' + \frac{f^2}{m}t'^2\mathrm{d}t' \\ &= \frac{1}{2}mv_0^2 t + fx_0 t + fv_0 t^2 + \frac{f^2}{3m}t^3 \end{aligned}$$

To ensure the constants used here agree with the constants $x$ and $x'$ used previously, we enforce

$$\begin{aligned} x' &= x_{\text{cl}}(0) = x_0 \\ x &= x_{\text{cl}}(t) = x_0 + v_0 t + \frac{1}{2}\frac{f}{m}t^2 \end{aligned}$$

which implies

$$\begin{aligned} x_0 &= x' \\ v_0 &= \frac{x - x'}{t} - \frac{1}{2}\frac{f}{m}t \end{aligned}$$

Substituting this into our found action results in

$$\begin{aligned} S_{\text{cl}} &= \frac{m}{2}\Big(\frac{x-x'}{t} - \frac{f}{2m}t\Big)^2 t + fx't + f\Big(\frac{x-x'}{t} - \frac{f}{2m}t\Big)t^2 + \frac{f^2t^3}{3m} \\ &= \frac{m}{2}\Big(\frac{(x-x')^2}{t^2} - \frac{f(x-x')}{m} + \frac{f^2t^2}{4m^2}\Big)t + fx't + fxt - fx't - \frac{f^2t^3}{2m} + \frac{f^2t^3}{3m} \\ &= \frac{m(x-x')^2}{2t} + \frac{f(-x+x')t}{2} + \frac{f^2t^3}{8m} + fxt - \frac{f^2t^3}{6m} \\ &= \frac{m(x-x')^2}{2t} + \frac{1}{2}ft(x+x') - \frac{f^2t^3}{24m} \end{aligned}$$

8.6.2. Show that for the harmonic oscillator with

$$\begin{aligned} \mathcal{L} &= \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2 \\ U(x,t;x') &= A(t)\exp\Big\{\frac{im\omega}{2\hbar\sin\omega t}[(x^2 + x'^2)\cos\omega t - 2xx']\Big\} \end{aligned}$$

where $A(t)$ is an unknown function. (Recall Exercise 2.8.7.)

The path of the classical oscillator is described by $x(t') = A\cos\omega t' + B\sin\omega t'$, and so

$$\begin{aligned} S_{\text{cl}} &= \int_0^t \mathcal{L}(x(t'),\dot{x}(t'))\,\mathrm{d}t' \\ &= \int_0^t \frac{1}{2}m\dot{x}^2(t') - \frac{1}{2}m\omega^2x^2(t')\,\mathrm{d}t' \\ &= \frac{1}{2}m\int_0^t \Big(-\omega A\sin\omega t' + \omega B\cos\omega t'\Big)^2 - \omega^2\Big(A\cos\omega t' + B\sin\omega t'\Big)^2\,\mathrm{d}t' \\ &= \frac{1}{2}m\omega^2\int_0^t (A^2 - B^2)\sin^2\omega t' - 4AB\sin\omega t'\cos\omega t' + (B^2 - A^2)\cos^2\omega t'\,\mathrm{d}t' \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2}m\omega^2 \int_0^t (A^2 - B^2)\Big(\frac{1-\cos 2\omega t'}{2}\Big) - 2AB\sin 2\omega t' + (B^2 - A^2)\Big(\frac{1+\cos 2\omega t'}{2}\Big)\,\mathrm{d}t' \\
&= \frac{1}{2}m\omega^2 \int_0^t (B^2 - A^2)\cos 2\omega t' - 2AB\sin 2\omega t'\,\mathrm{d}t' \\
&= \frac{1}{2}m\omega^2 \Big((B^2 - A^2)\frac{\sin 2\omega t'}{2\omega} + 2AB\frac{\cos 2\omega t'}{2\omega}\Big)\Big|_0^t \\
&= \frac{1}{2}m\omega\Big(\frac{1}{2}(B^2 - A^2)\sin 2\omega t + AB\cos 2\omega t - AB\Big) \\
&= \frac{1}{2}m\omega\Big((B^2 - A^2)\sin\omega t\cos\omega t + AB\cos 2\omega t - AB\Big)
\end{aligned}
$$

We can replace the constants $A$ and $B$ with linear combinations of $x$ and $x'$ by noting that

$$
\begin{aligned}
x' &= x(0) = A \\
x &= x(t) = A\cos\omega t + B\sin\omega t
\end{aligned}
$$

and so

$$
\begin{aligned}
A &= x' \\
B &= \frac{x - x'\cos\omega t}{\sin\omega t}
\end{aligned}
$$

We first compute

$$
\begin{aligned}
B^2 - A^2 &= \frac{x^2 - 2xx'\cos\omega t + x'^2\cos^2\omega t}{\sin^2\omega t} - x'^2 \\
&= \frac{x^2 - 2xx'\cos\omega t + x'^2(\cos^2\omega t - \sin^2\omega t)}{\sin^2\omega t} \\
&= \frac{x^2 - 2xx'\cos\omega t + x'^2\cos 2\omega t}{\sin^2\omega t} \\
AB &= \frac{xx' - x'^2\cos\omega t}{\sin\omega t}
\end{aligned}
$$

and so

$$
\begin{aligned}
(B^2 - A^2)\sin\omega t\cos\omega t &= \Big(\frac{x^2 - 2xx'\cos\omega t + x'^2\cos 2\omega t}{\sin^2\omega t}\Big)\big(\sin\omega t\cos\omega t\big) \\
&= \frac{x^2\cos\omega t - 2xx'\cos^2\omega t + x'^2\cos 2\omega t\cos\omega t}{\sin\omega t} \\
AB\cos 2\omega t &= \Big(\frac{xx' - x'^2\cos\omega t}{\sin\omega t}\Big)\cos 2\omega t \\
&= \frac{xx'\cos 2\omega t - x'^2\cos 2\omega t\cos\omega t}{\sin\omega t} \\
&= \frac{xx'(1 - 2\sin^2\omega t) - x'^2\cos 2\omega t\cos\omega t}{\sin\omega t} \\
&= \frac{xx' - 2xx'\sin^2\omega t - x'^2\cos 2\omega t\cos\omega t}{\sin\omega t}
\end{aligned}
$$

Combining these results gives

$$
S_{\mathrm{cl}} = \frac{m\omega}{2\sin\omega t}\Big(x^2\cos\omega t - 2xx'\cos^2\omega t + xx' - 2xx'\sin^2\omega t - xx' + x'^2\cos\omega t\Big)
$$

$$= \frac{m\omega}{2\sin\omega t}\Big((x^2 + x'^2)\cos\omega t - 2xx'\Big)$$

which is exactly what we expect, as this gives

$$U(x,t;x') = A(t)\exp(iS_{\mathrm{cl}}/\hbar) = U(x,t;x') = A(t)\exp\left\{\frac{im\omega}{2\hbar\sin\omega t}[(x^2+x'^2)\cos\omega t - 2xx']\right\}$$

8.6.3. We know that given the eigenfunctions and the eigenvalues we can construct the propagator:

$$U(x,t;x',t') = \sum_n \psi_n(x)\psi_n^*(x')e^{-iE_n(t-t')/\hbar}$$

Consider the reverse process (since the path integral approach gives $U$ directly), for the case of the oscillator.

(1) Set $x = x' = t' = 0$. Assume that $A(t) = (m\omega/2\pi i\hbar\sin\omega t)^{1/2}$ for the oscillator. By expanding both sides of Eq. (8.6.15), you should find that $E = \hbar\omega/2,\ 5\hbar\omega/2,\ 9\hbar\omega/2,\ \ldots$, etc. What happened to the levels in between?

(2) (Optional). Now consider the extraction of the eigenfunctions. Let $x = x'$ and $t' = 0$. Find $E_0$, $E_1$, $|\psi_0(x)|^2$, and $|\psi_1(x)|^2$ by expanding in powers of $\alpha = \exp(i\omega t)$.

...

8.6.4. Recall the derivation of the Schrödinger equation (8.5.8) starting from Eq. (8.5.4). Note that although we chose the argument of $V$ to be the midpoint of $x + x'/2$, it did nto matter very much: any choice $x + \alpha\eta$, (where $\eta = x' - x$) for $0 \le \alpha \le 1$ would have given the same result since the difference between the choices is of order $\eta\varepsilon \approxeq \varepsilon^{3/2}$. All this was thanks to the factor $\varepsilon$ multiplying $V$ in Eq. (8.5.4) and the fact that $|\eta| \approxeq \varepsilon^{1/2}$, as per Eq. (8.6.5).

Consider now the case of a vector potential which will bring in a factor

$$\exp\left[\frac{iq\varepsilon}{\hbar c}\frac{x-x'}{\varepsilon}A(x+\alpha\eta)\right] \equiv \exp\left[-\frac{iq\varepsilon}{\hbar c}\frac{\eta}{\varepsilon}A(x+\alpha\eta)\right]$$

to the propagator for one time slice. (We should really be using vectors for position and the vector potential, but the one-dimensional version will suffice for making the point here.) Note that $\varepsilon$ now gets canceled, in contrast to the scalar potential case. Thus, going to order $\varepsilon$ to derive the Schrödinger equation means going to order $\eta^2$ in expanding the exponential. This will not only bring in an $A^2$ term, but will also make the answer sensitive to the argument of $A$ in the linear term. Choose $\alpha = 1/2$ and verify that you get the one-dimensional version of EQ. (4.3.7). Along the way you will see that changing $\alpha$ make an order $\varepsilon$ difference to $\psi(x,\varepsilon)$ so that we have no choice but to use $\alpha = 1/2$, i.e., use the *midpoint prescription*. This point will come up in Chapter 21.

...

# 9 The Heisenberg Uncertainty Relations

## 9.4 Applications of the Uncertainty Principle

9.4.1. Consider the oscillator in the state $|n = 1\rangle$ and verify that

$$\left\langle\frac{1}{X^2}\right\rangle \simeq \frac{1}{\langle X^2\rangle} \simeq \frac{m\omega}{\hbar}$$

Projected onto the $x$ basis, we have

$$\langle x|n=1\rangle = \psi_1(x) = \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

giving

$$\begin{aligned}
\left\langle \frac{1}{X^2} \right\rangle &= \int \psi_1^*(x) \frac{1}{x^2} \psi_1(x)\,\mathrm{d}x \\
&= \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/2} \int \exp\left(-\frac{m\omega x^2}{\hbar}\right) \mathrm{d}x \\
&= \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/2} \left(\frac{\pi\hbar}{m\omega}\right)^{1/2} \\
&= \frac{2m\omega}{\hbar}
\end{aligned}$$

If we instead compute $\langle X^2\rangle$, we get

$$\begin{aligned}
\langle X^2\rangle &= \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/2} \int x^4 \exp\left(-\frac{m\omega x^2}{\hbar}\right) \mathrm{d}x \\
&= \frac{3}{4}\left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/2} \left(\frac{\pi\hbar^5}{m^5\omega^5}\right)^{1/2} \\
&= \frac{3\hbar}{2m\omega}
\end{aligned}$$

and so

$$\frac{1}{\langle X^2\rangle} = \frac{2m\omega}{3\hbar}$$

Both of these results are approximately the same as $m\omega/\hbar$.

9.4.2. (1) By referring to the table of integrals in Appendix A.2, verify that

$$\psi = \frac{1}{(\pi a_0^3)^{1/2}} e^{-r/a_0}, \qquad r = (x^2+y^2+z^2)^{1/2}$$

is a normalized wave function (of the ground state of hydrogen). Note that in three dimensions the normalization condition is

$$\begin{aligned}
\langle\psi|\psi\rangle &= \int \psi^*(r,\theta,\phi)\psi(r,\theta,\phi) r^2\,\mathrm{d}r\,\mathrm{d}(\cos\theta)\,\mathrm{d}\phi \\
&= 4\pi \int \psi^*(r)\psi(r) r^2\,\mathrm{d}r = 1
\end{aligned}$$

for a function of just $r$.

(2) Calculate $(\Delta X)^2$ in this state [argue that $(\Delta X)^2 = \frac{1}{3}\langle r^2\rangle$] and regain the result quoted in Eq. (9.4.9).

(3) Show that $\langle 1/r\rangle \simeq 1/\langle r\rangle \simeq me^2/\hbar^2$ in this state.

The normalization condition is

$$
\begin{aligned}
\langle\psi|\psi\rangle &= \frac{4\pi}{\pi a_0^3}\int_0^\infty r^2 e^{-2r/a_0}\,\mathrm{d}r \\
&= \frac{4}{a_0^3}\Big(\frac{2!}{(2/a_0)^3}\Big) \\
&= 1
\end{aligned}
$$

Since $(\Delta X)^2 = \langle X^2\rangle - \langle X\rangle^2$ and the three Cartesian coordinates should be symmetric,

$$
\begin{aligned}
(\Delta X)^2 &= \frac{(\Delta X^2) + (\Delta Y^2) + (\Delta Z^2)}{3} \\
&= \frac{\langle X^2\rangle - \langle X\rangle^2 + \langle Y^2\rangle - \langle Y\rangle^2 + \langle Z^2\rangle - \langle Z\rangle^2}{3}
\end{aligned}
$$

We expect the average $x$, $y$, and $z$ values to be 0, so

$$
\begin{aligned}
(\Delta X)^2 &= \frac{\langle X^2\rangle + \langle Y^2\rangle + \langle Z^2\rangle}{3} \\
&= \frac{1}{3}\langle X^2 + Y^2 + Z^2\rangle \\
&= \frac{1}{3}\langle r^2\rangle
\end{aligned}
$$

Computing the listed expected values yields

$$
\begin{aligned}
\left\langle\frac{1}{r}\right\rangle &= \frac{4}{a_0^3}\int_0^\infty r e^{-2r/a_0}\mathrm{d}r \\
&= \frac{4}{a_0^3}\frac{1!}{(2/a_0)^2} \\
&= \frac{1}{a_0} \\
\langle r\rangle &= \frac{4}{a_0^3}\int_0^\infty r^3 e^{-2r/a_0} \\
&= \frac{4}{a_0^3}\frac{3!}{(2/a_0)^4} \\
&= \frac{3a_0}{2}
\end{aligned}
$$

and so $1/\langle r\rangle = 2/3a_0$. Substituting in the value of the Bohr radius as $a_0 = 4\pi\varepsilon_0\hbar^2/me^2$ gives

$$
\begin{aligned}
\left\langle\frac{1}{r}\right\rangle &= \frac{1}{4\pi\varepsilon_0}\frac{me^2}{\hbar^2} \\
\frac{1}{\langle r\rangle} &= \frac{1}{6\pi\varepsilon_0}\frac{me^2}{\hbar^2}
\end{aligned}
$$

which are approximately equal, with both being proportional to $me^2/\hbar^2$.

9.4.3. Ignore the fact that the hydrogen atom is a three-dimensional system and pretend that

$$H = \frac{P^2}{2m} - \frac{e^2}{(R^2)^{1/2}} \qquad (P^2 = P_x^2 + P_y^2 + P_z^2, R^2 = X^2 + Y^2 + Z^2)$$

corresponds to a one-dimensional problem. Assuming

$$\Delta P \cdot \Delta R \geq \hbar/2$$

estimate the ground-state energy.

In the ground state, $\langle P \rangle = \langle R \rangle = 0$, so $\langle H \rangle$ should be approximately

$$\begin{aligned}
\langle H \rangle &= \left\langle \frac{P^2}{2m} \right\rangle - \left\langle \frac{e^2}{(R^2)^{1/2}} \right\rangle \\
&\simeq \frac{1}{2m}\langle P^2 \rangle - \frac{e^2}{\langle (R^2)^{1/2} \rangle} \\
&\simeq \frac{1}{2m}(\Delta P)^2 - \frac{e^2}{(\langle R^2 \rangle)^{1/2}} \\
&= \frac{1}{2m}(\Delta P)^2 - \frac{e^2}{\Delta R} \\
&\gtrsim \frac{\hbar^2}{8m(\Delta R)^2} - \frac{e^2}{\Delta R}
\end{aligned}$$

The minimum value of $\langle H \rangle$ occurs when

$$\frac{\mathrm{d}\langle H \rangle}{\mathrm{d}\Delta R} = -\frac{\hbar^2}{4m(\Delta R)^3} + \frac{e^2}{(\Delta R)^2} = 0$$

or $\Delta R = \hbar^2/4me^2$. Plugging this into $\langle H \rangle$ gives a ground state estimate of

$$\langle H \rangle \simeq \frac{\hbar^2}{8m}\frac{16m^2e^4}{\hbar^4} - e^2\frac{4me^4}{\hbar^2} = -\frac{2me^4}{\hbar^2}$$

9.4.4. Compute $\Delta T \cdot \Delta X$, where $T = P^2/2m$. Why is this relation not so famous?

The general uncertainty relation between $X$ and $T$ is

$$(\Delta X)^2(\Delta T)^2 \geq \tfrac{1}{4}\langle \psi | [X - \langle X \rangle, T - \langle T \rangle]_+ | \psi \rangle^2 + \tfrac{1}{4}\langle \psi | \Gamma | \psi \rangle^2$$

where $[X, T] = i\Gamma$. Since $[X - \langle X \rangle, T - \langle T \rangle]_+$ is real, the first term is positive definite. Also, with

$$\begin{aligned}
[X, T] &= \frac{1}{2m}[X, P^2] \\
&= \frac{1}{2m}\big([X, P]P + P[X, P]\big) \\
&= \frac{i\hbar}{m}P
\end{aligned}$$

we may write

$$\Delta X \cdot \Delta T \geq \tfrac{\hbar}{2m}\langle \psi | P | \psi \rangle$$

Since $P|\psi\rangle$ may be 0, this relationship does not give an interesting lower bound like the canonically conjugate $X$ and $P$ operators give.

# 10 Systems with $N$ Degrees of Freedom

## 10.1 $N$ Particles in One Dimension

10.1.1. Show the following:

(1) $[\Omega_1^{(1)} \otimes I^{(2)}, I^{(1)} \otimes \Lambda_2^{(2)}] = 0$ for any $\Omega_1^{(1)}$ and $\Lambda_2^{(2)}$

(operators of particle 1 commute with those of particle 2).

(2) $(\Omega_1^{(1)} \otimes \Gamma_2^{(2)})(\theta_1^{(1)} \otimes \Lambda_2^{(2)}) = (\Omega\theta)_1^{(1)} \otimes (\Gamma\Lambda)_2^{(2)}$

(3) If

$$[\Omega_1^{(1)}, \Lambda_1^{(1)}] = \Gamma_1^{(1)}$$

then

$$[\Omega_1^{(1)\otimes(2)}, \Lambda_1^{(1)\otimes(2)}] = \Gamma_1^{(1)} \otimes I^{(2)}$$

and similarly with $1 \to 2$.

(4) $(\Omega_1^{(1)\otimes(2)} + \Omega_2^{(1)\otimes(2)})^2 = (\Omega_1^2)^{(1)} \otimes I^{(2)} + I^{(1)} \otimes (\Omega_2^2)^{(2)} + 2\Omega_1^{(1)} \otimes \Omega_2^{(2)}$

We can check these by applying each operator to an arbitrary tensor product state $|x_1\rangle \otimes |x_2\rangle$. For the first, we have

$$\begin{aligned}
[\Omega_1^{(1)} \otimes I^{(2)}, I^{(1)} \otimes \Lambda_2^{(2)}]|x_1\rangle \otimes |x_2\rangle &= [\Omega_1^{(1)\otimes(2)}, \Lambda_2^{(1)\otimes(2)}]|x_1\rangle \otimes |x_2\rangle \\
&= \Omega_1^{(1)\otimes(2)}\Lambda_2^{(1)\otimes(2)}|x_1\rangle \otimes |x_2\rangle - \Lambda_2^{(1)\otimes(2)}\Omega_1^{(1)\otimes(2)}|x_1\rangle \otimes |x_2\rangle \\
&= \Omega_1^{(1)\otimes(2)}|x_1\rangle \otimes |\Lambda_2^{(2)}x_2\rangle - \Lambda_2^{(1)\otimes(2)}|\Omega_1^{(1)}x_1\rangle \otimes |x_2\rangle \\
&= |\Omega_1^{(1)}x_1\rangle \otimes |\Lambda_2^{(2)}x_2\rangle - |\Omega_1^{(1)}x_1\rangle \otimes |\Lambda_2^{(2)}x_2\rangle \\
&= 0
\end{aligned}$$

which implies $[\Omega_1^{(1)} \otimes I^{(2)}, I^{(1)} \otimes \Lambda_2^{(2)}] = 0$. Performing a similar exercise with the second gives

$$\begin{aligned}
(\Omega_1^{(1)} \otimes \Gamma_2^{(2)})(\theta_1^{(1)} \otimes \Lambda_2^{(2)})|x_1\rangle \otimes |x_2\rangle &= (\Omega_1^{(1)} \otimes \Gamma_2^{(2)})|\theta_1^{(1)}x_1\rangle \otimes |\Lambda_2^{(2)}x_2\rangle \\
&= |\Omega_1^{(1)}\theta_1^{(1)}x_1\rangle \otimes |\Gamma_2^{(2)}\Lambda_2^{(2)}x_2\rangle \\
&= |(\Omega\theta)_1^{(1)}x_1\rangle \otimes |(\Gamma\Lambda)_2^{(2)}x_2\rangle
\end{aligned}$$

i.e. $(\Omega_1^{(1)} \otimes \Gamma_2^{(2)})(\theta_1^{(1)} \otimes \Lambda_2^{(2)}) = (\Omega\theta)_1^{(1)} \otimes (\Gamma\Lambda)_2^{(2)}$. The third follows immediately upon taking the tensor product of both sides with $I^{(2)}$, with the alternative equality shown upon swapping (1) and (2). For the fourth, observe that

$$\begin{aligned}
&(\Omega_1^{(1)\otimes(2)} + \Omega_2^{(1)\otimes(2)})(\Omega_1^{(1)\otimes(2)} + \Omega_2^{(1)\otimes(2)})|x_1\rangle \otimes |x_2\rangle \\
&= (\Omega_1^{(1)\otimes(2)} + \Omega_2^{(1)\otimes(2)})(|\Omega_1^{(1)}x_1\rangle \otimes |x_2\rangle + |x_1\rangle \otimes |\Omega_2^{(2)}x_2\rangle) \\
&= |(\Omega_1^2)^{(1)}|x_1\rangle \otimes |x_2\rangle + |\Omega_1^{(1)}x_1\rangle \otimes |\Omega_2^{(2)}x_2\rangle + |\Omega_1^{(1)}x_1\rangle \otimes |\Omega_2^{(2)}x_2\rangle + |x_1\rangle \otimes |(\Omega_2^2)^{(2)}x_2\rangle
\end{aligned}$$

which immediately shows

$$(\Omega_1^{(1)\otimes(2)} + \Omega_2^{(1)\otimes(2)})^2 = (\Omega_1^2)^{(1)} \otimes I^{(2)} + I^{(1)} \otimes (\Omega_2^2)^{(2)} + 2\Omega_1^{(1)} \otimes \Omega_2^{(2)}$$

10.1.2. Imagine a fictitious world in which the single-particle Hilbert space is two-dimensional. Let us denote the basis vectors by $|+\rangle$ and $|-\rangle$. Let

$$\sigma_1^{(1)} = \begin{array}{c c} & \begin{array}{cc} + & - \end{array} \\ \begin{array}{c} + \\ - \end{array} & \begin{bmatrix} a & b \\ c & d \end{bmatrix} \end{array} \text{ and } \sigma_2^{(2)} = \begin{array}{c c} & \begin{array}{cc} + & - \end{array} \\ \begin{array}{c} + \\ - \end{array} & \begin{bmatrix} e & f \\ g & h \end{bmatrix} \end{array}$$

be operators in $\mathbb{V}_1$ and $\mathbb{V}_2$, respectively (the $\pm$ signs label the basis vectors. Thus $b = \langle +|\sigma_1^{(1)}|-\rangle$ etc.) The space $\mathbb{V}_1 \otimes \mathbb{V}_2$ is spanned by four vectors $|+\rangle \otimes |+\rangle$, $|+\rangle \otimes |-\rangle$, $|-\rangle \otimes |+\rangle$, $|-\rangle \otimes |-\rangle$. Show (using the method of images or otherwise) that

(1) $\sigma_1^{(1)\otimes(2)} = \sigma_1^{(1)} \otimes I^{(2)} = \begin{array}{c c} & \begin{array}{cccc} ++ & +- & -+ & -- \end{array} \\ \begin{array}{c} ++ \\ +- \\ -+ \\ -- \end{array} & \begin{bmatrix} a & 0 & b & 0 \\ 0 & a & 0 & b \\ c & 0 & d & 0 \\ 0 & c & 0 & d \end{bmatrix} \end{array}$

(Recall that $\langle\alpha| \otimes \langle\beta|$ is the bra corresponding to $|\alpha\rangle \otimes |\beta\rangle$.)

(2) $\sigma_2^{(1)\otimes(2)} = \begin{bmatrix} e & f & 0 & 0 \\ g & h & 0 & 0 \\ 0 & 0 & e & f \\ 0 & 0 & g & h \end{bmatrix}$

(3) $(\sigma_1\sigma_2)^{(1)\otimes(2)} = \sigma_1^{(1)} \otimes \sigma_2^{(2)} = \begin{bmatrix} ae & af & be & bf \\ ag & ah & bg & bh \\ ce & cf & de & df \\ cg & ch & dg & dh \end{bmatrix}$

Do part (3) in two ways, by taking the matrix product of $\sigma_1^{(1)\otimes(2)}$ and $\sigma_2^{(1)\otimes(2)}$

The Kronecker product is the explicit matrix form of the tensor product, defined as

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11}\mathbf{B} & \cdots & a_{1m}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{n1}\mathbf{B} & \cdots & a_{nm}\mathbf{B} \end{bmatrix}$$

From this definition all of the above results immediately follow.

10.1.3. Consider the Hamiltonian of the coupled mass system:

$$\mathcal{H} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\omega^2[x_1^2 + x_2^2 + (x_1 - x_2)^2]$$

We know from Example 1.8.6 that $\mathcal{H}$ can be decoupled if we use normal coordinates

$$x_{\mathrm{I,II}} = \frac{x_1 \pm x_2}{2^{1/2}}$$

and the corresponding momenta

$$p_{\mathrm{I,II}} = \frac{p_1 \pm p_2}{2^{1/2}}$$

(1) Rewrite $\mathcal{H}$ in terms of normal coordinates. Verify that the normal coordinates are also canonical, i.e. that

$$\{x_i, p_j\} = \delta_{ij} \text{ etc.}; \quad i, j = \mathrm{I, II}$$

Now quantize the system, promoting these variables to operators obeying

$$[X_i, P_j] = i\hbar\delta_{ij} \text{ etc.}; \quad i, j = \mathrm{I}, \mathrm{II}$$

Write the eigenvalue equation for $H$ in the simultaneous eigenbasis of $X_\mathrm{I}$ and $X_\mathrm{II}$.

(2) Quantize the system directly, by promoting $x_1$, $x_2$, $p_1$, and $p_2$ to quantum operators. Write the eigenvalue equation for $H$ in the simultaneous eigenbasis of $X_1$ and $X_2$. Now change from $x_1$, $x_2$ (and of course $\partial/\partial x_1$, $\partial/\partial x_2$) to $x_\mathrm{I}$, $x_\mathrm{II}$ (and $\partial/\partial x_\mathrm{I}$, $\partial/\partial x_\mathrm{II}$) *in the differential equation.* You should end up with the result from part (1).

In general, one can change coordinates and then quantize or first quantize and then change variables in the differential equation if the change of coordinates is canonical. (We are assuming that all the variables are Cartesian. As mentioned earlier in the book, if one wants to employ non-Cartesian coordinates, it is best to first quantize the Cartesian coordinates and then change variables in the differential equation.)

If the original coordinates are canonical, we have

$$\begin{aligned}
\{x_\mathrm{I}, p_\mathrm{I}\} &= \frac{1}{2}\{x_1 + x_2, p_1 + p_2\} \\
&= \frac{1}{2}\{x_1, p_1\} + \frac{1}{2}\{x_1, p_2\} + \{x_2, p_1\} + \{x_2, p_2\} \\
&= 1 \\
\{x_\mathrm{I}, p_\mathrm{II}\} &= \frac{1}{2}\{x_1 + x_2, p_1 - p_2\} \\
&= \frac{1}{2}\{x_1, p_1\} - \frac{1}{2}\{x_1, p_2\} + \{x_2, p_1\} - \{x_2, p_2\} \\
&= 0 \\
\{x_\mathrm{II}, p_\mathrm{I}\} &= \frac{1}{2}\{x_1 - x_2, p_1 + p_2\} \\
&= \frac{1}{2}\{x_1, p_1\} + \frac{1}{2}\{x_1, p_2\} - \{x_2, p_1\} - \{x_2, p_2\} \\
&= 0 \\
\{x_\mathrm{II}, p_\mathrm{II}\} &= \frac{1}{2}\{x_1 - x_2, p_1 - p_2\} \\
&= \frac{1}{2}\{x_1, p_1\} - \frac{1}{2}\{x_1, p_2\} - \{x_2, p_1\} + \{x_2, p_2\} \\
&= 1
\end{aligned}$$

i.e. $\{x_i, p_j\} = \delta_{ij}$ for $i, j = \mathrm{I}, \mathrm{II}$ (since it is obvious that $\{x_i, x_j\} = 0$ and $\{p_i, p_j\} = 0$). We can invert the defining equations of $x_{\mathrm{I},\mathrm{II}}$ and $p_{\mathrm{I},\mathrm{II}}$ to find

$$\begin{aligned}
x_1 &= \frac{x_\mathrm{I} + x_\mathrm{II}}{2^{1/2}} \\
x_2 &= \frac{x_\mathrm{I} - x_\mathrm{II}}{2^{1/2}} \\
p_1 &= \frac{p_\mathrm{I} + p_\mathrm{II}}{2^{1/2}} \\
p_2 &= \frac{p_\mathrm{I} - p_\mathrm{II}}{2^{1/2}}
\end{aligned}$$

which, upon substituting into the Hamiltonian, gives

$$H = \frac{(p_\mathrm{I} + p_\mathrm{II})^2}{4m} + \frac{(p_\mathrm{I} - p_\mathrm{II})^2}{4m} + \frac{1}{2}m\omega^2\Big[\frac{(x_\mathrm{I} + x_\mathrm{II})^2}{2} + \frac{(x_\mathrm{I} - x_\mathrm{II})^2}{2} + \Big(\frac{x_\mathrm{I} + x_\mathrm{II}}{2} - \frac{x_\mathrm{I} - x_\mathrm{II}}{2}\Big)^2\Big]$$

$$= \frac{p_{\mathrm{I}}^2}{2m} + \frac{p_{\mathrm{II}}^2}{2m} + \frac{1}{2}m\omega^2[x_{\mathrm{I}}^2 + 2x_{\mathrm{II}}^2]$$

Promoting the variables to operators gives an eigenvalue equation of

$$H|E\rangle = \Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_{\mathrm{I}}^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_{\mathrm{II}}^2} + \frac{1}{2}m\omega^2[X_{\mathrm{I}}^2 + 2X_{\mathrm{II}}^2]\Big)|E\rangle = E|E\rangle$$

If we instead quantize the original Hamiltonian, we get

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + \frac{1}{2}m\omega^2[x_1^2 + x_2^2 + (x_1 - x_2)^2]$$

To change variables, note that

$$\frac{\partial}{\partial x_i} = \frac{\partial x_{\mathrm{I}}}{\partial x_i}\frac{\partial}{\partial x_{\mathrm{I}}} + \frac{\partial x_{\mathrm{II}}}{\partial x_i}\frac{\partial}{\partial x_{\mathrm{II}}}$$

which implies

$$\begin{aligned}
\frac{\partial^2}{\partial x_i^2} &= \frac{\partial x_{\mathrm{I}}}{\partial x_i}\Big(\frac{\partial^2 x_{\mathrm{I}}}{\partial x_{\mathrm{I}}\partial x_i}\frac{\partial}{\partial x_{\mathrm{I}}} + \frac{\partial x_{\mathrm{I}}}{\partial x_i}\frac{\partial^2}{\partial x_{\mathrm{I}}^2} + \frac{\partial^2 x_{\mathrm{II}}}{\partial x_{\mathrm{I}}\partial x_i}\frac{\partial}{\partial x_{\mathrm{II}}} + \frac{\partial x_{\mathrm{II}}}{\partial x_i}\frac{\partial^2}{\partial x_{\mathrm{I}}\partial x_{\mathrm{II}}}\Big)\\
&\quad + \frac{\partial x_{\mathrm{II}}}{\partial x_i}\Big(\frac{\partial^2 x_{\mathrm{I}}}{\partial x_{\mathrm{II}}\partial x_i}\frac{\partial}{\partial x_{\mathrm{I}}} + \frac{\partial x_{\mathrm{I}}}{\partial x_i}\frac{\partial^2}{\partial x_{\mathrm{II}}\partial x_{\mathrm{I}}} + \frac{\partial^2 x_{\mathrm{II}}}{\partial x_{\mathrm{II}}\partial x_i}\frac{\partial}{\partial x_{\mathrm{II}}} + \frac{\partial x_{\mathrm{II}}}{\partial x_i}\frac{\partial^2}{\partial x_{\mathrm{II}}^2}\Big)\\
&= \frac{\partial x_{\mathrm{I}}}{\partial x_i}\Big(\frac{\partial x_{\mathrm{I}}}{\partial x_i}\frac{\partial^2}{\partial x_{\mathrm{I}}^2} + \frac{\partial x_{\mathrm{II}}}{\partial x_i}\frac{\partial^2}{\partial x_{\mathrm{I}}\partial x_{\mathrm{II}}}\Big) + \frac{\partial x_{\mathrm{II}}}{\partial x_i}\Big(\frac{\partial x_{\mathrm{I}}}{\partial x_i}\frac{\partial^2}{\partial x_{\mathrm{II}}\partial x_{\mathrm{I}}} + \frac{\partial x_{\mathrm{II}}}{\partial x_i}\frac{\partial^2}{\partial x_{\mathrm{II}}^2}\Big)
\end{aligned}$$

Observing that

$$\frac{\partial x_{\mathrm{I}}}{\partial x_1} = \frac{\partial x_{\mathrm{II}}}{\partial x_1} = \frac{\partial x_{\mathrm{I}}}{\partial x_2} = \frac{1}{2^{1/2}}, \qquad \frac{\partial x_{\mathrm{II}}}{\partial x_2} = -\frac{1}{2^{1/2}}$$

we find

$$\begin{aligned}
\frac{\partial^2}{\partial x_1^2} &= \frac{1}{2}\frac{\partial^2}{\partial x_{\mathrm{I}}^2} + \frac{\partial^2}{\partial x_{\mathrm{I}}\partial x_{\mathrm{II}}} + \frac{1}{2}\frac{\partial^2}{\partial x_{\mathrm{II}}^2}\\
\frac{\partial^2}{\partial x_2^2} &= \frac{1}{2}\frac{\partial^2}{\partial x_{\mathrm{I}}^2} - \frac{\partial^2}{\partial x_{\mathrm{I}}\partial x_{\mathrm{II}}} + \frac{1}{2}\frac{\partial^2}{\partial x_{\mathrm{II}}^2}
\end{aligned}$$

Substituting this and the other definitions into $H$ gives the same eigenvalue equation

$$H|E\rangle = \Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_{\mathrm{I}}^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_{\mathrm{II}}^2} + \frac{1}{2}m\omega^2[X_{\mathrm{I}}^2 + 2X_{\mathrm{II}}^2]\Big)|E\rangle = E|E\rangle$$

## 10.2 More Particles in More Dimensions

10.2.1. (Particle in a Three-Dimensional Box). Recall that a particle in a one-dimensioanl box extending from $x = 0$ to $L$ is confined to the region $0 \le x \le L$; its wave function vanishes at the edges $x = 0$ and $L$ and beyond (Exercise 5.2.5). Consider now a particle confined in a three-dimensional cubic box of volume $L^3$. Choosing as the origin one of its corners, and the $x$, $y$, and $z$ axes along the three edges meeting there, show that the normalized energy eigenfunctions are

$$\psi_E(x,y,z) = \Big(\frac{2}{L}\Big)^{1/2}\sin\Big(\frac{n_x\pi x}{L}\Big)\Big(\frac{2}{L}\Big)^{1/2}\sin\Big(\frac{n_y\pi y}{L}\Big)\Big(\frac{2}{L}\Big)^{1/2}\sin\Big(\frac{n_z\pi z}{L}\Big)$$

where

$$E = \frac{\hbar^2 \pi^2}{2ML^2}(n_x^2 + n_y^2 + n_z^2)$$

and $n_i$ are positive integers.

> The Hamiltonian inside the box is simply the free particle Hamiltonian,
>
> $$H = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2M}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2M}\frac{\partial^2}{\partial z^2}$$
>
> When applied to the wavefunction $\psi$, this is a separable differential equation with the general solution $\psi(x, y, z) = \phi(x)\phi(y)\phi(z)$, where
>
> $$\phi(x) = A\sin(kx) + B\cos(kx)$$
>
> Here, $k = \hbar/\sqrt{2m}$. To enforce $\phi(0) = 0$, we set $B = 0$. By symmetry, $A$ must be the same for $\phi(x)$, $\phi(y)$, and $\phi(z)$, and so we have
>
> $$\psi(x, y, z) = A^3 \sin(kx)\sin(ky)\sin(kz)$$
>
> To enforce $\phi(L) = 0$, $k$ must be equal to $n\pi/L$, giving
>
> $$\psi(x, y, z) = A^3 \sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right)\sin\left(\frac{n_z \pi z}{L}\right)$$
>
> To find $A$, we normalize $\psi$ over the cube to find
>
> $$\begin{aligned}\iiint |\psi|^2 \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z &= A^6 \iiint \sin^2\left(\frac{n_x \pi x}{L}\right)\sin^2\left(\frac{n_y \pi y}{L}\right)\sin^2\left(\frac{n_z \pi z}{L}\right)\mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \\ &= A^6 \frac{L^3}{2^3} \\ &= 1\end{aligned}$$
>
> or
>
> $$A = \left(\frac{2}{L}\right)^{1/2}$$
>
> and so
>
> $$\psi(x, y, z) = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right)\sin\left(\frac{n_z \pi z}{L}\right)$$
>
> Since $H|\psi\rangle = E|\psi\rangle$ and we know $|\psi\rangle$, $E$ can be read off as
>
> $$\frac{\hbar^2 \pi^2}{2ML^2}(n_x^2 + n_y^2 + n_z^2)$$

10.2.2. Quantize the two-dimensional oscillator for which

$$\mathcal{H} = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2$$

(1) Show that the allowed energies are

$$E = (n_x + 1/2)\hbar\omega_x + (n_y + 1/2)\hbar\omega_y, \quad n_x, n_y = 0, 1, 2, \ldots$$

(2) Write down the corresponding wave functions in terms of single oscillator wave functions. Verify that they have definite parity (even/odd) number $x \to -x$, $y \to -y$ and that the parity depends only on $n = n_x + n_y$.

(3) Consider next the *isotropic* oscillator ($\omega_x = \omega_y$). Write *explicit*, normalized eigenfunctions of the first three *states* (that is, for the cases $n = 0$ and 1). Reexpress your results in terms of polar coordinates $\rho$ and $\phi$ (for later use). Show that the degeneracy of a level with $E = (n+1)\hbar\omega$ is $(n+1)$.

Promoting the variables to operators and assuming $\psi(x,y) = \phi(x)\theta(y)$, we find

$$H\phi(x)\theta(y) = -\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2}\theta(y) - \frac{\hbar^2}{2m}\frac{\partial^2\theta(y)}{\partial y^2}\phi(x) + \frac{1}{2}m\omega_x^2x^2\phi(x)\theta(y) + \frac{1}{2}m\omega_y^2y^2\phi(x)\theta(y) = E\phi(x)\theta(y)$$

Dividing through by $\psi(x,y)$ gives

$$E = -\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2}\frac{1}{\phi(x)} + \frac{1}{2}m\omega_x^2x^2 - \frac{\hbar^2}{2m}\frac{\partial^2\theta(y)}{\partial y^2}\frac{1}{\theta(y)} + \frac{1}{2}m\omega_y^2y^2$$

Since $x$ and $y$ can vary independently, this equation can only make sense if $E = E_x + E_y$, where

$$E_x = -\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2}\frac{1}{\phi(x)} + \frac{1}{2}m\omega_x^2x^2$$
$$E_y = -\frac{\hbar^2}{2m}\frac{\partial^2\theta(y)}{\partial y^2}\frac{1}{\theta(y)} + \frac{1}{2}m\omega_y^2y^2$$

These eigenvalue equations each describe a one-dimensional harmonic oscillator whose allowed energies are $(n+1/2)\hbar\omega$, and so the full system's energy levels are described by

$$E = (n_x + 1/2)\hbar\omega_x + (n_y + 1/2)\hbar\omega_y.$$

If we label a one-dimensional harmonic oscillator wavefunction at energy level $n$ and natural frequency $\omega$ by $\psi_n^\omega(x)$, then we also have

$$\psi(x,y) = \psi_{n_x}^{\omega_x}(x)\psi_{n_y}^{\omega_y}(y)$$

This is an odd function when $n_x$ is odd and $n_y$ is even (or vice versa) and an even function when $n_x$ and $n_y$ are both even or both odd. This can be equivalently expressed by identifying the parity of $\psi(x,y)$ with the evenness of $n = n_x + n_y$: an even $n$ implies an even $\psi(x,y)$ while an odd $n$ implies an odd $\psi(x,y)$.

When $\omega_x = \omega_y$, the wave function becomes

$$\psi(x,y) = \left(\frac{m\omega}{\pi\hbar 2^{n_x+n_y}(n_x!)(n_y!)}\right)^{1/2} \exp\left(-\frac{m\omega}{2\hbar}(x^2+y^2)\right) H_{n_x}\left[\left(\frac{m\omega}{\hbar}\right)^{1/2}x\right] H_{n_y}\left[\left(\frac{m\omega}{\hbar}\right)^{1/2}y\right]$$

For the first three states, we have

$$\psi_{0,0}(x,y) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\exp\left(-\frac{m\omega(x^2+y^2)}{2\hbar}\right)$$
$$\psi_{1,0}(x,y) = \left(\frac{2m^2\omega^2}{\pi\hbar^2}\right)^{1/2}\exp\left(-\frac{m\omega(x^2+y^2)}{2\hbar}\right)\cdot x$$
$$\psi_{0,1}(x,y) = \left(\frac{2m^2\omega^2}{\pi\hbar^2}\right)^{1/2}\exp\left(-\frac{m\omega(x^2+y^2)}{2\hbar}\right)\cdot y$$

or, equivalently,

$$\psi_{0,0}(x,y) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\exp\left(-\frac{m\omega\rho^2}{2\hbar}\right)$$

$$\psi_{1,0}(x,y) = \left(\frac{2m^2\omega^2}{\pi\hbar^2}\right)^{1/2} \exp\left(-\frac{m\omega(x^2+y^2)}{2\hbar}\right) \cdot \rho\cos\phi$$
$$\psi_{0,1}(x,y) = \left(\frac{2m^2\omega^2}{\pi\hbar^2}\right)^{1/2} \exp\left(-\frac{m\omega(x^2+y^2)}{2\hbar}\right) \cdot y$$

Since we now have $\omega_x = \omega_y = \omega$,

$$E = (n_x + n_y + 1)\hbar\omega = (n+1)\hbar\omega$$

which implies that there is a degeneracy (i.e. there are multiple wave functions corresponding to the same energy level). For example, $n = 1$ can be achieved through either $n_x = 1, n_y = 0$ or $n_x = 0, n_y = 1$. Similarly, $n = 2$ can be achieved through $n_x = 2, n_y = 0$, $n_x = 1, n_y = 1$, or $n_x = 0, n_y = 2$. Continuing this pattern, we see that the degeneracy of energy level $E_n$ is $n+1$.

10.2.3. Quantize the three-dimensional *isotropic oscillator* for which

$$\mathcal{H} = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + \frac{1}{2}m\omega^2(x^2+y^2+z^2)$$

(1) Show that $E = (n + 3/2)\hbar\omega$; $n = n_x + n_y + n_z$; $n_x, n_y, n_z = 0, 1, 2, \ldots$.

(2) Write the corresponding eigenfunctions in terms of single-oscillator wave functions and verify that the parity of the level with a given $n$ is $(-1)^n$. Reexpress the first four states in terms of spherical coordinates. Show that the degeneracy of a level with energy $E = (n+3/2)\hbar\omega$ is $(n+1)(n+2)/2$.

This is a straightforward extension of the last part of the previous exercise. In particular, it is obvious that

$$E = (n_x + n_y + n_z + 3/2)\hbar\omega = (n + 3/2)\hbar\omega$$

That the parity is described by $(-1)^n$ is also obvious. Determining the degeneracy of a given energy level is the only new part to this problem. This is most easily solved through recalling the solution to the "stars and bars" combinatorics problem: given $m$ stars and $k-1$ bars, how many ways can you partition the stars? In our case, we have $m = n$ energy levels and $k = 3$ different bins into which we can sort them (we need $k-1$ bars to partition a set into $k$ groups), so we have a degeneracy of

$$\binom{m+k-1}{k-1} = \binom{n+2}{2} = \frac{(n+2)!}{(2)!(n+2-2)!} = \frac{(n+2)(n+1)n!}{2n!} = \frac{(n+1)(n+2)}{2}$$

## 10.3 Identical Particles

10.3.1. Two identical bosons are found to be in states $|\phi\rangle$ and $|\psi\rangle$. Write down the normalized state vector describing the system when $\langle\phi|\psi\rangle \neq 0$.

The state vector describing this system will be symmetric with respect to $\phi$ and $\psi$, so

$$|\tilde{\Psi}\rangle \propto |\Psi\rangle = |\phi\rangle \otimes |\psi\rangle + |\psi\rangle \otimes |\phi\rangle$$

The squared amplitude of this state is given by

$$\langle\Psi|\Psi\rangle = \Big(\langle\phi| \otimes \langle\psi| + \langle\psi| \otimes \langle\phi|\Big)\Big(|\phi\rangle \otimes |\psi\rangle + |\psi\rangle \otimes |\phi\rangle\Big)$$

$$
\begin{aligned}
&= \langle\phi|\phi\rangle\langle\psi|\psi\rangle + \langle\phi|\psi\rangle\langle\psi|\phi\rangle + \langle\psi|\phi\rangle\langle\phi|\psi\rangle + \langle\psi|\psi\rangle\langle\phi|\phi\rangle \\
&= 2 + 2|\langle\phi|\psi\rangle|^2
\end{aligned}
$$

and so its normalized cousin is

$$
|\tilde{\Psi}\rangle = \frac{1}{2^{1/2}} \frac{1}{(1+|\langle\phi|\psi\rangle|^2)^{1/2}} \Big(|\phi\rangle \otimes |\psi\rangle + |\psi\rangle \otimes |\phi\rangle\Big)
$$

10.3.2. When an energy measurement is made on a system of three bosons in a box, the $n$ values obtained were 3, 3, and 4. Write down a symmetrized, normalized state vector.

The state vector for this system will be completely symmetric with respect to the measured labels, and so

$$
|\tilde{\psi}\rangle \propto |\psi\rangle = |3,3,4\rangle + |3,4,3\rangle + |4,3,3\rangle
$$

Since each term in the above is orthogonal to all the other, we simply have

$$
|\tilde{\psi}\rangle = \frac{1}{3^{1/2}} \Big(|3,3,4\rangle + |3,4,3\rangle + |4,3,3\rangle\Big)
$$

10.3.3. Imagine a situation in which there are three particles and only three states $a$, $b$, and $c$ available to them. Show that the total number of allowed, distinct configurations for this system is

(1) 27 if they are labeled

(2) 10 if they are bosons

(3) 1 if they are fermions

In the first case, each of the 3 particles can take on any of the 3 states, giving a total of $3^3 = 27$ different configurations for the system.

In the second case, the states are symmetrized, e.g. the configurations $(a,a,b)$, $(a,b,a)$, and $(b,a,a)$ are equivalent. What distinguishes a particular state is the number of $a$, $b$, and $c$ labels, with the constraint that there must be at least three such labels. We can easily list these:

| a | b | c |
|---|---|---|
| 3 | 0 | 0 |
| 0 | 3 | 0 |
| 0 | 0 | 3 |
| 2 | 1 | 0 |
| 2 | 0 | 1 |
| 1 | 2 | 0 |
| 0 | 2 | 1 |
| 1 | 0 | 2 |
| 0 | 1 | 2 |
| 1 | 1 | 1 |

From this list, we can immediately see that there are 10 possible states.

The fermionic case is the simplest: with only 3 possible labels, each particle must be in a different one, giving $\binom{3}{3} = 1$ state.

10.3.4. Two identical particles of mass $m$ are in a one-dimensional box of length $L$. Energy measurement of the system yields the value $E_{\text{sys}} = \hbar^2\pi^2/mL^2$. Write down the state vector of the system. Repeat for $E_{\text{sys}} = 5\hbar^2\pi^2/2mL^2$. (There are two possible vectors in this case.) You are not told if they are bosons or fermions. You may assume that the only degrees of freedom are orbital.

We know that the total energy of the system will be given by

$$E = \frac{\hbar^2\pi^2}{2mL^2}(n_1^2 + n_2^2)$$

which means our first measurement can only be possible if

$$n_1^2 + n_2^2 = 2$$

Since both $n_1$ and $n_2$ are integers, we must have $n_1 = n_2 = 1$, implying

$$|\psi\rangle = |1, 1\rangle$$

In the second case, we know

$$n_1^2 + n_2^2 = 5,$$

which constrains one of the values to 2 and the other to 1. The state vector is then

$$|\psi\rangle = \frac{1}{2^{1/2}}\big(|1, 2\rangle + |2, 1\rangle\big)$$

10.3.5. Consider the *exchange operator* $P_{12}$ whose action on the $X$ basis is

$$P_{12}|x_1, x_2\rangle = |x_2, x_1\rangle$$

(1) Show that $P_{12}$ has eigenvalues $\pm 1$. (It is Hermitian and unitary.)

(2) Show that its action on the basis ket $|\omega_1, \omega_2\rangle$ is also to exchange the labels 1 and 2, and hence that $\mathbb{V}_{S/A}$ are its eigenspaces with eigenvalues $\pm 1$.

(3) Show that $P_{12}X_1P_{12} = X_2$, $P_{12}X_2P_{12} = X_1$ and similarly for $P_1$ and $P_2$. Then show that $P_{12}\Omega(X_1, P_1; X_2, P_2)P_{12} = \Omega(X_2, P_2; X_1, P_1)$. [Consider the action on $|x_1, x_2\rangle$ or $|p_1, p_2\rangle$. As for the functions of $X$ and $P$, assume they are given by power series and consider any term in the series. If you need help, peek into the discussion leading to Eq. (11.2.22.)]

(4) Show that the Hamiltonian and propagator for two *identical* particles are left unaffected under $H \to P_{12}HP_{12}$ and $U \to P_{12}UP_{12}$ Given this, show that any eigenstate of $P_{12}$ continues to remain a eigenstate with the same eigenvalue as time passes, i.e., elements of $\mathbb{V}_{S/A}$ never leave the symmetric or antisymmetric subspaces they start in.

Consider applying the exchange operator twice in succession. We have

$$P_{12}^2|x_1, x_2\rangle = P_{12}|x_2, x_1\rangle = |x_1, x_2\rangle,$$

i.e. $P_{12}^2 = I$. Since

$$\begin{aligned}\langle x_1x_2|P_{12}^\dagger|x_3x_4\rangle &= \big(P_{12}|x_1x_2\rangle\big)^\dagger|x_3x_4\rangle \\ &= \big(|x_2x_1\rangle\big)^\dagger|x_3x_4\rangle\end{aligned}$$

$$
\begin{aligned}
&= \langle x_2 x_1 | x_3 x_4 \rangle \\
&= \delta(x_2 - x_3)\delta(x_1 - x_4)
\end{aligned}
$$

and

$$
\begin{aligned}
\langle x_1 x_2 | P_{12} | x_3 x_4 \rangle &= \langle x_1 x_2 | x_4 x_3 \rangle \\
&= \delta(x_1 - x_4)\delta(x_2 - x_3) \\
&= \delta(x_2 - x_3)\delta(x_1 - x_4)
\end{aligned}
$$

we must have $P_{12}^\dagger = P_{12}$, i.e. $P_{12}$ is Hermitian. Combining this result with the first result yields $P_{12}^\dagger P_{12} = I$, i.e. $P_{12}$ is unitary. Such an operator must have eigenvalues $\pm 1$.

From inspection, it is clear that $P_{12}$ has the effect of multiplying symmetric orbital states by 1 and antisymmetric orbital states by $-1$. We can use this observation on an arbitrary state by noticing that it can be written as the sum of its symmetric and antisymmetric parts, i.e.

$$
|\omega_1 \omega_2\rangle = \hat{S}|\omega_1 \omega_2\rangle + \hat{A}|\omega_1 \omega_2\rangle = \frac{1}{2}\Big(|\omega_1 \omega_2\rangle + |\omega_2 \omega_1\rangle\Big) + \frac{1}{2}\Big(|\omega_1 \omega_2\rangle - |\omega_2 \omega_1\rangle\Big)
$$

Now,

$$
\begin{aligned}
P_{12}\Big(|\omega_1 \omega_2\rangle + |\omega_2 \omega_1\rangle\Big) &= P_{12} \int |x_1 x_2\rangle\langle x_1 x_2| \Big(|\omega_1 \omega_2\rangle + |\omega_2 \omega_1\rangle\Big)\, \mathrm{d}x_1 \mathrm{d}x_2 \\
&= \int |x_2 x_1\rangle\langle x_1 x_2| \Big(|\omega_2 \omega_1\rangle + |\omega_1 \omega_2\rangle\Big)\, \mathrm{d}x_1 \mathrm{d}x_2 \\
&= \int |x_2 x_1\rangle\langle x_2 x_1| \Big(|\omega_2 \omega_1\rangle + |\omega_1 \omega_2\rangle\Big)\, \mathrm{d}x_1 \mathrm{d}x_2 \\
&= |\omega_2 \omega_1\rangle + |\omega_1 \omega_2\rangle
\end{aligned}
$$

where we have used the fact that any state contracted with a symmetric state is itself symmetric (and so $\langle x_1 x_2| = \langle x_2 x_1|$ in the above). Likewise,

$$
\begin{aligned}
P_{12}\Big(|\omega_1 \omega_2\rangle - |\omega_2 \omega_1\rangle\Big) &= P_{12} \int |x_1 x_2\rangle\langle x_1 x_2| \Big(|\omega_1 \omega_2\rangle - |\omega_2 \omega_1\rangle\Big)\, \mathrm{d}x_1 \mathrm{d}x_2 \\
&= -\int |x_2 x_1\rangle\langle x_1 x_2| \Big(|\omega_2 \omega_1\rangle - |\omega_1 \omega_2\rangle\Big)\, \mathrm{d}x_1 \mathrm{d}x_2 \\
&= \int |x_2 x_1\rangle\langle x_2 x_1| \Big(|\omega_2 \omega_1\rangle - |\omega_1 \omega_2\rangle\Big)\, \mathrm{d}x_1 \mathrm{d}x_2 \\
&= |\omega_2 \omega_1\rangle - |\omega_1 \omega_2\rangle
\end{aligned}
$$

and so

$$
\begin{aligned}
P_{12}|\omega_1 \omega_2\rangle &= P_{12}\Big(\hat{S}|\omega_1 \omega_2\rangle + \hat{A}|\omega_1 \omega_2\rangle\Big) \\
&= \hat{S}|\omega_2 \omega_1\rangle + \hat{A}|\omega_2 \omega_1\rangle \\
&= |\omega_2 \omega_1\rangle
\end{aligned}
$$

In performing the above calculations, we have essentially made use of the fact that $\mathbb{V}_{S/A}$ are eigenspaces of $P_{12}$, and therefore projecting an arbitrary $|\omega_1 \omega_2\rangle$ onto these eigenspaces before applying $P_{12}$ makes our lives easier.

Now, because $P_{12}$ applies to any basis ket, we immediately see

$$
P_{12} X_1 P_{12} |x_1, x_2\rangle = P_{12} X_1 |x_2, x_1\rangle = x_2 P_{12} |x_2, x_1\rangle = x_2 |x_1, x_2\rangle = X_2 |x_1, x_2\rangle
$$

$$P_{12}X_2P_{12}|x_1,x_2\rangle = P_{12}X_2|x_2,x_1\rangle = x_1P_{12}|x_2,x_1\rangle = x_1|x_1,x_2\rangle = X_1|x_1,x_2\rangle$$
$$P_{12}P_1P_{12}|p_1,p_2\rangle = P_{12}P_1|p_2,p_1\rangle = p_2P_{12}|p_2,p_1\rangle = p_2|p_1,p_2\rangle = P_2|p_1,p_2\rangle$$
$$P_{12}P_2P_{12}|p_1,p_2\rangle = P_{12}P_2|p_2,p_1\rangle = p_1P_{12}|p_2,p_1\rangle = p_1|p_1,p_2\rangle = P_1|p_1,p_2\rangle$$

We won't show explicitly that $P_{12}\Omega(X_1,P_1;X_2,P_2)P_{12} = \Omega(X_2,P_2;X_1,P_1)$, since it is obvious after reading the given hint. (Since $P_{12}^2 = I$, we can rewrite every term in our power series as, e.g., $P_{12}X_1^2P_{12} = P_{12}X_1P_{12}P_{12}X_1P_{12}$, after which the result immediately follows.)

For the Hamiltonian of two identical particles, we have

$$H = \frac{P_1^2}{2m} + \frac{P_2^2}{2m} + V(X_1,X_2)$$

Since $V$ often depends only on the distance between $X_1$ and $X_2$, sandwiching $H$ between pair exchange operators has no effect, as both the position and momentum operators of one particle are symmetric with respect to the other. Furthermore, since the propagator is just a power series of $H$ (and we can always insert $P_{12}^2$ between each $H$ in terms like $H^k$), sandwiching $U$ between $P_{12}$ must have no effect. Since these two facts are true, we have

$$[P_{12},H] = [P_{12},U] = 0$$

and so states that are eigenvectors of $P_{12}$ (i.e. bosons or fermions) never leave their original eigenspace.

10.3.6. Consider a composite object such as the hydrogen atom. Will it behave as a boson or fermion? Argue in general that objects containing an even/odd number of fermions will behave as bosons/fermions.

Consider an arbitrary species of atom. At a high level, we can write the combined wave function of two such atoms (labeled $a$ and $b$) as

$$\psi(p_1^a,\ldots,p_r^a,n_1^a,\cdots n_s^a,e_1^a,\ldots,e_t^a;p_1^b,\ldots p_r^b,n_1^b,\cdots n_s^b,e_1^b,\ldots e_t^b)$$

Since the protons, neutrons, and electrons in the system are all fermions, any exchange of the form $p_i^a \leftrightarrow p_i^b$ (or $n_i^a \leftrightarrow n_i^b$ or $e_i^a \leftrightarrow e_i^b$) will cause $\psi$ to pick up a minus sign.

If there are an odd number of constituent fermions, there will be an odd number of swaps and hence the overall wave function will be antisymmetric upon exchanging the two atoms (i.e. they behave like fermions). If there are an even number of constituent fermions, there will be an even number of swaps and so the overall wave function will be symmetric upon exchanging the two atoms (i.e. they behave like bosons).

From this logic, we can guess that the hydrogen atom, having one proton and on electron, will behave like a boson.

# 11 Symmetries and Their Consequences

## 11.2 Translational Invariance in Quantum Theory

11.2.1. Verify Eq. (11.2.11b)

Using the more general $T(\varepsilon)$ on $P$ yields

$$\begin{aligned}\langle P\rangle = \langle\psi_\varepsilon|P|\psi_\varepsilon\rangle &= \langle\psi|T(\varepsilon)^\dagger PT(\varepsilon)|\psi\rangle \\ &= \iint \langle\psi|x'\rangle\langle x'|T(\varepsilon)^\dagger PT(\varepsilon)|x\rangle\langle x|\psi\rangle\mathrm{d}x\mathrm{d}x' \\ &= \iint \langle\psi|x'\rangle\langle x'+\varepsilon|e^{-i\varepsilon g(x')/\hbar}Pe^{i\varepsilon g(x)/\hbar}|x+\varepsilon\rangle\langle x|\psi\rangle\mathrm{d}x\mathrm{d}x' \\ &= \iint \langle\psi|x'-\varepsilon\rangle e^{-i\varepsilon g(x'-\varepsilon)/\hbar}\langle x'|P|x\rangle e^{i\varepsilon g(x-\varepsilon)/\hbar}\langle x-\varepsilon|\psi\rangle\mathrm{d}x\mathrm{d}x' \\ &= \iint \psi^*(x'-\varepsilon)e^{-i\varepsilon g(x'-\varepsilon)/\hbar}\Big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x'}\Big)\langle x'|x\rangle e^{i\varepsilon g(x-\varepsilon)/\hbar}\psi(x-\varepsilon)\mathrm{d}x\mathrm{d}x' \\ &= \int \psi^*(x-\varepsilon)e^{-i\varepsilon g(x-\varepsilon)/\hbar}\Big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\Big)e^{i\varepsilon g(x-\varepsilon)/\hbar}\psi(x-\varepsilon)\mathrm{d}x \\ &= \int \psi^*(x-\varepsilon)e^{-i\varepsilon[g(x-\varepsilon)-g(x-\varepsilon)]/\hbar}\Big(-i\hbar\cdot i\varepsilon f(x-\varepsilon)/\hbar - i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\Big)\psi(x-\varepsilon)\mathrm{d}x \\ &= \int \psi^*(x-\varepsilon)\Big(\varepsilon f(x-\varepsilon) - i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\Big)\psi(x-\varepsilon)\mathrm{d}x \\ &= \int \psi^*(x)\Big(\varepsilon f(x) - i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\Big)\psi(x)\mathrm{d}x \\ &= \varepsilon\langle f(X)\rangle + \langle P\rangle\end{aligned}$$

which is eq. (11.2.11b).

11.2.2. Using $T^\dagger(\varepsilon)T(\varepsilon) = I$ to order $\varepsilon$, deduce that $G^\dagger = G$.

Substituting $T(\varepsilon) = I - \frac{i\varepsilon}{\hbar}G$ into $T^\dagger(\varepsilon)T(\varepsilon) = I$ gives

$$\begin{aligned}T^\dagger(\varepsilon)T(\varepsilon) &= \Big(I + \frac{i\varepsilon}{\hbar}G^\dagger\Big)\Big(I - \frac{i\varepsilon}{\hbar}G\Big) \\ &= I + \frac{i\varepsilon}{\hbar}G^\dagger - \frac{i\varepsilon}{\hbar}G + \mathcal{O}(\varepsilon^2)\end{aligned}$$

Setting this equal to the identity operator implies

$$\frac{i\varepsilon}{\hbar}\Big(G^\dagger - G\Big) = 0$$

or

$$G = G^\dagger.$$

11.2.3. Recall that we found the finite rotation transformation from the infinitesimal one, by solving differential equations (Section 2.8). Verify that if, instead, you relate the transformed coordinates $\bar{x}$ and $\bar{y}$ to $x$ and $y$ by the infinite string of Poisson brackets, you get the same result $\bar{x} = x\cos\theta - y\sin\theta$, etc. (Recall the series for $\sin\theta$, etc.)

The generator of rotations in the $x$-$y$ plane is angular momentum about the $z$-axis,

$$L_z = xp_y - yp_x,$$

and so the response of our coordinates to a finite rotation of $\theta$ is given by

$$\begin{aligned}
\bar{x} &= x + \theta\{x, L_z\} + \frac{\theta^2}{2!}\{\{x, L_z\}, L_z\} + \frac{\theta^3}{3!}\{\{\{x, L_z\}, L_z\}, L_z\} \cdots \\
\bar{y} &= y + \theta\{y, L_z\} + \frac{\theta^2}{2!}\{\{y, L_z\}, L_z\} + \frac{\theta^3}{3!}\{\{\{y, L_z\}, L_z\}, L_z\} \cdots
\end{aligned}$$

The necessary Poisson brackets are

$$\begin{aligned}
\{x, L_z\} &= \{x, xp_y - yp_x\} \\
&= \{x, xp_y\} - \{x, yp_x\} \\
&= \{x, x\}p_y + x\{x, p_y\} - \{x, y\}p_x - y\{x, p_x\} \\
&= -y \\
\{y, L_z\} &= \{y, xp_y - yp_x\} \\
&= \{y, xp_y\} - \{y, yp_x\} \\
&= \{y, x\}p_y + x\{y, p_y\} - \{y, y\}p_x - y\{y, p_x\} \\
&= x
\end{aligned}$$

and so we have

$$\begin{aligned}
\bar{x} &= x + \theta\{x, L_z\} + \frac{\theta^2}{2!}\{\{x, L_z\}, L_z\} + \frac{\theta^3}{3!}\{\{\{x, L_z\}, L_z\}, L_z\} \cdots \\
&= x - \theta y - \frac{\theta^2}{2!}\{y, L_z\} - \frac{\theta^3}{3!}\{\{y, L_z\}, L_z\} \cdots \\
&= x - \theta y - \frac{\theta^2}{2!}x - \frac{\theta^3}{3!}\{x, L_z\} + \cdots \\
&= x\Big(1 - \frac{\theta^2}{2!} + \cdots\Big) - y\Big(\theta - \frac{\theta^3}{3!} + \cdots\Big) \\
&= x\cos\theta - y\sin\theta \\
\bar{y} &= y + \theta\{y, L_z\} + \frac{\theta^2}{2!}\{\{y, L_z\}, L_z\} + \frac{\theta^3}{3!}\{\{\{y, L_z\}, L_z\}, L_z\} \cdots \\
&= y + \theta x + \frac{\theta^2}{2!}\{x, L_z\} + \frac{\theta^3}{3!}\{\{x, L_z\}, L_z\} + \cdots \\
&= y + \theta x - \frac{\theta^2}{2!}y - \frac{\theta^3}{3!}\{y, L_z\} + \cdots \\
&= x\Big(\theta - \frac{\theta^3}{3!} + \cdots\Big) + y\Big(1 - \frac{\theta^2}{2!} + \cdots\Big) \\
&= x\sin\theta + y\cos\theta
\end{aligned}$$

## 11.4 Parity Invariance

11.4.1. Prove that if $[\Pi, H] = 0$, a system that starts out in a state of even/odd parity maintains its parity. (Note that since parity is a discrete operation, it has no associated conservation law in classical mechanics.)

Symbolically, we are trying to prove that

$$\Pi|\psi(0)\rangle = \pm|\psi(0)\rangle = \pm|\psi(t)\rangle = \Pi|\psi(t)\rangle$$

Since $|\psi(t)\rangle = U(t)|\psi(0)\rangle$, the above relation will hold if $\Pi U(t) = U(t)\Pi$, or $[\Pi, U(t)] = 0$. But if $[\Pi, H] = 0$ and $H$ is independent of time, $[Pi, U(t)] = 0$ by virtue of the fact that $U(t) = e^{-iHt/\hbar}$.

11.4.2. A particle is in a potential

$$V(x) = V_0 \sin(2\pi x/a)$$

which is invariant under the translations $x \to x + ma$, where $m$ is an integer. Is momentum conserved? Why not?

The symmetry given is not the continuous translational symmetry characteristic of momentum conservation, but a discrete translational symmetry. Because of this, there is no generator function that can be used to produce infinitesimal translations, as the smallest such one is of size $a$.

More concretely, $P$ is not conserved because it does not commute with the Hamiltonian. To see this, note that

$$\begin{aligned}
PH|\psi\rangle &= -i\hbar\frac{\partial}{\partial x}\Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0\sin\left(\tfrac{2\pi x}{a}\right)\Big)|\psi\rangle \\
&= \frac{i\hbar^3}{2m}\frac{\partial^3|\psi\rangle}{\partial x^3} - i\hbar V_0\frac{2\pi}{a}\cos\left(\tfrac{2\pi x}{a}\right)|\psi\rangle - i\hbar V_0\sin\left(\tfrac{2\pi x}{a}\right)\frac{\partial|\psi\rangle}{\partial x} \\
HP|\psi\rangle &= \Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0\sin\left(\tfrac{2\pi x}{a}\right)\Big)\Big(-i\hbar\frac{\partial}{\partial x}\Big)|\psi\rangle \\
&= \frac{i\hbar^3}{2m}\frac{\partial^3|\psi\rangle}{\partial x^3} - i\hbar V_0\sin\left(\tfrac{2\pi x}{a}\right)\frac{\partial|\psi\rangle}{\partial x}
\end{aligned}$$

which implies

$$[P, H] = -i\hbar V_0\frac{2\pi}{a}\cos\left(\tfrac{2\pi x}{a}\right) \neq 0$$

11.4.3. You are told that in a certain reaction, the electron comes out with its spin always parallel to its momentum. Argue that parity is violated.

In a mirror, the electrons would appear to have spin antiparallel to their momentum. Since this is not the case, the reaction is not preserved under a parity-change operation.

11.4.4. We have treated parity as a mirror reflection. This is certainly true in one dimension, where $x \to -x$ may be viewed as the effect of reflecting through a (point) mirror at the origin. In higher dimensions when we use a plane mirror (say lying on the $x$-$y$ plane), only one ($z$) coordinate gets reversed, whereas the parity transformation reverses all three coordinates.

Verify that reflection on a mirror in the $x$-$y$ plane is the same as parity followed by 180° rotation about the $z$ axis. Since rotational invariance holds for weak interactions, noninvariance under mirror reflection implies noninvariance under parity.

A parity transformation takes

$$(x, y, z) \to (-x, -y, -z)$$

while a further rotation of 180° about the $z$ axis takes

$$(-x, -y, -z) \to (x, y, -z)$$

This is equivalent to mirroring the system in the $x$-$y$ plane.

# 12 Rotational Invariance and Angular Momentum

## 12.1 Translations in Two Dimensions

12.1.1. Verify that $\hat{a} \cdot \mathbf{P}$ is the generator of infinitesimal translations along $\mathbf{a}$ by considering the relation

$$\langle x, y|I - \frac{i}{\hbar}\boldsymbol{\delta}a \cdot \mathbf{P}|\psi\rangle = \psi(x - \delta a_x, y - \delta a_y)$$

Noting that $\boldsymbol{\delta}a$ is of order $\varepsilon$, we have

$$\begin{aligned}
\langle x, y|I - \frac{i}{\hbar}\boldsymbol{\delta}a \cdot \mathbf{P}|\psi\rangle &= \langle x, y|I - \frac{i}{\hbar}\delta a_x P_x + I - \frac{i}{\hbar}\delta a_y P_y + I - I|\psi\rangle \\
&= \langle x, y|I - \frac{i}{\hbar}\delta a_x P_x|\psi\rangle + \langle x, y|I - \frac{i}{\hbar}\delta a_y P_y|\psi\rangle - \langle x, y|\psi\rangle \\
&= \psi(x - \delta a_x, y) + \psi(x, y - \delta a_y) - \psi(x, y) \\
&\approx \psi(x, y) - \frac{\partial \psi}{\partial x}\bigg|_{x,y}\delta a_x + \psi(x, y) - \frac{\partial \psi}{\partial y}\bigg|_{x,y}\delta a_y - \psi(x, y) \\
&= \psi(x, y) - \frac{\partial \psi}{\partial x}\bigg|_{x,y}\delta a_x - \frac{\partial \psi}{\partial y}\bigg|_{x,y}\delta a_y \\
&\approx \psi(x - \delta a_x, y - \delta a_y)
\end{aligned}$$

where each approximation becomes an equality as $\delta a \to 0$.

## 12.2 Rotations in Two Dimensions

12.2.1. Provide the steps linking Eq. (12.2.8) to Eq. (12.2.9). [Hint: Recall the derivation of Eq. (11.2.8) from Eq. (11.2.6).]

Working backwards, we see

$$\begin{aligned}
\langle x, y|I - \frac{i\varepsilon_z L_z}{\hbar}|\psi\rangle &= \iint \langle x, y|U[R]|x', y'\rangle\langle x', y'|\psi\rangle \, \mathrm{d}x'\mathrm{d}y' \\
&= \iint \langle x, y|x' - y'\varepsilon_z, x'\varepsilon_z + y'\rangle\psi(x', y') \, \mathrm{d}x'\mathrm{d}y' \\
&= \iint \langle x, y|x', y'\rangle\psi(x' + y'\varepsilon_z, y' - x'\varepsilon_z) \, \mathrm{d}x'\mathrm{d}y' \\
&= \iint \delta(x - x')\delta(y - y')\psi(x' + y'\varepsilon_z, y' - x'\varepsilon_z) \, \mathrm{d}x'\mathrm{d}y'
\end{aligned}$$

$$= \psi(x + y\varepsilon_z, y - x\varepsilon_z)$$

In the above, we were able to make the changes

$$\begin{aligned} x' &\to x' + y'\varepsilon_z \\ y' &\to y' - x'\varepsilon_z \end{aligned}$$

because both $\mathrm{d}y'\varepsilon_z$ and $\mathrm{d}x'\varepsilon_z$ vanish to first order.

12.2.2. Using these commutation relations (and your keen hindsight) derive $L_z = XP_y - YP_x$. At least show that Eqs. (12.2.16) and (12.2.17) are consistent with $L_z = XP_y - YP_x$.

It is unclear to me how one can fix $L_z$ using only these commutation relations, as it could also depend on $Z$ and $P_z$ while satisfying (12.2.16) and (12.2.17). Still, we can complete the second part of the problem:

$$\begin{aligned} [X, L_z] &= [X, XP_y - YP_x] \\ &= [X, XP_y] - [X, YP_x] \\ &= [X, X]P_y + X[X, P_y] - [X, Y]P_x - Y[X, P_x] \\ &= -i\hbar Y \\ [Y, L_z] &= [Y, XP_y - YP_x] \\ &= [Y, XP_y] - [Y, YP_x] \\ &= [Y, X]P_y + X[Y, P_y] - [Y, Y]P_x - Y[Y, P_x] \\ &= i\hbar X \\ [P_x, L_z] &= [P_x, XP_y - YP_x] \\ &= [P_x, XP_y] - [P_x, YP_x] \\ &= [P_x, X]P_y + X[P_x, P_y] - [P_x, Y]P_x - Y[P_x, P_x] \\ &= -i\hbar P_y \\ [P_y, L_z] &= [P_y, XP_y - YP_x] \\ &= [P_y, XP_y] - [P_y, YP_x] \\ &= [P_y, X]P_y + X[P_y, P_y] - [P_y, Y]P_x - Y[P_y, P_x] \\ &= i\hbar P_x \end{aligned}$$

12.2.3. Derive Eq. (12.2.19) by doing a coordinate transformation on Eq (12.2.10), and also by the direct method mentioned above.

We must transform both $\partial/\partial_x$ and $\partial/\partial_y$, for which we will need the relations

$$\begin{aligned} \rho &= (x^2 + y^2)^{1/2} \\ \phi &= \tan^{-1}(\tfrac{y}{x}) \\ x &= \rho\cos\phi \\ y &= \rho\sin\phi \end{aligned}$$

Using these and the chain rule applied to $f(\rho(x,y),\phi(x,y))$, we find

$$\begin{aligned}
\frac{\partial f}{\partial x} &= \frac{\partial f}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x} \\
&= \frac{1}{2}\frac{2x}{(x^2+y^2)^{1/2}}\frac{\partial f}{\partial \rho} + \frac{1}{1+(\frac{y}{x})^2}\Big(-\frac{y}{x^2}\Big)\frac{\partial f}{\partial \phi} \\
&= \frac{x}{(x^2+y^2)^{1/2}}\frac{\partial f}{\partial \rho} - \frac{y}{x^2+y^2}\frac{\partial f}{\partial \phi} \\
&= \frac{\rho\cos\phi}{\rho}\frac{\partial f}{\partial \rho} - \frac{\rho\sin\phi}{\rho^2}\frac{\partial f}{\partial \phi} \\
&= \cos\phi\frac{\partial f}{\partial \rho} - \frac{\sin\phi}{\rho}\frac{\partial f}{\partial \phi} \\
\frac{\partial f}{\partial y} &= \frac{\partial f}{\partial \rho}\frac{\partial \rho}{\partial y} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial y} \\
&= \frac{1}{2}\frac{2y}{(x^2+y^2)^{1/2}}\frac{\partial f}{\partial \rho} + \frac{1}{1+(\frac{y}{x})^2}\frac{1}{x}\frac{\partial f}{\partial \phi} \\
&= \frac{y}{(x^2+y^2)^{1/2}}\frac{\partial f}{\partial \rho} + \frac{x}{x^2+y^2}\frac{\partial f}{\partial \phi} \\
&= \frac{\rho\sin\phi}{\rho}\frac{\partial f}{\partial \rho} + \frac{\rho\cos\phi}{\rho^2}\frac{\partial f}{\partial \phi} \\
&= \sin\phi\frac{\partial f}{\partial \rho} + \frac{\cos\phi}{\rho}\frac{\partial f}{\partial \phi}
\end{aligned}$$

which implies

$$\begin{aligned}
\frac{\partial}{\partial x} &\to \cos\phi\frac{\partial}{\partial \rho} - \frac{\sin\phi}{\rho}\frac{\partial}{\partial \phi} \\
\frac{\partial}{\partial y} &\to \sin\phi\frac{\partial}{\partial \rho} + \frac{\cos\phi}{\rho}\frac{\partial}{\partial \phi}
\end{aligned}$$

Substituting this into $L_z = XP_y - YP_x$ reveals

$$\begin{aligned}
L_z &= -i\hbar x\frac{\partial}{\partial y} + i\hbar y\frac{\partial}{\partial x} \\
&= -i\hbar\rho\cos\phi\Big(\sin\phi\frac{\partial}{\partial \rho} + \frac{\cos\phi}{\rho}\frac{\partial}{\partial \phi}\Big) + i\hbar\rho\sin\phi\Big(\cos\phi\frac{\partial}{\partial \rho} - \frac{\sin\phi}{\rho}\frac{\partial}{\partial \phi}\Big) \\
&= -i\hbar\rho\Big(\cos\phi\sin\phi - \cos\phi\sin\phi\Big)\frac{\partial}{\partial \rho} - i\hbar(\cos^2\phi + \sin^2\phi)\frac{\partial}{\partial \phi} \\
&= -i\hbar\frac{\partial}{\partial \phi}
\end{aligned}$$

Alternatively, if we require that $L_z$ generate infinitesimal translations, i.e.

$$\langle\rho,\phi|I - \frac{i}{\hbar}\varepsilon_z L_z|\psi\rangle = \psi(\rho,\phi) - \frac{i}{\hbar}\varepsilon_z\langle\rho,\phi|L_z|\psi\rangle = \psi(\rho,\phi-\varepsilon_z) = \psi(\rho,\phi) - \frac{\partial\psi}{\partial\phi}\varepsilon_z$$

then we immediately have

$$L_z = -i\hbar\frac{\partial}{\partial \phi}$$

12.2.4. Rederive the equivalent of Eq. (12.2.23) keeping terms of order $\varepsilon_x\varepsilon_z^2$. (You may assume $\varepsilon_y = 0$.) Use this information to rewrite Eq. (12.2.24) to order $\varepsilon_x\varepsilon_z^2$. By equating coefficients of this term deduce the constraint

$$-2L_zP_xL_z + P_xL_z^2 + L_z^2P_x = \hbar^2 P_x$$

This seems to conflict with statement (1) made above, but not really, in view of the identity

$$-2\Lambda\Omega\Lambda + \Omega\Lambda^2 + \Lambda^2\Omega \equiv [\Lambda, [\Lambda, \Omega]]$$

Using the identity, verify that the new constraint coming from the $\varepsilon_x\varepsilon_z^2$ term is satisfied given the commutation relations between $P_x$, $P_y$, and $L_z$.

Tracing the steps outlined in the text, we consider the following sequence of operators

$$U[R(-\varepsilon_z\mathbf{k})]T(-\varepsilon_x\mathbf{i})U[R(\varepsilon_z\mathbf{k})]T(\varepsilon_x\mathbf{i})$$

Applied to a point $(x, y)$, this has the effect of

$$\begin{aligned}\begin{bmatrix}x\\y\end{bmatrix} &\to \begin{bmatrix}x+\varepsilon_x\\y\end{bmatrix}\\ &\to \begin{bmatrix}(x+\varepsilon_x)-y\varepsilon_z\\(x+\varepsilon_x)\varepsilon_z+y\end{bmatrix}\\ &\to \begin{bmatrix}x-y\varepsilon_z\\(x+\varepsilon_x)\varepsilon_z+y\end{bmatrix}\\ &\to \begin{bmatrix}(x-y\varepsilon_z)+(x\varepsilon_z+\varepsilon_x\varepsilon_z+y)\varepsilon_z\\-(x-y\varepsilon_z)\varepsilon_z+x\varepsilon_z+\varepsilon_x\varepsilon_z+y\end{bmatrix}\\ &= \begin{bmatrix}x(1+\varepsilon_z^2)+\varepsilon_x\varepsilon_z^2\\y(1+\varepsilon_z^2)+\varepsilon_x\varepsilon_z\end{bmatrix}\end{aligned}$$

Writing this out in terms of operators, we see that we must have

$$\left(I+\frac{i}{\hbar}\varepsilon_zL_z\right)\left(I+\frac{i}{\hbar}\varepsilon_xP_x\right)\left(I-\frac{i}{\hbar}\varepsilon_zL_z\right)\left(I-\frac{i}{\hbar}\varepsilon_xP_x\right) = I + I\varepsilon_z^2 - \frac{i}{\hbar}\varepsilon_x\varepsilon_z^2P_x - \frac{i}{\hbar}\varepsilon_x\varepsilon_zP_y$$

We can expand the lefthand side (keeping terms up to $\mathcal{O}(\varepsilon^3)$) to find

$$\frac{i}{\hbar}\frac{\varepsilon_x^2\varepsilon_z}{\hbar^2}[L_z,P_x]P_x + \frac{i}{\hbar}\frac{\varepsilon_x\varepsilon_z^2}{\hbar^2}L_z[P_x,L_z] + \frac{\varepsilon_x^2}{\hbar^2}P_x^2 + \frac{\varepsilon_x\varepsilon_z}{\hbar^2}[P_x,L_z] + \frac{\varepsilon_z^2}{\hbar^2}L_z^2 + I$$

As this problem is formulated, I believe it is unsolvable. At the very least, there is some necessary step that cannot be found by looking at the mathematics, as using a CAS yields multiple untrue requirements.

## 12.3 The Eigenvalue Problem of $L_z$

12.3.1. Provide the steps linking Eq. (12.3.5) to Eq. (12.3.6).

Imposing the Hermiticity of $L_z$ gives

$$-i\hbar\int_0^\infty\int_0^{2\pi}\psi_1^*\frac{\partial\psi_2}{\partial\phi}\rho\,\mathrm{d}\phi\,\mathrm{d}\rho = \left[-i\hbar\int_0^\infty\int_0^{2\pi}\psi_2^*\frac{\partial\psi_1}{\partial\phi}\rho\,\mathrm{d}\phi\,\mathrm{d}\rho\right]^*$$

$$= i\hbar \int_0^\infty \int_0^{2\pi} \psi_2 \frac{\partial \psi_1^*}{\partial \phi} \rho \, \mathrm{d}\phi \, \mathrm{d}\rho$$

$$= i\hbar \int_0^\infty \left(\psi_1^* \psi_2\right)\Big|_{\phi=0}^{\phi=2\pi} \rho \, \mathrm{d}\rho - i\hbar \int_0^\infty \int_0^{2\pi} \psi_1^* \frac{\partial \psi_2}{\partial \phi} \rho \, \mathrm{d}\phi \, \mathrm{d}\rho$$

Clearly, this equality holds only if

$$\psi_1^*(\rho, 0)\psi_2(\rho, 0) = \psi_1^*(\rho, 2\pi)\psi_2(\rho, 2\pi)$$

which, given each $\psi_i$ is arbitrary, implies that

$$\psi(\rho, 0) = \psi(\rho, 2\pi).$$

12.3.2. Let us try to deduce the restriction on $l_z$ from another angle. Consider a superposition of two allowed $l_z$ eigenstates:

$$\psi(\rho, \phi) = A(\rho)e^{i\phi l_z/\hbar} + B(\rho)e^{i\phi l_z'/\hbar}$$

By demanding that upon a $2\pi$ rotation we get the same physical state (not necessarily the same state vector), show that $l_z - l_z' = m\hbar$, where $m$ is an integer. By arguing on the grounds of symmetry that the allowed values of $l_z$ must be symmetric about zero, show that these values are *either* $\ldots, 3\hbar/2, \hbar/2, -\hbar/2, -3\hbar/2, \ldots$ or $\ldots, 2\hbar, \hbar, 0 - \hbar, -2\hbar, \ldots$. It is not possible to restrict $l_z$ any further this way.

The physical state of the system is described by its probability distribution,

$$|\psi(\rho, \phi)|^2 = A^2(\rho) + A(\rho)B^*(\rho)e^{i\phi(l_z - l_z')/\hbar} + A^*(\rho)B(\rho)e^{-i\phi(l_z - l_z')/\hbar} + B(\rho)^2$$

In order for this to remain undisturbed under a rotation by $2\pi$, we must have

$$e^{i2\pi(l_z - l_z')/\hbar} = 1$$

and

$$e^{-i2\pi(l_z - l_z')/\hbar} = 1$$

or, equivalently,

$$l_z - l_z' = m\hbar, \quad m \in \mathbb{Z}.$$

Given that there is no preference to positive or negative $l_z$ values in nature, the eigenvalues of $L_z$ should be spaced evenly about 0. The only possibilities for $l_z$ that satisfy these two constraints are

$$l_z = m\hbar$$

or

$$l_z = \frac{m\hbar}{2}$$

12.3.3. A particle is described by a wave function

$$\psi(\rho, \phi) = Ae^{-\rho^2/2\Delta^2} \cos^2 \phi$$

Show (by expressing $\cos^2 \phi$ in terms of $\Phi_m$) that

$$P(l_z = 0) = 2/3$$

$$P(l_z = 2\hbar) = 1/6$$
$$P(l_z = -2\hbar) = 1/6$$

(Hint: Argue that the radial part $e^{-\rho^2/2\Delta^2}$ is irrelevant here.)

First, note that we can use

$$\Phi_m(\phi) = (2\pi)^{-1/2} e^{im\phi},$$

to write

$$\begin{aligned}
\cos^2\phi &= \left(\frac{e^{i\phi} + e^{-i\phi}}{2}\right)^2 \\
&= \frac{1}{2} + \frac{e^{i2\phi}}{4} + \frac{e^{-i2\phi}}{4} \\
&= \frac{(2\pi)^{1/2}}{2}\Phi_0(\phi) + \frac{(2\pi)^{1/2}}{4}\Phi_2(\phi) + \frac{(2\pi)^{1/2}}{4}\Phi_{-2}(\phi)
\end{aligned}$$

Now, given the fact that the wave function is separable, we may write $\psi(\rho, \phi) = \Omega(\rho)\theta(\phi)$ and focus only on the angular component, $\theta(\phi)$. We can normalize this as

$$\begin{aligned}
\int_0^{2\pi} |\theta(\phi)|^2 \, \mathrm{d}\phi &= B^2 \int_0^{2\pi} \cos^4(\phi) \, \mathrm{d}\phi \\
&= B^2 \int_0^{2\pi} \left(\frac{1}{2} + \frac{1}{2}\cos(2\phi)\right)^2 \mathrm{d}\phi \\
&= B^2 \int_0^{2\pi} \frac{1}{4} + \frac{1}{2}\cos(2\phi) + \frac{1}{4}\cos^2(2\phi) \, \mathrm{d}\phi \\
&= B^2 \int_0^{2\pi} \frac{1}{4} + \frac{1}{2}\cos(2\phi) + \frac{1}{8} + \frac{1}{8}\cos(4\phi) \, \mathrm{d}\phi \\
&= B^2 \cdot \frac{6\pi}{8}
\end{aligned}$$

or $B = (4/3\pi)^{1/2}$. Putting everything together, the angular wave function is

$$\theta(\phi) = \left(\frac{2}{3}\right)^{1/2} \left(\Phi_0(\phi) + \frac{1}{2}\Phi_2(\phi) + \frac{1}{2}\Phi_{-2}(\phi)\right)$$

The probabilities associated with finding the particle in various states of definite angular momentum are

$$\begin{aligned}
P(l_z = 0) &= \frac{2}{3}\left| \int_0^{2\pi} \Phi_0^*(\phi)\left(\Phi_0(\phi) + \frac{1}{2}\Phi_2(\phi) + \frac{1}{2}\Phi_{-2}(\phi)\right) \mathrm{d}\phi \right|^2 \\
&= \frac{2}{3} \cdot 1 \\
&= \frac{2}{3} \\
P(l_z = 2\hbar) &= \frac{2}{3}\left| \int_0^{2\pi} \Phi_2^*(\phi)\left(\Phi_0(\phi) + \frac{1}{2}\Phi_2(\phi) + \frac{1}{2}\Phi_{-2}(\phi)\right) \mathrm{d}\phi \right|^2 \\
&= \frac{2}{3} \cdot \frac{1}{4} \\
&= \frac{1}{6} \\
P(l_z = -2\hbar) &= \frac{2}{3}\left| \int_0^{2\pi} \Phi_{-2}^*(\phi)\left(\Phi_0(\phi) + \frac{1}{2}\Phi_2(\phi) + \frac{1}{2}\Phi_{-2}(\phi)\right) \mathrm{d}\phi \right|^2
\end{aligned}$$

$$= \frac{2}{3} \cdot \frac{1}{4}$$
$$= \frac{1}{6}$$

12.3.4. A particle is described by a wave function

$$\psi(\rho, \phi) = Ae^{-\rho^2/2\Delta^2}\left(\frac{\rho}{\Delta}\cos\phi + \sin\phi\right)$$

Show that

$$P(l_z = \hbar) = P(l_z = -\hbar) = \tfrac{1}{2}$$

Though it is not required to solve the problem, we first find the normalization factor $A$,

$$\begin{aligned}
&A^2 \int_0^\infty\!\!\int_0^{2\pi} e^{-\rho^2/\Delta^2}\left(\frac{\rho}{\Delta}\cos\phi + \sin\phi\right)^2 \rho \, \mathrm{d}\phi \, \mathrm{d}\rho \\
&= A^2 \int_0^\infty\!\!\int_0^{2\pi} e^{-\rho^2/\Delta^2}\left(\frac{\rho^2}{\Delta^2}\cos^2\phi + \frac{2\rho}{\Delta}\cos\phi\sin\phi + \sin^2\phi\right)\rho \, \mathrm{d}\phi \, \mathrm{d}\rho \\
&= A^2 \int_0^\infty\!\!\int_0^{2\pi} e^{-\rho^2/\Delta^2}\left[\frac{\rho^2}{\Delta^2}\left(\frac{1}{2} + \frac{1}{2}\cos(2\phi)\right) + \frac{\rho}{\Delta}\sin(2\phi) + \left(\frac{1}{2} - \frac{1}{2}\cos(2\phi)\right)\right]\rho \, \mathrm{d}\phi \, \mathrm{d}\rho \\
&= \pi A^2 \int_0^\infty e^{-\rho^2/\Delta^2}\left[\frac{\rho^2}{\Delta^2} + 1\right]\rho \, \mathrm{d}\rho \\
&= \pi A^2\left(\frac{1}{\Delta^2}\int_0^\infty \rho^3 e^{-\rho^2/\Delta^2}\mathrm{d}\rho + \int_0^\infty \rho e^{-\rho^2/\Delta^2}\mathrm{d}\rho\right) \\
&= \pi A^2\left(\frac{1}{\Delta^2}\frac{\Delta^4}{2} + \frac{\Delta^2}{2}\right) \\
&= \pi A^2\Delta^2
\end{aligned}$$

i.e. $A = (\pi\Delta^2)^{-1/2}$. Now we rewrite $\psi(\rho, \phi)$ in terms of $\Phi_m(\phi)$ as

$$\begin{aligned}
\psi(\rho, \phi) &= \frac{e^{-\rho^2/2\Delta^2}}{(\pi\Delta^2)^{1/2}}\left(\frac{\rho}{2\Delta}(e^{i\phi} + e^{-i\phi}) - \frac{i}{2}(e^{i\phi} - e^{-i\phi})\right) \\
&= \frac{e^{-\rho^2/2\Delta^2}}{(\pi\Delta^2)^{1/2}}\frac{(2\pi)^{1/2}}{2}\left(\frac{\rho}{\Delta}\Phi_1(\phi) + \frac{\rho}{\Delta}\Phi_{-1}(\phi) - i\Phi_1(\phi) + i\Phi_{-1}(\phi)\right) \\
&= \frac{e^{-\rho^2/2\Delta^2}}{(2\Delta^2)^{1/2}}\left(\Phi_1(\phi)\left[\frac{\rho}{\Delta} - i\right] + \Phi_{-1}(\phi)\left[\frac{\rho}{\Delta} + i\right]\right)
\end{aligned}$$

This is a superposition of two angular momentum eigenstates: one of $l_z = \hbar$ and the other of $l_z = -\hbar$. Since these states are orthogonal to one another, we know

$$\int_0^{2\pi} \Phi_1^*(\phi)\psi(\rho, \phi)\mathrm{d}\phi = \frac{e^{-\rho^2/2\Delta^2}}{(2\Delta^2)^{1/2}}\left(\frac{\rho}{\Delta} - i\right)$$
$$\int_0^{2\pi} \Phi_2^*(\phi)\psi(\rho, \phi)\mathrm{d}\phi = \frac{e^{-\rho^2/2\Delta^2}}{(2\Delta^2)^{1/2}}\left(\frac{\rho}{\Delta} + i\right)$$

Since the magnitude of the inner product of the wave function with the $l_z = \hbar$ and $l_z = -\hbar$ angular momentum eigenfunctions is the same no matter which one we choose, they are equally likely to occur. That is, $P(l_z = \hbar) = P(l_z = -\hbar) = \frac{1}{2}$.

12.3.5. Note that the angular momentum seems to generate a repulsive potential in Eq. (12.3.13). Calculate its gradient and identify it as the centrifugal force.

Isolating $V(\rho)$ gives

$$\begin{aligned}V(\rho) &= \frac{1}{R(\rho)}\Big[ER(\rho) + \frac{\hbar^2}{2\mu}\Big(\frac{\mathrm{d}^2R(\rho)}{\mathrm{d}\rho^2} + \frac{1}{\rho}\frac{\mathrm{d}R(\rho)}{\mathrm{d}\rho} - \frac{m^2}{\rho^2}R(\rho)\Big)\Big] \\ &= E + \frac{\hbar^2}{2\mu}\frac{1}{R(\rho)}\frac{\mathrm{d}^2R(\rho)}{\mathrm{d}\rho^2} + \frac{\hbar^2}{2\mu}\frac{1}{\rho R(\rho)}\frac{\mathrm{d}R(\rho)}{\mathrm{d}\rho} - \frac{\hbar^2}{2\mu}\frac{m^2}{\rho^2}\end{aligned}$$

The gradient of this is

$$\begin{aligned}\frac{\mathrm{d}V(\rho)}{\mathrm{d}\rho}\mathbf{e}_\rho &= \frac{\hbar^2}{2\mu}\Big(-\frac{1}{R^2}\frac{\mathrm{d}^2R}{\mathrm{d}\rho^2}\frac{\mathrm{d}R}{\mathrm{d}\rho} + \frac{1}{R}\frac{\mathrm{d}^3R}{\mathrm{d}\rho^3} - \frac{1}{\rho^2R}\frac{\mathrm{d}R}{\mathrm{d}\rho} - \frac{1}{\rho R^2}\frac{\mathrm{d}R}{\mathrm{d}\rho} + \frac{1}{\rho R}\frac{\mathrm{d}^2R}{\mathrm{d}\rho^2} + 2\frac{m^2}{\rho^3}\Big)\mathbf{e}_\rho \\ &= \frac{\hbar^2}{2\mu}\Big(\frac{\mathrm{d}^3R}{\mathrm{d}\rho^3}\frac{1}{R} + \frac{\mathrm{d}^2R}{\mathrm{d}\rho^2}\Big[\frac{1}{\rho R} - \frac{1}{R^2}\frac{\mathrm{d}R}{\mathrm{d}\rho}\Big] - \frac{\mathrm{d}R}{\mathrm{d}\rho}\Big[\frac{1}{\rho^2R} + \frac{1}{\rho R^2}\Big] + 2\frac{m^2}{\rho^3}\Big)\mathbf{e}_\rho\end{aligned}$$

12.3.6. Consider a particle of mass $\mu$ constrained to move on a circle of radius $a$. Show that $H = L_z^2/2\mu a^2$. Solve the eigenvalue problem of $H$ and interpret the degeneracy.

For a (quasi) free particle constrained to move on a circle of radius $a$, the kinetic energy (and thus classical Hamiltonian) is given by

$$\begin{aligned}T &= \frac{1}{2}\mu v^2 \\ &= \frac{1}{2}\mu a^2\dot{\phi}^2 \\ &= \frac{1}{2}\mu a^2\Big(\frac{\mathrm{d}}{\mathrm{d}t}\tan^{-1}(\tfrac{y}{x})\Big)^2 \\ &= \frac{1}{2}\mu a^2\Big[\frac{1}{1+(\frac{y}{x})^2}\Big(\frac{\dot{y}}{x} - \frac{y}{x^2}\dot{x}\Big)\Big]^2 \\ &= \frac{1}{2}\mu a^2\Big(\frac{x\dot{y} - y\dot{x}}{x^2+y^2}\Big)^2 \\ &= \frac{1}{2}\frac{a^2}{\mu}\Big(\frac{x\mu\dot{y} - y\mu\dot{x}}{a^2}\Big)^2 \\ &= \frac{(xp_y - yp_x)^2}{2\mu a^2}\end{aligned}$$

Identifying the classical angular momentum operator with its quantum variant gives

$$H = \frac{L_z^2}{2\mu a^2}$$

We know that rotationally invariant Hamiltonians permit solutions of the form

$$\psi_m(\rho,\phi) = R_{Em}(\rho)\Phi_m(\phi)$$

From the problem statement, $R_{Em}(\rho) \propto \delta(\rho - a)$. Using the angular coordinate form of $L_z$ produces the time-independent equation

$$-\frac{\hbar^2}{2\mu a^2}\frac{\partial^2}{\partial\phi^2}\psi_m(\rho,\phi) = \frac{m^2\hbar^2}{2\mu a^2}\psi_m(\rho,\phi) = E_m\psi(\rho,\phi)$$

i.e.

$$E_m = \frac{m^2\hbar^2}{2\mu a^2}$$

Clearly, states of $m = k$ have the same energy as states of $m = -k$. This makes sense, as the sign of $m$ corresponds only to the direction of rotation.

12.3.7. (*The Isotropic Oscillator*). Consider the Hamiltonian

$$H = \frac{P_x^2 + P_y^2}{2\mu} + \frac{1}{2}\mu\omega^2(X^2 + Y^2)$$

(1) Convince yourself $[H, L_z] = 0$ and reduce the eigenvalue problem of $H$ to the radial differential equation for $R_{Em}(\rho)$.

(2) Examine the equation as $\rho \to 0$ and show that

$$R_{Em}(\rho) \xrightarrow[\rho\to 0]{} \rho^{|m|}$$

(3) Show likewise that up to powers of $\rho$

$$R_{Em}(\rho) \xrightarrow[\rho\to \infty]{} e^{-\mu\omega\rho^2/2\hbar}$$

So assume that $R_{Em}(\rho) = \rho^{|m|}e^{-\mu\omega\rho^2/2\hbar}U_{Em}(\rho)$.

(4) Switch to dimensionless variables $\varepsilon = E/\hbar\omega$, $y = (\mu\omega/\hbar)^{1/2}\rho$.

(5) Convert the equation for $R$ into an equation for $U$. (I suggest proceeding in two stages: $R = y^{|m|}f$, $f = e^{-y^2/2}U$.) You should end up with

$$U'' + \left[\left(\frac{2|m|+1}{y}\right) - 2y\right]U' + (2\varepsilon - 2|m| - 2)U = 0$$

(6) Argue that a power series for $U$ of the form

$$U(y) = \sum_{r=0}^{\infty} C_r y^r$$

will lead to a *two-term* recursion relation.

(7) Find the relation between $C_{r+2}$ and $C_r$. Argue that the series must terminate at some finite $r$ if the $y \to \infty$ behavior of the solution is to be acceptable. Show that $\varepsilon = r + |m| + 1$ leads to termination after $r$ terms. Now argue that $r$ is necessarily even—i.e., $r = 2k$. (Show that if $r$ is odd, the behavior of $R$ as $\rho \to 0$ is not $\rho^{|m|}$.) So finally you must end up with

$$E = (2k + |m| + 1)\hbar\omega, \qquad k = 0, 1, 2, \ldots$$

Define $n = 2k + |m|$, so that

$$E_n = (n+1)\hbar\omega$$

(8) For a given $n$, what are the allowed values of $|m|$? Given this information show that for a given $n$, the degeneracy is $n + 1$. Compare this to what you found in Cartesian coordinates (Exercise 10.2.2).

(9) Write down all the normalized eigenfunctions corresponding to $n = 0, 1$.

(10) Argue that the $n = 0$ function *must* equal the corresponding one found in Cartesian coordinates. Show that the two $n = 1$ solutions are linear combinations of their counterparts in Cartesian coordinates. Verify that the parity of the states is $(-1)^n$ as you found in Cartesian coordinates.

First, we compute the commutators of squared state variables with $L_z$,

$$\begin{aligned}
[X^2, L_z] &= X[X, L_z] + [X, L_z]X \\
&= -i\hbar XY - i\hbar YX \\
&= -2i\hbar XY \\
[Y^2, L_z] &= Y[Y, L_z] + [Y, L_z]Y \\
&= i\hbar YX + i\hbar XY \\
&= 2i\hbar XY \\
[P_x^2, L_z] &= P_x[P_x, L_z] + [P_x, L_z]P_x \\
&= -i\hbar P_x P_y - i\hbar P_y P_x \\
&= -2i\hbar P_x P_y \\
[P_y^2, L_z] &= P_y[P_y, L_z] + [P_y, L_z]P_y \\
&= i\hbar P_y P_x + i\hbar P_x P_y \\
&= 2i\hbar P_x P_y
\end{aligned}$$

From this, we note that $[P_x^2 + P_y^2, L_z] = [X^2 + Y^2, L_z] = 0$, and thus $[H, L_z] = 0$.

The potential in angular coordinates is $V(\rho) = \frac{1}{2}\mu\omega^2\rho^2$, and thus the radial equation is

$$\Big[-\frac{\hbar^2}{2\mu}\Big(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho} - \frac{m^2}{\rho^2}\Big) + \frac{1}{2}\mu\omega^2\rho^2\Big]R_{Em}(\rho) = ER_{Em}(\rho)$$

As $\rho$ goes to 0, the $\rho^2$ and $E$ terms become negligible, outshined by terms proportional to $\rho^{-1}$ and $\rho^{-2}$. Since we do not know the second derivative of the radial part of the wave function we keep that term as well, giving a limiting equation of

$$\frac{\mathrm{d}^2 R}{\mathrm{d}\rho^2} + \frac{1}{\rho}\frac{\mathrm{d}R}{\mathrm{d}\rho} - \frac{m^2}{\rho^2}R = 0$$

Using the ansatz $R = \rho^k$ gives

$$k(k-1)\rho^{k-2} + k\rho^{k-2} - m^2\rho^{k-2} = 0$$

or $k^2 - m^2 = 0$, i.e. $k = |m|$ (the exponent must be positive to ensure decent behavior at $\rho = 0$). If we now examine the behavior as $\rho$ goes to $\infty$, the $\rho^2$ term is much larger than all others (the term proportional only to $R_{Em}(\rho)$ must go to 0 at infinity), with the possible exception of the term containing $\mathrm{d}^2/\mathrm{d}\rho^2$, so we have

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2 R}{\mathrm{d}\rho^2} + \frac{1}{2}\mu\omega^2\rho^2 R = 0$$

Knowing that $f'(x) \propto xf(x)$ when $f(x) \propto e^{\pm\alpha x^2/2}$, we substitute this into the above to find

$$\begin{aligned}
-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}}{\mathrm{d}\rho}\Big(\pm\alpha\rho e^{\pm\alpha\rho^2/2}\Big) + \frac{1}{2}\mu\omega^2\rho^2 e^{\pm\alpha\rho^2/2} &= \mp\frac{\alpha\hbar^2}{2\mu}e^{\pm\alpha\rho^2/2} - \frac{\alpha^2\hbar^2}{2\mu}\rho^2 e^{\pm\alpha\rho^2/2} + \frac{1}{2}\mu\omega^2\rho^2 e^{\pm\alpha\rho^2/2} \\
&\approx -\frac{\alpha^2\hbar^2}{2\mu}\rho^2 e^{\pm\alpha\rho^2/2} + \frac{1}{2}\mu\omega^2\rho^2 e^{\pm\alpha\rho^2/2}
\end{aligned}$$

where we have used the approximate equality since $\rho^2 e^{\pm\alpha\rho^2/2} \gg e^{\pm\alpha\rho^2/2}$ as $\rho$ goes to infinity. Now, for a well-behaved $R(\rho)$, we must take the negative exponent in our ansatz. Choosing $\alpha = \mu\omega/\hbar$ satisfies the limiting differential equation.

From these limiting answers, we assume

$$R(\rho) = \rho^{|m|} e^{-\mu\omega\rho^2/2\hbar} U(\rho)$$

To switch to the given dimensionless variables, we make the usual replacements, as well as

$$\frac{\mathrm{d}}{\mathrm{d}\rho} \to \Big(\frac{\mu\omega}{\hbar}\Big)^{1/2} \frac{\mathrm{d}}{\mathrm{d}y}$$

Altogether, we find

$$\Big[-\frac{\hbar^2}{2\mu}\Big(\frac{\mu\omega}{\hbar}\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{\mu\omega}{\hbar}\frac{1}{y}\frac{\mathrm{d}}{\mathrm{d}y} - \frac{\mu\omega}{\hbar}\frac{m^2}{y^2}\Big) + \frac{1}{2}\mu\omega^2\frac{\hbar}{\mu\omega}y^2\Big] R_{Em}(\rho) = \varepsilon\hbar\omega R_{Em}(\rho)$$

or

$$\Big(-\frac{\mathrm{d}^2}{\mathrm{d}y^2} - \frac{1}{y}\frac{\mathrm{d}}{\mathrm{d}y} + \frac{m^2}{y^2} + y^2 - 2\varepsilon\Big) R_{Em}(\rho) = 0$$

Taking Shankar's suggestion to first substitute $R = y^{|m|} f$ gives term-wise results of

$$\begin{aligned}
-\frac{\mathrm{d}^2}{\mathrm{d}y^2}\big(y^{|m|}f\big) &= -\frac{\mathrm{d}}{\mathrm{d}y}\big(|m|y^{|m|-1}f + y^{|m|}f'\big) \\
&= -|m|(|m|-1)y^{|m|-2}f - |m|y^{|m|-1}f' - |m|y^{|m|-1}f' - y^{|m|}f'' \\
&= (|m| - m^2)y^{|m|-2}f - 2|m|y^{|m|-1}f' - y^{|m|}f'' \\
-\frac{1}{y}\frac{\mathrm{d}}{\mathrm{d}y}\big(y^{|m|}f\big) &= -|m|y^{|m|-2}f - y^{|m|-1}f' \\
\frac{m^2}{y^2}\big(y^{|m|}f\big) &= m^2 y^{|m|-2} f \\
y^2\big(y^{|m|}f\big) &= y^{|m|+2} f
\end{aligned}$$

and a total result of

$$-y^{|m|}f'' - (2|m|+1)y^{|m|-1}f' + (y^2 - 2\varepsilon)y^{|m|}f = 0$$

Given that

$$\begin{aligned}
f &= Ue^{-y^2/2} \\
f' &= (-yU + U')e^{-y^2/2} \\
f'' &= \big((y^2-1)U - 2yU' + U''\big)e^{-y^2/2}
\end{aligned}$$

we have

$$y^{|m|}\Big(-U'' + \big(2y - \tfrac{2|m|-1}{y}\big)U' + (2|m| + 2 - 2\varepsilon)U\Big)e^{-y^2/2} = 0$$

Dividing by $-y^{|m|}e^{-y^2/2}$ gives the form in the problem statement,

$$U'' + \Big[\Big(\frac{2|m|+1}{y}\Big) - 2y\Big]U' + (2\varepsilon - 2|m| - 2)U = 0$$

Assuming that $U$ can be expanded in a power series,

$$U = \sum_{r=0}^{\infty} C_r y^r$$

the above differential equation becomes

$$
\begin{aligned}
&\sum_{r=0}^{\infty}\Big[C_r r(r-1)y^{r-2}+C_r r(2|m|+1)y^{r-2}-2C_r r y^r+C_r(2\varepsilon-2|m|-2)y^r\Big]\\
&=\sum_{k=0}^{\infty}C_{k+2}\big((k+2)(k+1)+(k+2)(2|m|+1)\big)y^k+\sum_{r=0}^{\infty}C_r(2\varepsilon-2|m|-2r-2)y^r\\
&=\sum_{r=0}^{\infty}\Big[C_{r+2}\Big((r+2)(r+1)+(k+2)(2|m|+1)\Big)+C_r\Big(2\varepsilon-2|m|-2r-2\Big)\Big]y^r\\
&=0
\end{aligned}
$$

This will be true only if

$$
C_{r+2}=C_r\frac{2(|m|+r+1-\varepsilon)}{r^2+2r|m|+4r+4|m|+4}
$$

which is our two-term recurrence relation. Explicitly, given $C_0$ and $C_1$, we have

$$
\begin{aligned}
U(y)=&C_0\Big(1+\frac{|m|+1-\varepsilon}{2|m|+2}y^2+\Big[\frac{|m|+1-\varepsilon}{2|m|+2}\Big]\Big[\frac{|m|+3-\varepsilon}{4|m|+8}\Big]y^4+\cdots\Big)\\
&+C_1\Big(y+\frac{2|m|+4-2\varepsilon}{6|m|+9}y^3+\Big[\frac{2|m|+4-2\varepsilon}{6|m|+9}\Big]\Big[\frac{2|m|+8-2\varepsilon}{10|m|+25}\Big]y^5+\cdots\Big)
\end{aligned}
$$

Now, to ensure that $e^{-y^2/2}$ dies faster than $U(y)$ grows, the parenthesized expressions must contain a finite number of terms. This is because the $C_r$ coefficients die more slowly than $1/r!$—which have the approximate relation $C_{r+2}=C_r/r^2$—and so an untruncated $U(y)$ grows at a faster-than-exponential rate. From inspection, we can guarantee that $U(y)$ contains a finite number of terms by choosing $\varepsilon=|m|+r+1$.

Now, to first order, the odd $r$ terms in $U(y)$ must be made zero to avoid $R(\rho)$ behaving like $\rho^{|m|+1}$ as $\rho\to 0$. Keeping only the terms proportional to $C_0$, we rewrite $\varepsilon=|m|+2k+1$, where $k\in\mathbb{N}$. Defining $n=|m|+2k$ and reinstating units gives

$$
E_n=(n+1)\hbar\omega.
$$

Let us now consider the allowed values of $m$ for a given $n$. Since $n-2k=|m|$, valid $m$ values will each be separated by 2 and centered around the origin. That is,

$$
\begin{aligned}
n=0&\implies m=0\\
n=1&\implies m=-1,1\\
n=2&\implies m=-2,0,2\\
n=3&\implies m=-3,-1,1,3\\
&\vdots
\end{aligned}
$$

Thus, $m$ has $n+1$ degrees of freedom, which is exactly what we found in 10.2.2. The first few eigenfunctions are

$$
\begin{aligned}
\psi_{E0}(\rho,\phi)&=R_{E0}(\rho)\Phi_0(\phi)\\
&=\frac{C_0}{(2\pi)^{1/2}}e^{-\mu\omega\rho^2/2\hbar}\\
\psi_{E(-1)}(\rho,\phi)&=R_{E(-1)}(\rho)\Phi_{-1}(\phi)
\end{aligned}
$$

$$= \frac{C_0}{(2\pi)^{1/2}} \rho e^{-\mu\omega\rho^2/2\hbar} e^{-i\phi}$$

$$\psi_{E1}(\rho,\phi) = R_{E1}(\rho)\Phi_1(\phi)$$

$$= \frac{C_0}{(2\pi)^{1/2}} \rho e^{-\mu\omega\rho^2/2\hbar} e^{i\phi}$$

Given that we have used the same Hamiltonian as that of 10.2.2, all solutions we find here should be linear combinations of those we found before. In particular, the solution for $n = 0$ should be exactly the same, being perfectly isotropic. We find that this is indeed the case, with the $n = 1$ eigenfunctions differing only by $e^{\pm i\phi}$ weighted by $\cos\phi$ or $\sin\phi$.

12.3.8. Consider a particle of mass $\mu$ and charge $q$ in a vector potential

$$\mathbf{A} = \frac{B}{2}(-y\mathbf{i} + x\mathbf{j})$$

(1) Show that the magnetic field is $\mathbf{B} = B\mathbf{k}$.

(2) Show that a classical particle in this potential will move in circles at an angular frequency $\omega_0 = qB/\mu c$.

(3) Consider the Hamiltonian for the corresponding quantum problem:

$$H = \frac{[P_x + qYB/2c]^2}{2\mu} + \frac{[P_y - qXB/2c]^2}{2\mu}$$

Show that $Q = (cP_x + qYB/2)/qB$ and $P = (P_y - qXB/2c)$ are canonical. Write $H$ in terms of $P$ and $Q$ and show that allowed levels are $E = (n + 1/2)\hbar\omega_0$.

(4) Expand $H$ out in terms of the original variables and show

$$H = H\Big(\frac{\omega_0}{2}, \mu\Big) - \frac{\omega_0}{2} L_z$$

where $H(\omega_0/2, \mu)$ is the Hamiltonian for an isotropic two-dimensional harmonic oscillator of mass $\mu$ and frequency $\omega_0/2$. Argue that the same basis that diagonalized $H(\omega_0/2, \mu)$ will diagonalize $H$. By thinking in terms of this basis, show that the allowed levels for $H$ are $E = (k + \frac{1}{2}|m| - \frac{1}{2}m + \frac{1}{2})\hbar\omega_0$, where $k$ is any integer and $m$ is the angular momentum. Convince yourself that you get the same levels from this formula as from the earlier one [$E = (n + 1/2)\hbar\omega_0$]. We shall return to this problem in Chapter 21.

From basic electromagnetism, the magnetic field is given by

$$\begin{aligned}
\mathbf{B} &= \nabla \times \mathbf{A} \\
&= (\partial_y A_z - \partial_z A_y)\mathbf{i} - (\partial_x A_z - \partial_z A_x)\mathbf{j} + (\partial_x A_y - \partial_y A_x)\mathbf{k} \\
&= \Big(\frac{B}{2} + \frac{B}{2}\Big)\mathbf{k} \\
&= B\mathbf{k}
\end{aligned}$$

The force on a classical particle moving in this field is described, in CGS units, by

$$\mathbf{F} = \mu\dot{\mathbf{v}} = \frac{q}{c}\mathbf{v} \times \mathbf{B}$$

which, componentwise, can be written as

$$\mu \begin{bmatrix} \dot{v}_x \\ \dot{v}_y \\ \dot{v}_z \end{bmatrix} = \frac{q}{c} \begin{bmatrix} v_y B \\ -v_x B \\ 0 \end{bmatrix}$$

Taking the time derivative of both sides of this and using the definitions of $\dot{v}_i$ given above, we find

$$\mu\ddot{v}_x = \frac{q}{c}\dot{v}_y B = -\frac{q}{c}\Big(\frac{q}{\mu c}v_x B\Big)B = -\frac{q^2B^2}{\mu c^2}v_x$$
$$\mu\ddot{v}_y = -\frac{q}{c}\dot{v}_x B = -\frac{q}{c}\Big(\frac{q}{\mu c}v_y B\Big)B = -\frac{q^2B^2}{\mu c^2}v_y$$

where we have left out the $z$ component on account of its clear solution. Recognizing both the $x$ and $y$ components of the velocity to be undergoing simple harmonic motion with $\omega_0 = qB/\mu c$, we may write

$$\mathbf{v} = v_0\cos(\omega_0 t + \phi_0)\mathbf{i} - v_0\sin(\omega_0 t + \phi_0)\mathbf{j} + v_1\mathbf{k}$$

which immediately implies the position of the particle is given by

$$\mathbf{x} = \frac{v_0}{\omega_0}\sin(\omega_0 t + \phi_0)\mathbf{i} + \frac{v_0}{\omega_0}\cos(\omega_0 t + \phi_0) + v_1 t\mathbf{k}$$

i.e. the particle gyrates around the magnetic field lines with frequency $\omega_0$.

To confirm the canonical nature of the given $Q$ and $P$ coordinates, we need to verify that $[Q,P] = i\hbar$,

$$\begin{aligned}
[Q,P] &= \frac{1}{qB}[cP_x + \frac{q}{2}YB, P_y - \frac{q}{2c}XB] \\
&= \frac{1}{qB}\Big(c[P_x,P_y] - \frac{q}{2}[P_x,X]B + \frac{q}{2}[Y,P_y]B - \frac{q^2}{4c}[Y,X]B^2\Big) \\
&= \frac{1}{qB}\Big(\frac{qB}{2}(i\hbar) + \frac{qB}{2}(i\hbar)\Big) \\
&= i\hbar
\end{aligned}$$

We can rewrite $H$ in terms of $Q$ and $P$ as

$$H = \Big(\frac{qB}{c}\Big)^2\frac{Q^2}{2\mu} + \frac{P^2}{2\mu} = \frac{P^2}{2\mu} + \frac{1}{2}\mu\omega_0^2 Q^2$$

which is exactly the Hamiltonian of the harmonic oscillator, implying the allowable energy levels are $E = (n + \frac{1}{2})\hbar\omega_0$.

Returning to the original Hamiltonian, we may expand it to find

$$\begin{aligned}
H &= \frac{[P_x + qYB/2c]^2}{2\mu} + \frac{[P_y - qXB/2c]^2}{2\mu} \\
&= \frac{1}{2\mu}\Big[P_x^2 + \frac{qB}{c}P_xY + \Big(\frac{qB}{2c}\Big)^2Y^2\Big] + \frac{1}{2\mu}\Big[P_y^2 - \frac{qB}{c}P_yX + \Big(\frac{qB}{2c}\Big)^2X^2\Big] \\
&= \frac{P_x^2}{2\mu} + \frac{P_y^2}{2\mu} + \frac{1}{2}\mu\Big(\frac{qB}{2\mu c}\Big)^2X^2 + \frac{1}{2}\mu\Big(\frac{qB}{2\mu c}\Big)^2Y^2 - \frac{qB}{2\mu c}\Big(XP_y - YP_x\Big) \\
&= \frac{P_x^2}{2\mu} + \frac{P_y^2}{2\mu} + \frac{1}{2}\mu\Big(\frac{\omega_0}{2}\Big)^2X^2 + \frac{1}{2}\mu\Big(\frac{\omega_0}{2}\Big)^2Y^2 - \frac{\omega_0}{2}L_z \\
&= H\Big(\frac{\omega_0}{2},\mu\Big) - \frac{\omega_0}{2}L_z
\end{aligned}$$

where $H\big(\frac{\omega_0}{2},\mu\big)$ is the isotropic two-dimensional oscillator from with mass $\mu$ and frequency $\omega_0/2$. These components of the overall Hamiltonian share a common, diagonal basis if they commute. Since

$$[X^2 + Y^2, L_z] = [X^2 + Y^2, XP_y - YP_x]$$

$$
\begin{aligned}
&= [X^2, XP_y] - [X^2, YP_x] + [Y^2, XP_y] - [Y^2, YP_x] \\
&= -\Big(X[X,X]P_y + [X,Y]XP_x + YX[X,P_x] + Y[X,P_x]X\Big) \\
&\quad + \Big(Y[Y,X]P_y + [Y,X]YP_y + XY[Y,P_y] + X[Y,P_y]Y\Big) \\
&= -i\hbar YX - i\hbar YX + i\hbar XY + i\hbar XY \\
&= 0
\end{aligned}
$$

and

$$
\begin{aligned}
[P_x^2 + P_y^2, L_z] &= [P_x^2 + P_y^2, XP_y - YP_x] \\
&= [P_x^2, XP_y] - [P_x^2, YP_x] + [P_y^2, XP_y] - [P_y^2, YP_x] \\
&= \Big(P_x[P_x,X]P_y + [P_x,X]P_xP_y + [X,P_x]P_xP_y + X[P_x,P_y]P_x\Big) \\
&\quad - \Big(P_y[P_y,Y]P_x + [P_y,Y]P_yP_x + [Y,P_y]P_yP_x + Y[P_y,P_x]P_y\Big) \\
&= -i\hbar P_xP_y - i\hbar P_xP_y + i\hbar P_xP_y + i\hbar P_yP_x + i\hbar P_yP_x - i\hbar P_yP_x \\
&= 0
\end{aligned}
$$

the two parts of the Hamiltonian *do* commute, and hence can be diagonalize by a common basis. Given that the eigenfunctions of $H\big(\frac{\omega_0}{2}, \mu\big)$ can be written as $R(\rho)\Phi(\phi)$ (where $\Phi(\phi)$ are the eigenfunctions of $L_z$) and $L_z$ commutes with any function of $\rho$, it is clear that the two parts of the Hamiltonian can, more specifically, be diagonalized by the same basis as that found in the previous problems on the isotropic two-dimensional oscillator. If we apply this Hamiltonian to a state built from that basis, we find

$$
\begin{aligned}
H|\psi_{Em}\rangle &= H\Big(\frac{\omega_0}{2}, \mu\Big)|\psi_{Em}\rangle - \frac{\omega_0}{2}L_z|\psi_{Em}\rangle \\
&= (2k + |m| + 1)\frac{\hbar\omega_0}{2}|\psi_{Em}\rangle - \frac{\omega_0}{2}m\hbar|\psi_{Em}\rangle \\
&= \Big(k + \frac{1}{2}|m| - \frac{1}{2}m + \frac{1}{2}\Big)\hbar\omega_0|\psi_{Em}\rangle
\end{aligned}
$$

which implies the energy is quantized as

$$
E = \Big(k + \frac{1}{2}|m| - \frac{1}{2}m + \frac{1}{2}\Big)\hbar\omega_0
$$

Since $k \in \mathbb{N}$ and $|m| - m \geq 0$, this expression gives the exact same energy levels as $E = (n + 1/2)\hbar\omega_0$.

## 12.4 Angular Momentum in Three Dimensions

12.4.1. (1) Verify that Eqs. (12.4.9) and Eq. (12.4.8) are equivalent, given the definition of $\varepsilon_{ijk}$.

(2) Let $U_1$, $U_2$, and $U_3$ be three energy eigenfunctions of a single particle in some potential. Construct the wave function $\psi_A(x_1, x_2, x_3)$ fo three fermions in this potential, one of which is in $U_1$, one in $U_2$, and one in $U_3$, using the $\varepsilon_{ijk}$ tensor.

Since

$$
\mathbf{c} = c_x\mathbf{i} + c_y\mathbf{j} + c_z\mathbf{k} = \mathbf{a} \times \mathbf{b}
$$

$$
\begin{aligned}
&= \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix} \\
&= (a_y b_z - a_z b_y)\mathbf{i} + (a_z b_x - a_x b_z)\mathbf{j} + (a_x b_y - a_y b_x)\mathbf{k}
\end{aligned}
$$

we may write

$$
\begin{aligned}
c_1 &= a_2 b_3 - a_3 b_2 \\
c_2 &= a_3 b_1 - a_1 b_3 \\
c_3 &= a_1 b_2 - a_2 b_1
\end{aligned}
$$

If we want to find each $c_i$ with (12.4.9), we evaluate

$$
\begin{aligned}
c_1 &= \sum_{j=1}^{3} \sum_{k=1}^{3} \varepsilon_{1jk} a_j b_k \\
&= \varepsilon_{123} a_2 b_3 + \varepsilon_{132} a_3 b_2 \\
&= a_2 b_3 - a_3 b_2 \\
c_2 &= \sum_{j=1}^{3} \sum_{k=1}^{3} \varepsilon_{2jk} a_j b_k \\
&= \varepsilon_{213} a_1 b_3 + \varepsilon_{231} a_3 b_1 \\
&= -a_1 b_3 + a_3 b_1 \\
c_3 &= \sum_{j=1}^{3} \sum_{k=1}^{3} \varepsilon_{3jk} a_j b_k \\
&= \varepsilon_{312} a_1 b_2 + \varepsilon_{321} a_2 b_1 \\
&= a_1 b_2 - a_2 b_1
\end{aligned}
$$

which is equivalent to the first set of $c_i$ values.

For the second part of this problem, we are looking to write a wavefunction that is completely antisymmetric with respect to $U_1$, $U_2$, and $U_3$. This can be done with the antisymmetric tensor via

$$
\psi_A(x_1, x_2, x_3) = \frac{1}{6} \varepsilon_{ijk} U_i(x_1) U_j(x_2) U_k(x_3)
$$

where we have invoked the Einstein summation convention. The 1/6 is present for normalization purposes.

12.4.2. (1) Verify Eq. (12.4.2) by first constructing the $3 \times 3$ matrices corresponding to $R(\varepsilon_x \mathbf{i})$ and $R(\varepsilon_y \mathbf{j})$, to order $\varepsilon$.

(2) Provide the steps connecting Eqs. (12.4.3) and (12.4.4a).

(3) Verify that $L_x$ and $L_y$ defined in Eq. (12.4.1) satisfy Eq. (12.4.4a). The proof for other commutators follows by cyclic permutation.

If we define positive rotations as anticlockwise, the requested rotation matrices are

$$R(\varepsilon_x\mathbf{i}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varepsilon_x & -\sin\varepsilon_x \\ 0 & \sin\varepsilon_x & \cos\varepsilon_x \end{bmatrix}$$
$$R(\varepsilon_y\mathbf{j}) = \begin{bmatrix} \cos\varepsilon_y & 0 & \sin\varepsilon_y \\ 0 & 1 & 0 \\ -\sin\varepsilon_y & 0 & \cos\varepsilon_y \end{bmatrix}$$

As we take both $\varepsilon_x$ and $\varepsilon_y$ to 0, these become

$$\lim_{\varepsilon_x\to 0} R(\varepsilon_x\mathbf{i}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -\varepsilon_x \\ 0 & \varepsilon_x & 1 \end{bmatrix}$$
$$\lim_{\varepsilon_y\to 0} R(\varepsilon_y\mathbf{j}) = \begin{bmatrix} 1 & 0 & \varepsilon_y \\ 0 & 1 & 0 \\ -\varepsilon_y & 0 & 1 \end{bmatrix}$$

We can now write out (12.4.2) in matrix form as

$$\begin{aligned}
R(-\varepsilon_y\mathbf{j})R(-\varepsilon_x\mathbf{i})R(\varepsilon_y\mathbf{j})R(\varepsilon_x\mathbf{i}) &= \begin{bmatrix} 1 & 0 & -\varepsilon_y \\ 0 & 1 & 0 \\ \varepsilon_y & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \varepsilon_x \\ 0 & -\varepsilon_x & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & \varepsilon_y \\ 0 & 1 & 0 \\ -\varepsilon_y & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -\varepsilon_x \\ 0 & \varepsilon_x & 1 \end{bmatrix} \\
&= \begin{bmatrix} 1 & \varepsilon_x\varepsilon_y & -\varepsilon_y \\ 0 & 1 & \varepsilon_x \\ \varepsilon_y & -\varepsilon_x & 1 \end{bmatrix} \begin{bmatrix} 1 & \varepsilon_x\varepsilon_y & \varepsilon_y \\ 0 & 1 & -\varepsilon_x \\ -\varepsilon_y & \varepsilon_x & 1 \end{bmatrix} \\
&= \begin{bmatrix} 1+\varepsilon_y^2 & \varepsilon_x\varepsilon_y & -\varepsilon_x^2\varepsilon_y \\ -\varepsilon_x\varepsilon_y & 1+\varepsilon_x^2 & 0 \\ 0 & \varepsilon_x\varepsilon_y^2 & \varepsilon_y^2+\varepsilon_x^2+1 \end{bmatrix} \\
&\approx \begin{bmatrix} 1 & \varepsilon_x\varepsilon_y & 0 \\ -\varepsilon_x\varepsilon_y & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= R(-\varepsilon_x\varepsilon_y\mathbf{k})
\end{aligned}$$

where the last line follows from the fact that

$$\lim_{\varepsilon_z\to 0} R(\varepsilon_z\mathbf{k}) = \lim_{\varepsilon_z\to 0} \begin{bmatrix} \cos\varepsilon_z & -\sin\varepsilon_z & 0 \\ \sin\varepsilon_z & \cos\varepsilon_z & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & -\varepsilon_z & 0 \\ \varepsilon_z & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Starting from (12.4.3), we have

$$\begin{aligned}
U[R(-\varepsilon_y\mathbf{j})]\cdots U[R(\varepsilon_x\mathbf{i})] &= e^{i\varepsilon_y L_y/\hbar} e^{i\varepsilon_x L_x/\hbar} e^{-i\varepsilon_y L_y/\hbar} e^{-i\varepsilon_x L_x/\hbar} \\
&\approx (1 + \tfrac{i\varepsilon_y}{\hbar}L_y)(1 + \tfrac{i\varepsilon_x}{\hbar}L_x)(1 - \tfrac{i\varepsilon_y}{\hbar}L_y)(1 - \tfrac{i\varepsilon_x}{\hbar}L_x) \\
&= (1 + \tfrac{i\varepsilon_y}{\hbar}L_y + \tfrac{i\varepsilon_x}{\hbar}L_x - \tfrac{\varepsilon_x\varepsilon_y}{\hbar^2}L_yL_x)(1 - \tfrac{i\varepsilon_y}{\hbar}L_y - \tfrac{i\varepsilon_x}{\hbar}L_x - \tfrac{\varepsilon_x\varepsilon_y}{\hbar^2}L_yL_x) \\
&= 1 - \tfrac{i\varepsilon_y}{\hbar}L_y - \tfrac{i\varepsilon_x}{\hbar}L_x - \tfrac{\varepsilon_x\varepsilon_y}{\hbar^2}L_yL_x \\
&\quad + \tfrac{i\varepsilon_y}{\hbar}L_y + \tfrac{\varepsilon_y^2}{\hbar^2}L_y^2 + \tfrac{\varepsilon_x\varepsilon_y}{\hbar^2}L_yL_x - \tfrac{i\varepsilon_x\varepsilon_y^2}{\hbar^3}L_y^2L_x \\
&\quad + \tfrac{i\varepsilon_x}{\hbar}L_x + \tfrac{\varepsilon_x\varepsilon_y}{\hbar^2}L_xL_y + \tfrac{\varepsilon_x^2}{\hbar^2}L_x^2 - \tfrac{i\varepsilon_x^2\varepsilon_y}{\hbar^3}L_xL_yL_x \\
&\quad - \tfrac{\varepsilon_x\varepsilon_y}{\hbar^2}L_yL_x + \tfrac{i\varepsilon_x\varepsilon_y^2}{\hbar^3}L_yL_xL_y + \tfrac{i\varepsilon_x^2\varepsilon_y}{\hbar^3}L_yL_x^2 + \tfrac{\varepsilon_x^2\varepsilon_y^2}{\hbar^4}L_yL_xL_yL_x
\end{aligned}$$

After canceling terms and neglecting those of order $\varepsilon_x^2$ or $\varepsilon_y^2$, we find

$$\begin{aligned}U[R(-\varepsilon_y\mathbf{j})]U[R(-\varepsilon_x\mathbf{i})]U[R(\varepsilon_y\mathbf{j})]U[R(\varepsilon_x\mathbf{i})] &\approx 1+\tfrac{\varepsilon_x\varepsilon_y}{\hbar^2}L_xL_y-\tfrac{\varepsilon_x\varepsilon_y}{\hbar^2}L_yL_x\\ &=1+\tfrac{\varepsilon_x\varepsilon_y}{\hbar^2}[L_x,L_y]\\ &=U[R(-\varepsilon_x\varepsilon_y\mathbf{k})]\end{aligned}$$

which only works if

$$[L_x,L_y]=i\hbar L_z$$

To verify that this is actually the case, we compute

$$\begin{aligned}[L_x,L_y] &=[YP_z-ZP_y,ZP_x-XP_z]\\ &=[YP_z,ZP_x]-[YP_z,XP_z]-[ZP_y,ZP_x]+[ZP_y,XP_z]\\ &=[YP_z,ZP_x]+[ZP_y,XP_z]\\ &=Y[P_z,Z]P_x+[Y,Z]P_zP_x+ZY[P_z,P_x]+Z[Y,P_x]P_z\\ &\quad+Z[P_y,X]P_z+[Z,X]P_yP_z+XZ[P_y,P_z]+X[Z,P_z]P_y\\ &=-i\hbar YP_x+i\hbar XP_y\\ &=i\hbar(XP_y-YP_x)\\ &=i\hbar L_z\end{aligned}$$

12.4.3. We would like to show that $\hat{\theta}\cdot\mathbf{L}$ generates rotations about the axis parallel to $\hat{\theta}$. Let $\delta\boldsymbol{\theta}$ be an infinitesimal rotation parallel to $\boldsymbol{\theta}$.

(1) Show that when a vector $\mathbf{r}$ is rotated by an angle $\delta\boldsymbol{\theta}$, it changes to $\mathbf{r}+\delta\boldsymbol{\theta}\times\mathbf{r}$. (It might help to start with $\mathbf{r}\perp\delta\boldsymbol{\theta}$ and then generalize.)

(2) We therefore demand that (to first order, as usual)

$$\psi(\mathbf{r})\xrightarrow[U[R(\delta\boldsymbol{\theta})]]{}\psi(\mathbf{r}-\delta\boldsymbol{\theta}\times\mathbf{r})=\psi(\mathbf{r})-(\delta\boldsymbol{\theta}\times\mathbf{r})\cdot\nabla\psi$$

Comparing to $U[R(\delta\boldsymbol{\theta})]=I-(i\delta\theta/\hbar)L_{\hat{\theta}}$, show that $L_{\hat{\theta}}=\hat{\theta}\cdot\mathbf{L}$.

We can encode a rotation of $\theta$ about an arbitrary axis via

$$R(\theta\boldsymbol{\theta})=R(-\phi_z\mathbf{k})R(-\phi_y\mathbf{j})R(\theta\mathbf{i})R(\phi_y\mathbf{j})R(\phi_z\mathbf{k})$$

where $\phi_y$ and $\phi_z$ are suitably chosen to align the rotation axis first within the $x$-$z$ plane, and then along the $x$ axis. That is, if the rotation axis is given by $\mathbf{u}=\begin{bmatrix}u_x & u_y & u_z\end{bmatrix}^T$ (where $\|\mathbf{u}\|=1$), then $R(\phi_z\mathbf{k})$ should zero out $y$ component and $R(\phi_y\mathbf{j})$ should zero out the (resulting) $z$ component. Since

$$\begin{aligned}R(\phi_z\mathbf{k})\mathbf{u} &=\begin{bmatrix}\cos\phi_z & -\sin\phi_z & 0\\ \sin\phi_z & \cos\phi_z & 0\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}u_x\\ u_y\\ u_z\end{bmatrix}\\ &=\begin{bmatrix}u_x\cos\phi_z-u_y\sin\phi_z\\ u_x\sin\phi_z+u_y\cos\phi_z\\ u_z\end{bmatrix}\end{aligned}$$

this first condition is satisfied when

$$u_x\sin\phi_z+u_y\cos\phi_z=0$$

i.e. $\tan\phi_z = -u_y/u_x$. Since rotations preserve length, we know immediately the this rotation must take $\mathbf{u}$ to $\mathbf{u} = \begin{bmatrix}(u_x^2+u_y^2)^{1/2} & 0 & u_z\end{bmatrix}^T$. Applying the next rotation moves this vector to

$$\begin{aligned}
R(\phi_y\mathbf{j})\mathbf{u} &= \begin{bmatrix}\cos\phi_y & 0 & \sin\phi_y\\ 0 & 1 & 0\\ -\sin\phi_y & 0 & \cos\phi_y\end{bmatrix}\begin{bmatrix}(u_x^2+u_y^2)^{1/2}\\ 0\\ u_z\end{bmatrix}\\
&= \begin{bmatrix}(u_x^2+u_y^2)^{1/2}\cos\phi_y + u_z\sin\phi_y\\ 0\\ -(u_x^2+u_y^2)^{1/2}\sin\phi_y + u_z\cos\phi_y\end{bmatrix}
\end{aligned}$$

The second condition is met when

$$-(u_x^2+u_y^2)^{1/2}\sin\phi_y + u_z\cos\phi_y = 0$$

or $\tan\phi_y = u_z/(u_x^2+u_y^2)^{1/2}$. Using basic trigonometry, we know

$$\begin{aligned}
\cos\phi_z &= \cos\arctan\left(-\frac{u_y}{u_x}\right) = \frac{u_x}{(u_x^2+u_y^2)^{1/2}}\\
\sin\phi_z &= \sin\arctan\left(-\frac{u_y}{u_x}\right) = -\frac{u_y}{(u_x^2+u_y^2)^{1/2}}\\
\cos\phi_y &= \cos\arctan\left(\frac{u_z}{(u_x^2+u_y^2)^{1/2}}\right) = \frac{(u_x^2+u_y^2)^{1/2}}{(u_x^2+u_y^2+u_z^2)^{1/2}}\\
\sin\phi_y &= \sin\arctan\left(\frac{u_z}{(u_x^2+u_y^2)^{1/2}}\right) = \frac{u_z}{(u_x^2+u_y^2+u_z^2)^{1/2}}
\end{aligned}$$

and so

$$\begin{aligned}
R(\phi_y\mathbf{j})R(\phi_z\mathbf{k}) &= \frac{1}{(1-u_z^2)^{1/2}}\begin{bmatrix}(1-u_z^2)^{1/2} & 0 & u_z\\ 0 & 1 & 0\\ -u_z & 0 & (1-u_z^2)^{1/2}\end{bmatrix}\begin{bmatrix}u_x & u_y & 0\\ -u_y & u_x & 0\\ 0 & 0 & (1-u_z^2)^{1/2}\end{bmatrix}\\
&= \frac{1}{(1-u_z^2)^{1/2}}\begin{bmatrix}u_x(1-u_z^2)^{1/2} & u_y(1-u_z^2)^{1/2} & u_z(1-u_z^2)^{1/2}\\ -u_y & u_x & 0\\ -u_xu_z & -u_yu_z & 1-u_z^2\end{bmatrix}
\end{aligned}$$

Since $R(-\phi_z\mathbf{k})R(-\phi_y\mathbf{j}) = R(\phi_z\mathbf{k})^T R(\phi_y\mathbf{j})^T = [R(\phi_y\mathbf{j})R(\phi_z\mathbf{k})]^T$, we can immediately write

$$R(-\phi_z\mathbf{k})R(-\phi_y\mathbf{j}) = \frac{1}{(1-u_z^2)^{1/2}}\begin{bmatrix}u_x(1-u_z^2)^{1/2} & -u_y & -u_xu_z\\ u_y(1-u_z^2)^{1/2} & u_x & -u_yu_z\\ u_z(1-u_z^2)^{1/2} & 0 & 1-u_z^2\end{bmatrix}$$

Now, when $\delta\theta$ is small, the central $R(\delta\theta\mathbf{i})$ matrix becomes

$$R(\theta\mathbf{i}) = \begin{bmatrix}1 & 0 & 0\\ 0 & 1 & -\delta\theta\\ 0 & \delta\theta & 1\end{bmatrix}$$

and so a small rotation about an arbitrary axis can be written as

$$\begin{aligned}
&\frac{1}{1-u_z^2}\begin{bmatrix}u_x(1-u_z^2)^{1/2} & -u_y & -u_xu_z\\ u_y(1-u_z^2)^{1/2} & u_x & -u_yu_z\\ u_z(1-u_z^2)^{1/2} & 0 & 1-u_z^2\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & -\delta\theta\\ 0 & \delta\theta & 1\end{bmatrix}\begin{bmatrix}u_x(1-u_z^2)^{1/2} & u_y(1-u_z^2)^{1/2} & u_z(1-u_z^2)^{1/2}\\ -u_y & u_x & 0\\ -u_xu_z & -u_yu_z & 1-u_z^2\end{bmatrix}\\
&= \frac{1}{1-u_z^2}\begin{bmatrix}u_x(1-u_z^2)^{1/2} & -u_y & -u_xu_z\\ u_y(1-u_z^2)^{1/2} & u_x & -u_yu_z\\ u_z(1-u_z^2)^{1/2} & 0 & 1-u_z^2\end{bmatrix}\begin{bmatrix}u_x(1-u_z^2)^{1/2} & u_y(1-u_z^2)^{1/2} & u_z(1-u_z^2)^{1/2}\\ -u_y+\delta\theta u_xu_z & u_x+\delta\theta u_yu_z & -\delta\theta(1-u_z^2)\\ -u_xu_z-\delta\theta u_y & -u_yu_z+\delta\theta u_x & 1-u_z^2\end{bmatrix}
\end{aligned}$$

$$= \frac{1}{1-u_z^2}\begin{bmatrix} 1-u_z^2 & -\delta\theta u_z(1-u_z^2) & \delta\theta u_y(1-u_z^2) \\ \delta\theta u_z(1-u_z^2) & 1-u_z^2 & -\delta\theta u_x(1-u_z^2) \\ -\delta\theta u_y(1-u_z^2) & \delta\theta u_x(1-u_z^2) & 1-u_z^2 \end{bmatrix}$$
$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \delta\theta \begin{bmatrix} 0 & -u_z & u_y \\ u_z & 0 & -u_x \\ -u_y & u_x & 0 \end{bmatrix}$$

which is the operator $(I + \delta\boldsymbol{\theta}\times)$, i.e. a small rotation of $\mathbf{r}$ by an angle $\delta\theta$ about $\mathbf{u}$ can be written as

$$\mathbf{r} + \delta\boldsymbol{\theta} \times \mathbf{r}$$

This fact can also be seen geometrically, as the rotated vector moves perpendicularly to both $\delta\boldsymbol{\theta}$ and $\mathbf{r}$ with a displacement proportional to $\|\mathbf{r}\|\|\delta\boldsymbol{\theta}\|\sin\delta\theta$, the magnitude of $\delta\boldsymbol{\theta}\times\mathbf{r}$.

To first order, we can Taylor expand $\psi(\mathbf{r})$ under a small rotation as

$$\begin{aligned}
\psi(\mathbf{r} - \delta\boldsymbol{\theta}\times\mathbf{r}) &= \psi(\mathbf{r}) - (\delta\boldsymbol{\theta}\times\mathbf{r})\cdot\nabla\psi \\
&= \psi(\mathbf{r}) - (\delta\theta_y z - \delta\theta_z y)\frac{\partial\psi}{\partial x} - (\delta\theta_z x - \delta\theta_x z)\frac{\partial\psi}{\partial y} - (\delta\theta_x y - \delta\theta_y x)\frac{\partial\psi}{\partial z} \\
&= \psi(\mathbf{r}) - \delta\theta_x\Big(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\Big)\psi(\mathbf{r}) - \delta\theta_y\Big(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\Big)\psi(\mathbf{r}) - \delta\theta_z\Big(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\Big)\psi(\mathbf{r}) \\
&= \Big[I - \frac{i}{\hbar}\Big(\delta\theta_x(YP_z - ZP_y) - \delta\theta_y(ZP_x + XP_z) + \delta\theta_z(XP_y - YP_x)\Big)\Big]\psi(\mathbf{r}) \\
&= \Big(I - \frac{i}{\hbar}\delta\boldsymbol{\theta}\cdot\mathbf{L}\Big)\psi(\mathbf{r})
\end{aligned}$$

Equating this operator to $I - i\delta\theta L_{\hat{\theta}}/\hbar$, we see

$$L_{\hat{\theta}} = \hat{\theta}\cdot\mathbf{L}$$

where $\hat{\theta} = \mathbf{u}$.

12.4.4. Recall that $\mathbf{V}$ is a vector operator if its components $V_i$ transform as

$$U^\dagger[R]V_iU[R] = \sum_j R_{ij}V_j$$

(1) For an infinitesimal rotation $\delta\boldsymbol{\theta}$, show, on the basis of the previous exercise, that

$$\sum_j R_{ij}V_j = V_i + (\delta\boldsymbol{\theta}\times\mathbf{V})_i = V_i + \sum_j\sum_k \varepsilon_{ijk}(\delta\theta)_jV_k$$

(2) Feed in $U[R] = 1 - (i/\hbar)\delta\boldsymbol{\theta}\cdot\mathbf{L}$ into the left-hand side of Eq. (12.4.13) and deduce that

$$[V_i, L_j] = i\hbar\sum_k \varepsilon_{ijk}V_k$$

This is as good a definition of a vector operator as Eq. (12.4.13). By setting $\mathbf{V} = \mathbf{L}$, we can obtain the commutation rules among the $L$'s.

The first part of this exercise was accomplished in the previous question's solution. In indicial notation, a small rotation of $\delta\theta$ about an arbitrary axis $\hat{\theta}$ can be written (in index notation) as

$$V_i + \sum_j \sum_k \varepsilon_{ijk}(\delta\theta)_j V_k$$

Feeding the given $U[R]$ into $U^\dagger[R]V_iU[R]$ and expanding gives

$$\begin{aligned} U^\dagger[R]V_iU[R] &= (1-(i/\hbar)\delta\boldsymbol{\theta}\cdot\mathbf{L})^\dagger V_i(1-(i/\hbar)\delta\boldsymbol{\theta}\cdot\mathbf{L}) \\ &= (1+\tfrac{i}{\hbar}(\delta\theta)_jL_j)V_i(1-\tfrac{i}{\hbar}(\delta\theta)_kL_k) \\ &= V_i + \tfrac{i}{\hbar}(\delta\theta)_jL_jV_i - \tfrac{i}{\hbar}(\delta\theta)_kV_iL_k + \tfrac{1}{\hbar^2}(\delta\theta)_j(\delta\theta)_kL_jV_iL_k \end{aligned}$$

Equating this to the first equation, canceling $V_i$, and dropping the term proportional to $(\delta\theta)^2$ gives the requirement

$$-\tfrac{i}{\hbar}(\delta\theta)_j(V_iL_j - L_jV_i) = -\tfrac{i}{\hbar}(\delta\theta)_j[V_i, L_j] = \varepsilon_{ijk}(\delta\theta)_jV_k$$

or

$$[V_i, L_j] = i\hbar\varepsilon_{ijk}V_k$$

## 12.5 The Eigenvalue Problem of $L^2$ and $L_z$

12.5.1. Consider a vector field $\mathbf{\Psi}(x,y)$ in two dimensions. From Fig. 12.1 it follows that under an infinitesimal rotation $\varepsilon_z\mathbf{k}$,

$$\begin{aligned} \psi_x \to \psi'_x(x,y) &= \psi_x(x+y\varepsilon_z, y-x\varepsilon_z) - \psi_y(x+y\varepsilon_z, y-x\varepsilon_z)\varepsilon_z \\ \psi_y \to \psi'_y(x,y) &= \psi_x(x+y\varepsilon_z, y-x\varepsilon_z)\varepsilon_z + \psi_y(x+y\varepsilon_z, y-x\varepsilon_z) \end{aligned}$$

Show that (to order $\varepsilon_z$)

$$\begin{bmatrix}\psi'_x\\ \psi'_y\end{bmatrix} = \left(\begin{bmatrix}1&0\\0&1\end{bmatrix} - \frac{i\varepsilon_z}{\hbar}\begin{bmatrix}L_z&0\\0&L_z\end{bmatrix} - \frac{i\varepsilon_z}{\hbar}\begin{bmatrix}0&-i\hbar\\ i\hbar&0\end{bmatrix}\right)\begin{bmatrix}\psi_x\\ \psi_y\end{bmatrix}$$

so that

$$\begin{aligned} J_z &= L_z^{(1)}\otimes I^{(2)} + I^{(1)}\otimes S_z^{(2)} \\ &= L_z + S_z \end{aligned}$$

where $I^{(2)}$ is a $2\times 2$ identity matrix with respect to the vector components, $I^{(1)}$ is the identity operator with respect to the argument $(x,y)$ of $\mathbf{\Psi}(x,y)$. This example only illustrates the fact that $J_z = L_z + S_z$ if the wave function is not a scalar. An example of half-integral eigenvalues will be provided when we consider spin in a later chapter. (In the present example, $S_z$ has eigenvalues $\pm\hbar$.)

Since $\varepsilon_k$ is an infinitesimal value, we may Taylor expand the transformed components of $\mathbf{\Psi}(x,y)$ to find

$$\begin{aligned} \psi'_x &= \psi_x + \frac{\partial\psi_x}{\partial x}y\varepsilon_z - \frac{\partial\psi_x}{\partial y}x\varepsilon_z - \Big(\psi_y + \frac{\partial\psi_y}{\partial x}y\varepsilon_z - \frac{\partial\psi_y}{\partial y}x\varepsilon_z\Big)\varepsilon_z \\ &= \psi_x + \frac{i\varepsilon_z}{\hbar}YP_x\psi_x - \frac{i\varepsilon_z}{\hbar}XP_y\psi_x - \psi_y\varepsilon_z \\ &= \psi_x - \frac{i\varepsilon_z}{\hbar}(XP_y - YP_x)\psi_x - \frac{i\varepsilon_z}{\hbar}(-i\hbar\psi_y) \end{aligned}$$

$$
\begin{aligned}
&= \psi_x - \frac{i\varepsilon_z}{\hbar} L_z \psi_x - \frac{i\varepsilon_z}{\hbar}(-i\hbar\psi_y) \\
\psi'_y &= \Big(\psi_x + \frac{\partial \psi_x}{\partial x} y\varepsilon_z - \frac{\partial \psi_x}{\partial y} x\varepsilon_z\Big)\varepsilon_z + \psi_y + \frac{\partial \psi_y}{\partial x} y\varepsilon_z - \frac{\partial \psi_y}{\partial y} x\varepsilon_z \\
&= \psi_x\varepsilon_z + \psi_y + \frac{i\varepsilon_z}{\hbar} Y P_x \psi_y - \frac{i\varepsilon_z}{\hbar} X P_y \psi_y \\
&= \psi_y - \frac{i\varepsilon_z}{\hbar}(X P_y - Y P_x)\psi_y - \frac{i\varepsilon_z}{\hbar}(i\hbar\psi_x)
\end{aligned}
$$

where we have suppressed the arguments to $\psi_x(x,y)$ and $\psi_y(x,y)$. We can collect these equations in matrix form as

$$
\begin{bmatrix} \psi'_x \\ \psi'_y \end{bmatrix} = \left( \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{i\varepsilon_z}{\hbar} \begin{bmatrix} L_z & 0 \\ 0 & L_z \end{bmatrix} - \frac{i\varepsilon_z}{\hbar} \begin{bmatrix} 0 & -i\hbar \\ i\hbar & 0 \end{bmatrix} \right) \begin{bmatrix} \psi_x \\ \psi_y \end{bmatrix}
$$

Now, the matrix containing $L_z$ terms acts to rotate the argument of $\mathbf{\Psi}(x,y)$, while the matrix containing $i\hbar$ terms rotates the components of $\mathbf{\Psi}$ itself. Thinking of these components as two separate 'spaces' (the domain and codomain), we can write the generator of vectorial rotations as

$$
J_z = L_z^{(1)} \otimes I^{(2)} + I^{(1)} \otimes S_z^{(2)} = L_z + S_z
$$

12.5.2. (1) Verify that the $2\times 2$ matrices $J_x^{(1/2)}$, $J_y^{(1/2)}$, and $J_z^{(1/2)}$ obey the commutation rule $[J_x^{(1/2)}, J_y^{(1/2)}] = i\hbar J_z^{(1/2)}$.

(2) Do the same for the $3 \times 3$ matrices $J_i^{(1)}$.

(3) Construct the $4 \times 4$ matrices and verify that

$$
[J_x^{(3/2)}, J_y^{(3/2)}] = i\hbar J_z^{(3/2)}
$$

From what we have learned of the raising and lowering operators $J_+$ and $J_-$, we know that, for a given $j$,

$$
\begin{aligned}
\langle jm'|J_x|jm\rangle &= \langle jm'|\frac{J_+ + J_-}{2}|jm\rangle \\
&= \frac{\hbar}{2}\{\delta_{m',m+1}[(j-m)(j+m+1)]^{1/2} + \delta_{m',m-1}[(j+m)(j-m+1)]^{1/2}\} \\
\langle jm'|J_y|jm\rangle &= \langle jm'|\frac{J_+ - J_-}{2i}|jm\rangle \\
&= \frac{\hbar}{2i}\{\delta_{m',m+1}[(j-m)(j+m+1)]^{1/2} - \delta_{m',m-1}[(j+m)(j-m+1)]^{1/2}\} \\
\langle jm'|J_z|jm\rangle &= \delta_{m',m} m\hbar
\end{aligned}
$$

Recalling that $m$ takes on integer spacing between $-j$ and $j$, we choose the matrix indices $k$ and $l$ (i.e. $[J_x^{(j)}]_{kl}$, etc.) such that $m = j - (l-1)$ and $m' = j - (k-1)$. Both indices start at 1. With this choice, the index forms of our matrices are

$$
\begin{aligned}
[J_x^{(j)}]_{kl} &= \frac{\hbar}{2}\{\delta_{k,l-1}[(l-1)(2j-l+2)]^{1/2} + \delta_{k,l+1}[l(2j-l+1)]^{1/2}\} \\
[J_y^{(j)}]_{kl} &= -\frac{i\hbar}{2}\{\delta_{k,l-1}[(l-1)(2j-l+2)]^{1/2} - \delta_{k,l+1}[l(2j-l+1)]^{1/2}\}
\end{aligned}
$$

$$[J_z^{(j)}]_{kl} = \delta_{kl}(j - l + 1)\hbar$$

We can now produce the set of $2 \times 2$ matrices corresponding to $j = 1/2$.

$$J_x^{(1/2)} = \begin{bmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{bmatrix}$$
$$J_y^{(1/2)} = \begin{bmatrix} 0 & -i\hbar/2 \\ i\hbar/2 & 0 \end{bmatrix}$$
$$J_z^{(1/2)} = \begin{bmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{bmatrix}$$

The commutator is

$$\begin{aligned}
[J_x^{(1/2)}, J_y^{(1/2)}] &= \frac{i\hbar^2}{4} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} - \frac{i\hbar^2}{4} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\
&= \frac{i\hbar^2}{4} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - \frac{i\hbar^2}{4} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \\
&= \frac{i\hbar^2}{4} \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix} \\
&= i\hbar \begin{bmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{bmatrix} \\
&= i\hbar J_z^{(1/2)}
\end{aligned}$$

The set of $3 \times 3$ matrices is

$$J_x^{(1)} = \begin{bmatrix} 0 & \hbar/2^{1/2} & 0 \\ \hbar/2^{1/2} & 0 & \hbar/2^{1/2} \\ 0 & \hbar/2^{1/2} & 0 \end{bmatrix}$$
$$J_y^{(1)} = \begin{bmatrix} 0 & -i\hbar/2^{1/2} & 0 \\ i\hbar/2^{1/2} & 0 & -i\hbar/2^{1/2} \\ 0 & i\hbar/2^{1/2} & 0 \end{bmatrix}$$
$$J_z^{(1)} = \begin{bmatrix} \hbar & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\hbar \end{bmatrix}$$

Their commutator is

$$\begin{aligned}
[J_x^{(1)}, J_y^{(1)}] &= \frac{i\hbar^2}{2} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} - \frac{i\hbar^2}{2} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \\
&= \frac{i\hbar^2}{2} \begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{bmatrix} - \frac{i\hbar^2}{2} \begin{bmatrix} -1 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix} \\
&= \frac{i\hbar^2}{2} \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{bmatrix} \\
&= i\hbar \begin{bmatrix} \hbar & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\hbar \end{bmatrix} \\
&= i\hbar J_z^{(1)}
\end{aligned}$$

Finally, the set of $4 \times 4$ matrices is

$$J_x^{(3/2)} = \frac{\hbar}{2} \begin{bmatrix} 0 & 3^{1/2} & 0 & 0 \\ 3^{1/2} & 0 & 2 & 0 \\ 0 & 2 & 0 & 3^{1/2} \\ 0 & 0 & 3^{1/2} & 0 \end{bmatrix}$$

$$J_y^{(3/2)} = \frac{i\hbar}{2} \begin{bmatrix} 0 & -3^{1/2} & 0 & 0 \\ 3^{1/2} & 0 & -2 & 0 \\ 0 & 2 & 0 & -3^{1/2} \\ 0 & 0 & 3^{1/2} & 0 \end{bmatrix}$$

$$J_z^{(3/2)} = \frac{\hbar}{2} \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix}$$

Their commutation relation is

$$\begin{aligned} [J_x^{(3/2)}, J_y^{(3/2)}] &= \frac{i\hbar^2}{4} \begin{bmatrix} 0 & 3^{1/2} & 0 & 0 \\ 3^{1/2} & 0 & 2 & 0 \\ 0 & 2 & 0 & 3^{1/2} \\ 0 & 0 & 3^{1/2} & 0 \end{bmatrix} \begin{bmatrix} 0 & -3^{1/2} & 0 & 0 \\ 3^{1/2} & 0 & -2 & 0 \\ 0 & 2 & 0 & -3^{1/2} \\ 0 & 0 & 3^{1/2} & 0 \end{bmatrix} \\ &\quad - \frac{i\hbar^2}{4} \begin{bmatrix} 0 & -3^{1/2} & 0 & 0 \\ 3^{1/2} & 0 & -2 & 0 \\ 0 & 2 & 0 & -3^{1/2} \\ 0 & 0 & 3^{1/2} & 0 \end{bmatrix} \begin{bmatrix} 0 & 3^{1/2} & 0 & 0 \\ 3^{1/2} & 0 & 2 & 0 \\ 0 & 2 & 0 & 3^{1/2} \\ 0 & 0 & 3^{1/2} & 0 \end{bmatrix} \\ &= \frac{i\hbar^2}{4} \begin{bmatrix} 3 & 0 & -2 \cdot 3^{1/2} & 0 \\ 0 & 1 & 0 & -2 \cdot 3^{1/2} \\ 2 \cdot 3^{1/2} & 0 & -1 & 0 \\ 0 & 2 \cdot 3^{1/2} & 0 & -3 \end{bmatrix} \\ &\quad - \frac{i\hbar^2}{4} \begin{bmatrix} -3 & 0 & -2 \cdot 3^{1/2} & 0 \\ 0 & -1 & 0 & -2 \cdot 3^{1/2} \\ 2 \cdot 3^{1/2} & 0 & 1 & 0 \\ 0 & 2 \cdot 3^{1/2} & 0 & 3 \end{bmatrix} \\ &= \frac{i\hbar^2}{4} \begin{bmatrix} 6 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & -6 \end{bmatrix} \\ &= i\hbar \cdot \frac{\hbar}{2} \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix} \\ &= i\hbar J_z^{(3/2)} \end{aligned}$$

12.5.3. (1) Show that $\langle J_x \rangle = \langle J_y \rangle = 0$ in a state $|jm\rangle$.

(2) Show that in these states

$$\langle J_x^2 \rangle = \langle J_y^2 \rangle = \tfrac{1}{2}\hbar^2[j(j+1) - m^2]$$

(use symmetry arguments to relate $\langle J_x^2 \rangle$ to $\langle J_y^2 \rangle$).

(3) Check that $\Delta J_x \cdot \Delta J_y$ from part (2) satisfies the inequality imposed by the uncertainty principle [Eq. (9.2.9)].

(4) Show that the uncertainty bound is saturated in the state $|j, \pm j\rangle$.

The first problem is a simple exercise in algebra,

$$\begin{aligned}
\langle J_x\rangle &= \langle jm|\frac{J_+ + J_-}{2}|jm\rangle \\
&= \frac{C_+(j,m)}{2}\langle jm|j,m+1\rangle + \frac{C_-(j,m)}{2}\langle jm|j,m-1\rangle \\
&= 0 \\
\langle J_y\rangle &= \langle jm|\frac{J_+ - J_-}{2i}|jm\rangle \\
&= \frac{C_+(j,m)}{2i}\langle jm|j,m+1\rangle - \frac{C_-(j,m)}{2i}\langle jm|j,m-1\rangle \\
&= 0
\end{aligned}$$

For the second, note that

$$\begin{aligned}
\left(\frac{J_+ + J_-}{2}\right)^2 &= \frac{1}{4}\Big(J_+^2 + J_+J_- + J_-J_+ + J_-^2\Big) \\
&= \frac{1}{4}\Big(J_+^2 + (J^2 - J_z^2 + \hbar J_z) + (J^2 - J_z^2 - \hbar J_z) + J_-^2)\Big) \\
&= \frac{1}{4}\Big(J_+^2 + J_-^2 + 2J^2 - 2J_z^2\Big) \\
\left(\frac{J_+ - J_-}{2i}\right)^2 &= -\frac{1}{4}\Big(J_+^2 - J_+J_- - J_-J_+ + J_-^2\Big) \\
&= -\frac{1}{4}\Big(J_+^2 - (J^2 - J_z^2 + \hbar J_z) - (J^2 - J_z^2 - \hbar J_z) + J_-^2)\Big) \\
&= -\frac{1}{4}\Big(J_+^2 + J_-^2 - 2J^2 + 2J_z^2\Big)
\end{aligned}$$

and so

$$\begin{aligned}
\langle J_x^2\rangle &= \frac{1}{4}\langle jm|J_+^2 + J_-^2 + 2J^2 - 2J_z^2|jm\rangle \\
&= \frac{1}{2}\langle jm|J^2 - J_z^2|jm\rangle \\
&= \frac{1}{2}\langle jm|\hbar^2 j(j+1) - \hbar^2 m^2|jm\rangle \\
&= \frac{1}{2}\hbar^2[j(j+1) - m^2] \\
\langle J_y^2\rangle &= -\frac{1}{4}\langle jm|J_+^2 + J_-^2 - 2J^2 + 2J_z^2|jm\rangle \\
&= \frac{1}{2}\langle jm|J^2 - J_z^2|jm\rangle \\
&= \frac{1}{2}\hbar^2[j(j+1) - m^2]
\end{aligned}$$

Further noting that

$$J_xJ_y = \frac{1}{4i}(J_+ + J_-)(J_+ - J_-)$$

$$
\begin{aligned}
&= \frac{1}{4i}(J_+^2 + J_-J_+ - J_+J_- - J_-^2) \\
J_yJ_x &= \frac{1}{4i}(J_+ - J_-)(J_+ + J_-) \\
&= \frac{1}{4i}(J_+^2 + J_+J_- - J_-J_+ - J_-^2)
\end{aligned}
$$

and thus

$$[J_x, J_y]_+ = J_xJ_y + J_yJ_x = \frac{1}{2i}(J_+^2 - J_-^2) \implies \langle jm|[J_x, J_y]_+|jm\rangle = 0,$$

the uncertainty principle tells us that

$$\Delta J_x \cdot \Delta J_y = \frac{1}{2}\hbar^2|j(j+1) - m^2| \geq \frac{1}{2}|\langle jm|\hbar J_z|jm\rangle| = \frac{|m|\hbar^2}{2}$$

which effectively says

$$j^2 + j \geq |m^2 + m|,$$

a statement we know to be true (as $j$—the total angular momentum—must always be greater than or equal in magnitude to $m$—the $z$ component of angular momentum). Clearly, this reaches an equality when $m = j$.

12.5.4. (1) Argue that the eigenvalues of $J_x^{(i)}$ and $J_y^{(i)}$ are the same as those of $J_z^{(i)}$, namely, $j\hbar, (j-1)\hbar, \ldots, (-j\hbar)$. Generalize the result to $\hat{\theta} \cdot \mathbf{J}^{(j)}$.

(2) Show that

$$(J - j\hbar)[J - (j-1)\hbar][J - (j-2)\hbar] \cdots (J + j\hbar) = 0$$

where $J \equiv \hat{\theta} \cdot \mathbf{J}^{(j)}$. (Hint: In the case $J = J_z$ what happens when both sides are applied to an arbitrary eigenket $|jm\rangle$? What about an arbitrary superposition of such kets?)

(3) It follows from (2) that $J^{2j+1}$ is a linear combination of $J^0, J^1, \ldots, J^{2j}$. Argue that the same goes for $J^{2j+k}$, $k = 1, 2, \ldots$.

As there is no preferred direction and we may have just as easily chosen $\hat{\theta} \cdot \mathbf{J}$ as $J_z$ to be diagonal in the shared $J^2$, $J_i$ basis, all $\hat{\theta} \cdot \mathbf{J}^{(j)}$ must have the same eigenvalues as $J_z^{(j)}$. The fact that

$$(J - j\hbar)[J - (j-1)\hbar][J - (j-2)\hbar] \cdots (J + j\hbar) = 0$$

is a consequence of angular momentum being quantized to some value of $m$ along *any* axis. That is, it is a restatement of the observation made in the first sentence.

The linear dependence of $J^{2j+k}$ can be seen by writing those factors of $J$ whose powers exceed $2j$ as a linear combination of lower powers of $J$.

12.5.5. (*Hard*). Using results from the previous exercise and Eq. (12.5.23), show that

(1) $D^{(1/2)}[R] = \exp(-i\hat{\theta} \cdot \mathbf{J}^{(1/2)}/\hbar) = \cos(\theta/2)I^{1/2} - (2i/\hbar)\sin(\theta/2)\hat{\theta} \cdot \mathbf{J}^{(1/2)}$

(2) $D^{(1)}[R] = \exp(-i\theta_x J_x^{(1)}/\hbar) = (\cos\theta_x - 1)\left(\frac{J_x^{(1)}}{\hbar}\right)^2 - i\sin\theta_x\left(\frac{J_x^{(1)}}{\hbar}\right) + I^{(1)}$

From the previous problem, we know that

$$(\hat{\theta}\cdot\mathbf{J}^{(1/2)} - \tfrac{1}{2}\hbar)(\hat{\theta}\cdot\mathbf{J}^{(1/2)} + \tfrac{1}{2}\hbar) = 0$$

or

$$(\hat{\theta}\cdot\mathbf{J}^{(1/2)})^2 = \tfrac{1}{4}\hbar^2$$

Armed with this piece of information (and calling $\hat{\theta}\cdot\mathbf{J}^{(1/2)} \equiv J$), we can expand $D^{(1/2)}[R]$ as

$$\begin{aligned}
D^{(1/2)}[R] &= \sum_{n=0}^{\infty}\left(\frac{-i\theta}{\hbar}\right)^n J^n \frac{1}{n!} \\
&= I - i\Big(\frac{\theta}{\hbar}\Big)J - \frac{1}{2!}\Big(\frac{\theta}{\hbar}\Big)^2 J^2 + i\frac{1}{3!}\Big(\frac{\theta}{\hbar}\Big)^3 J^3 + \frac{1}{4!}\Big(\frac{\theta}{\hbar}\Big)^4 J^4 - i\frac{1}{5!}\Big(\frac{\theta}{\hbar}\Big)^5 J^5 - \cdots \\
&= \Big[I - \frac{1}{2!}\Big(\frac{\theta}{\hbar}\Big)^2 J^2 + \frac{1}{4!}\Big(\frac{\theta}{\hbar}\Big)^4 J^4 - \cdots\Big] - i\Big[\Big(\frac{\theta}{\hbar}\Big)J - \frac{1}{3!}\Big(\frac{\theta}{\hbar}\Big)^3 J^3 + \frac{1}{5!}\Big(\frac{\theta}{\hbar}\Big)^5 J^5 - \cdots\Big] \\
&= \Big[I - \frac{1}{2!}\Big(\frac{\theta}{\hbar}\Big)^2\Big(\frac{\hbar}{2}\Big)^2 + \frac{1}{4!}\Big(\frac{\theta}{\hbar}\Big)^4\Big(\frac{\hbar}{2}\Big)^4 - \cdots\Big] - i\Big[\Big(\frac{\theta}{\hbar}\Big)J - \frac{1}{3!}\Big(\frac{\theta}{\hbar}\Big)^3\Big(\frac{\hbar}{2}\Big)^2 J + \frac{1}{5!}\Big(\frac{\theta}{\hbar}\Big)^5\Big(\frac{\hbar}{2}\Big)^4 J - \cdots\Big] \\
&= \Big[I - \frac{1}{2!}\Big(\frac{\theta}{2}\Big)^2 + \frac{1}{4!}\Big(\frac{\theta}{2}\Big)^4 - \cdots\Big] - \frac{2i}{\hbar}\Big[\Big(\frac{\theta}{2}\Big) - \frac{1}{3!}\Big(\frac{\theta}{2}\Big)^3 + \frac{1}{5!}\Big(\frac{\theta}{2}\Big)^5 - \cdots\Big]J \\
&= \cos(\theta/2)I^{(1/2)} - (2i/\hbar)\sin(\theta/2)\hat{\theta}\cdot\mathbf{J}^{(1/2)}
\end{aligned}$$

For the second part, we draw upon the previous problem to write

$$(J_x^{(1)} - \hbar)J_x^{(1)}(J_x^{(1)} + \hbar) = 0$$

or

$$(J_x^{(1)})^3 = \hbar^2 J_x^{(1)}$$

Calling $J_x^{(1)} \equiv J$, we find

$$\begin{aligned}
D^{(1)}[R] &= \sum_{n=0}^{\infty}\left(\frac{-i\theta}{\hbar}\right)^n J^n \frac{1}{n!} \\
&= I - i\Big(\frac{\theta}{\hbar}\Big)J - \frac{1}{2!}\Big(\frac{\theta}{\hbar}\Big)^2 J^2 + i\frac{1}{3!}\Big(\frac{\theta}{\hbar}\Big)^3 J^3 + \frac{1}{4!}\Big(\frac{\theta}{\hbar}\Big)^4 J^4 - i\frac{1}{5!}\Big(\frac{\theta}{\hbar}\Big)^5 J^5 - \cdots \\
&= I - i\Big(\frac{\theta}{\hbar}\Big)J - \frac{1}{2!}\Big(\frac{\theta}{\hbar}\Big)^2 J^2 + i\frac{1}{3!}\Big(\frac{\theta}{\hbar}\Big)^3 \hbar^2 J + \frac{1}{4!}\Big(\frac{\theta}{\hbar}\Big)^4 \hbar^2 J^2 - i\frac{1}{5!}\Big(\frac{\theta}{\hbar}\Big)^5 \hbar^4 J - \cdots \\
&= I + \Big[-\frac{1}{2!}\theta^2\frac{J^2}{\hbar^2} + \frac{1}{4!}\theta^4\frac{J^2}{\hbar^2} - \cdots\Big] - i\Big[\theta\frac{J}{\hbar} - \frac{1}{3!}\theta^3\frac{J}{\hbar} + \frac{1}{5!}\theta^5\frac{J}{\hbar} - \cdots\Big] \\
&= I + (1 - \frac{1}{2!}\theta^2 + \frac{1}{4!}\theta^4 - \cdots - 1)\frac{J^2}{\hbar^2} - i\Big[\theta - \frac{1}{3!}\theta^3 + \frac{1}{5!}\theta^5 - \cdots\Big]\frac{J}{\hbar} \\
&= I^{(1)} + (\cos\theta_x - 1)\Big(\frac{J_x^{(1)}}{\hbar}\Big)^2 - i\sin\theta_x\Big(\frac{J_x^{(1)}}{\hbar}\Big)
\end{aligned}$$

12.5.6. Consider the family of states $|jj\rangle, \dots, |jm\rangle, \dots, |j,-j\rangle$. One refers to them as states of the same magnitude but different orientations of angular momentum. If one takes this remark literally, i.e., in the classical sense, one is led to believe that one may rotate these into each other, as is the case for classical states with these properties. Consider, for instance, the family $|1,1\rangle$, $|1,0\rangle$, $|1,-1\rangle$. It may seem, for example, that the state with zero angular momentum along the $z$ axis, $|1,0\rangle$, may be obtained by rotating $|1,1\rangle$ by some suitable ($\frac{1}{2}\pi$?) angle about the $x$ axis. Using $D^{(1)}[R(\theta_x\mathbf{i})]$ from part (2) in the last exercise show that

$$|1,0\rangle \neq D^{(1)}[R(\theta_x\mathbf{i})]|1,1\rangle \quad \text{for any } \theta_x$$

The error stems from the fact that classical reasoning should be applied to $\langle \mathbf{J}\rangle$, which responds to rotations like an ordinary vector, and not directly to $|jm\rangle$, which is a vector in Hilbert space. Verify that $\langle \mathbf{J}\rangle$ responds to rotations like its classical counterpart, by showing that $\langle \mathbf{J}\rangle$ in the state $D^{(1)}[R(\theta_x\mathbf{i})]|1,1\rangle$ is $\hbar[-\sin\theta_x\mathbf{j} + \cos\theta_x\mathbf{k}]$.

It is not too hard to see why we can't always satisfy

$$|jm'\rangle = D^{(j)}[R]|jm\rangle$$

or more generally, for two normalized kets $|\psi_j'\rangle$ and $|\psi_j\rangle$, satisfy

$$|\psi_j'\rangle = D^{(j)}[R]|\psi_j\rangle$$

by any choice of $R$. These abstract equations imply $(2j+1)$ linear, complex relations between the components of $|\psi_j'\rangle$ and $|\psi_j\rangle$ that can't be satisfied by varying $R$, which depends on only three parameters, $\theta_x$, $\theta_y$, and $\theta_z$. (Of course one can find a unitary matrix in $\mathbb{V}_J$ that takes $|jm\rangle$ into $|jm'\rangle$ or $|\psi_j\rangle$ in $\psi_j'\rangle$, but it will not be a *rotation* matrix corresponding to $U[R]$.

Using the results from the previous exercise and (12.5.23), we have

$$\begin{aligned}
D^{(1)}[R(\theta_x\mathbf{i})] &= \frac{1}{\hbar^2}(\cos\theta_x - 1)\begin{bmatrix} 0 & \hbar/2^{1/2} & 0 \\ \hbar/2^{1/2} & 0 & \hbar/2^{1/2} \\ 0 & \hbar/2^{1/2} & 0 \end{bmatrix}^2 - \frac{i}{\hbar}\sin\theta_x \begin{bmatrix} 0 & \hbar/2^{1/2} & 0 \\ \hbar/2^{1/2} & 0 & \hbar/2^{1/2} \\ 0 & \hbar/2^{1/2} & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= (\cos\theta_x - 1)\begin{bmatrix} 1/2 & 0 & 1/2 \\ 0 & 1 & 0 \\ 1/2 & 0 & 1/2 \end{bmatrix} - i\sin\theta_x \begin{bmatrix} 0 & 2^{-1/2} & 0 \\ 2^{-1/2} & 0 & 2^{-1/2} \\ 0 & 2^{-1/2} & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} (\cos\theta_x + 1)/2 & -i\sin(\theta_x)/2^{1/2} & (\cos\theta_x - 1)/2 \\ -i\sin(\theta_x)/2^{1/2} & \cos\theta_x & -i\sin(\theta_x)/2^{1/2} \\ (\cos\theta_x - 1)/2 & -i\sin(\theta_x)/2^{1/2} & (\cos\theta_x + 1)/2 \end{bmatrix}
\end{aligned}$$

where the basis is represented as

$$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = |1,1\rangle, \qquad \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = |1,0\rangle, \qquad \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = |1,-1\rangle$$

Applying the rotation matrix to $|1,1\rangle$ gives

$$D^{(1)}[R(\theta_x\mathbf{i})]|1,1\rangle = \begin{bmatrix} (\cos\theta_x + 1)/2 \\ -i\sin(\theta_x)/2^{1/2} \\ (\cos\theta_x - 1)/2 \end{bmatrix}$$

As the first and third entries cannot be simultaneously nonzero, this operation will never change $|1,1\rangle$ into $|1,0\rangle$.

What of the expectation values of $J_x^{(1)}$, $J_y^{(1)}$, and $J_z^{(1)}$ in this rotated state? For these we have

$$\begin{aligned}
\langle J_x\rangle &= \begin{bmatrix} (\cos\theta_x + 1)/2 & i\sin(\theta_x)/2^{1/2} & (\cos\theta_x - 1)/2 \end{bmatrix} \begin{bmatrix} 0 & \hbar/2^{1/2} & 0 \\ \hbar/2^{1/2} & 0 & \hbar/2^{1/2} \\ 0 & \hbar/2^{1/2} & 0 \end{bmatrix} \begin{bmatrix} (\cos\theta_x + 1)/2 \\ -i\sin(\theta_x)/2^{1/2} \\ (\cos\theta_x - 1)/2 \end{bmatrix} \\
&= \begin{bmatrix} (\cos\theta_x + 1)/2 & i\sin(\theta_x)/2^{1/2} & (\cos\theta_x - 1)/2 \end{bmatrix} \begin{bmatrix} -i\hbar\sin(\theta_x)/2 \\ \hbar\cos\theta_x/2^{1/2} \\ -i\hbar\sin(\theta_x)/2 \end{bmatrix}
\end{aligned}$$

$$
\begin{aligned}
&= -i\hbar(\cos\theta_x - 1)\sin(\theta_x)/4 - i\hbar(\cos\theta_x + 1)\sin(\theta_x)/4 + i\hbar\sin(\theta_x)\cos(\theta_x)/2 \\
&= 0
\end{aligned}
$$

$$
\begin{aligned}
\langle J_y \rangle &= \begin{bmatrix}(\cos\theta_x + 1)/2 & i\sin(\theta_x)/2^{1/2} & (\cos\theta_x - 1)/2\end{bmatrix} \begin{bmatrix} 0 & -i\hbar/2^{1/2} & 0 \\ i\hbar/2^{1/2} & 0 & -i\hbar/2^{1/2} \\ 0 & i\hbar/2^{1/2} & 0 \end{bmatrix} \begin{bmatrix} (\cos\theta_x + 1)/2 \\ -i\sin(\theta_x)/2^{1/2} \\ (\cos\theta_x - 1)/2 \end{bmatrix} \\
&= \begin{bmatrix}(\cos\theta_x + 1)/2 & i\sin(\theta_x)/2^{1/2} & (\cos\theta_x - 1)/2\end{bmatrix} \begin{bmatrix} -\hbar\sin(\theta_x)/2 \\ i\hbar/2^{1/2} \\ \hbar\sin(\theta_x)/2 \end{bmatrix} \\
&= \hbar(\cos\theta_x - 1)\sin(\theta_x)/4 - \hbar(\cos\theta_x + 1)\sin(\theta_x)/4 - \hbar\sin(\theta_x)/2 \\
&= -\hbar\sin\theta_x
\end{aligned}
$$

$$
\begin{aligned}
\langle J_z \rangle &= \begin{bmatrix}(\cos\theta_x + 1)/2 & i\sin(\theta_x)/2^{1/2} & (\cos\theta_x - 1)/2\end{bmatrix} \begin{bmatrix} \hbar & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\hbar \end{bmatrix} \begin{bmatrix} (\cos\theta_x + 1)/2 \\ -i\sin(\theta_x)/2^{1/2} \\ (\cos\theta_x - 1)/2 \end{bmatrix} \\
&= \begin{bmatrix}(\cos\theta_x + 1)/2 & i\sin(\theta_x)/2^{1/2} & (\cos\theta_x - 1)/2\end{bmatrix} \begin{bmatrix} \hbar(\cos\theta_x + 1)/2 \\ 0 \\ -\hbar(\cos\theta_x - 1)/2 \end{bmatrix} \\
&= \hbar[(\cos\theta_x + 1)/2]^2 - \hbar[(\cos\theta_x - 1)/2]^2 \\
&= \hbar\cos^2(\theta_x/2) - \hbar\sin^2(\theta_x/2) \\
&= \hbar\cos\theta_x
\end{aligned}
$$

or, compactly,

$$
\langle \mathbf{J} \rangle = \hbar \begin{bmatrix} 0 \\ -\sin\theta_x \\ \cos\theta_x \end{bmatrix}
$$

where the basis is now in physical space, not Hilbert space. In words, while we are not able to naïvely rotate the state into $|1,0\rangle$, we are able to rotate the expectation value until.

12.5.7. *Euler Angles.* Rather than parameterize an arbitrary rotation by the angle $\boldsymbol{\theta}$, which describes a *single* rotation by $\theta$ about an axis parallel to $\boldsymbol{\theta}$, we may parameterize it by three angles, $\gamma$, $\beta$, and $\alpha$ called *Euler angles*, which define three successive rotations:

$$
U[R(\alpha,\beta,\gamma)] = e^{-i\alpha J_z/\hbar} e^{-i\beta J_y/\hbar} e^{-i\gamma J_z/\hbar}
$$

(1) Construct $D^{(1)}[R(\alpha,\beta,\gamma)]$ explicitly as a product of three $3\times 3$ matrices. (Use the result from Exercise 12.5.5 with $J_x \to J_y$.)

(2)Let it act on $|1,1\rangle$ and show that $\langle \mathbf{J} \rangle$ in the resulting state is

$$
\langle \mathbf{J} \rangle = \hbar(\sin\beta\cos\alpha\mathbf{i} + \sin\beta\sin\alpha\mathbf{j} + \cos\beta\mathbf{k})
$$

(3) Show that for no value of $\alpha$, $\beta$, and $\gamma$ can one rotate $|1,1\rangle$ into just $|1,0\rangle$.

(4) Show that one can always rotate any $|1,m\rangle$ into a linear combination that involves $|1,m'\rangle$, i.e.

$$
\langle 1,m'|D^{(1)}[R(\alpha,\beta,\gamma)]|1,m\rangle \neq 0
$$

for some $\alpha$, $\beta$, $\gamma$ and any $m$, $m'$.

(5) To see that one can occasionally rotate $|jm\rangle$ into $|jm'\rangle$, verify that a 180° rotation about the $y$ axis applied to $|1,1\rangle$ turns it into $|1,-1\rangle$.

The $J_z^{(1)}$ matrix is easy to exponentiate,

$$e^{-i\alpha J_z^{(1)}/\hbar} = \begin{bmatrix} e^{-i\alpha} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e^{i\alpha} \end{bmatrix}, \qquad e^{-i\gamma J_z^{(1)}/\hbar} = \begin{bmatrix} e^{-i\gamma} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e^{i\gamma} \end{bmatrix}$$

The compact form of $e^{-i\beta J_y/\hbar}$ is

$$\begin{aligned}
D^{(1)}[R(\beta\mathbf{j})] &= \frac{1}{\hbar^2}(\cos\beta - 1)\begin{bmatrix} 0 & -i\hbar/2^{1/2} & 0 \\ i\hbar/2^{1/2} & 0 & -i\hbar/2^{1/2} \\ 0 & i\hbar/2^{1/2} & 0 \end{bmatrix}^2 - \frac{i}{\hbar}\sin\beta\begin{bmatrix} 0 & -i\hbar/2^{1/2} & 0 \\ i\hbar/2^{1/2} & 0 & -i\hbar/2^{1/2} \\ 0 & i\hbar/2^{1/2} & 0 \end{bmatrix} \\
&\quad + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= (\cos\beta - 1)\begin{bmatrix} 1/2 & 0 & -1/2 \\ 0 & 1 & 0 \\ -1/2 & 0 & 1/2 \end{bmatrix} + \frac{1}{2^{1/2}}\sin\beta\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} (\cos\beta + 1)/2 & -\sin(\beta)/2^{1/2} & -(\cos\beta - 1)/2 \\ \sin(\beta)/2^{1/2} & \cos\beta & -\sin(\beta)/2^{1/2} \\ -(\cos\beta - 1)/2 & \sin(\beta)/2^{1/2} & (\cos\beta + 1)/2 \end{bmatrix}
\end{aligned}$$

and so

$$\begin{aligned}
D^{(1)}[R(\alpha,\beta,\gamma)] &= \begin{bmatrix} e^{-i\alpha} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e^{i\alpha} \end{bmatrix}\begin{bmatrix} (\cos\beta + 1)/2 & -\sin(\beta)/2^{1/2} & -(\cos\beta - 1)/2 \\ \sin(\beta)/2^{1/2} & \cos\beta & -\sin(\beta)/2^{1/2} \\ -(\cos\beta - 1)/2 & \sin(\beta)/2^{1/2} & (\cos\beta + 1)/2 \end{bmatrix}\begin{bmatrix} e^{-i\gamma} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e^{i\gamma} \end{bmatrix} \\
&= \begin{bmatrix} e^{-i\alpha} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e^{i\alpha} \end{bmatrix}\begin{bmatrix} e^{-i\gamma}(\cos\beta + 1)/2 & -\sin(\beta)/2^{1/2} & -e^{i\gamma}(\cos\beta - 1)/2 \\ e^{-i\gamma}\sin(\beta)/2^{1/2} & \cos\beta & -e^{i\gamma}\sin(\beta)/2^{1/2} \\ -e^{-i\gamma}(\cos\beta - 1)/2 & \sin(\beta)/2^{1/2} & e^{i\gamma}(\cos\beta + 1)/2 \end{bmatrix} \\
&= \begin{bmatrix} e^{-i(\alpha+\gamma)}(\cos\beta + 1)/2 & -e^{-i\alpha}\sin(\beta)/2^{1/2} & -e^{-i(\alpha-\gamma)}(\cos\beta - 1)/2 \\ e^{-i\gamma}\sin(\beta)/2^{1/2} & \cos\beta & -e^{i\gamma}\sin(\beta)/2^{1/2} \\ -e^{i(\alpha-\gamma)}(\cos\beta - 1)/2 & e^{i\alpha}\sin(\beta)/2^{1/2} & e^{i(\alpha+\gamma)}(\cos\beta + 1)/2 \end{bmatrix} \\
&= \begin{bmatrix} e^{-i(\alpha+\gamma)}\cos^2(\beta/2) & -e^{-i\alpha}\sin(\beta)/2^{1/2} & e^{-i(\alpha-\gamma)}\sin^2(\beta/2) \\ e^{-i\gamma}\sin(\beta)/2^{1/2} & \cos\beta & -e^{i\gamma}\sin(\beta)/2^{1/2} \\ e^{i(\alpha-\gamma)}\sin^2(\beta/2) & e^{i\alpha}\sin(\beta)/2^{1/2} & e^{i(\alpha+\gamma)}\cos^2(\beta/2) \end{bmatrix}
\end{aligned}$$

To find $\langle \mathbf{J} \rangle$, we calculate $\langle 1,1|D^{(1)}[R(\alpha,\beta,\gamma)]^\dagger J_i^{(1)} D^{(1)}[R(\alpha,\beta,\gamma)]|1,1\rangle$ for $i = x, y, z$. The algebra is tedious and not particularly enlightening, so we use a CAS to find

$$\begin{aligned}
\langle J_x^{(1)} \rangle &= \hbar\sin\beta\cos\alpha \\
\langle J_y^{(1)} \rangle &= \hbar\sin\alpha\sin\beta \\
\langle J_z^{(1)} \rangle &= \hbar\cos\beta
\end{aligned}$$

i.e.

$$\langle \mathbf{J} \rangle = \hbar(\sin\beta\cos\alpha\mathbf{i} + \sin\beta\sin\alpha\mathbf{j} + \cos\beta\mathbf{k})$$

By examining

$$D^{(1)}[R(\alpha,\beta,\gamma)]|1,1\rangle = \begin{bmatrix} e^{-i(\alpha+\gamma)}\cos^2(\beta/2) \\ e^{-i\gamma}\sin(\beta)/2^{1/2} \\ e^{i(\alpha-\gamma)}\sin^2(\beta/2) \end{bmatrix}$$

we find that the middle entry can never be 1 for any choice of $\alpha$, $\beta$, $\gamma$, i.e. this state can never be $|1,0\rangle$. In fact, when $\beta$ is chosen to be $\pi/2$ (so that the middle entry takes on its largest value), both the first and third entries are nonzero, meaning the closest we can get to $|1,0\rangle$ is a linear combination of states containing a bit of $|1,0\rangle$.

Part 4 follows from the fact that any entry of $D^{(1)}[R(\alpha,\beta,\gamma)]|1,1\rangle$ can be made nonzero through an appropriate choice of $\alpha,\beta,\gamma$, and thus we can always perform a rotation from $|1,m\rangle$ into a state that contains $|1,m'\rangle$. (Of course, the rotated state may contain more than just $|1,m'\rangle$, as we saw above.)

From $D^{(1)}[R(\alpha,\beta,\gamma)]|1,1\rangle$ (see above), it is immediately clear that $\beta=\pi$ takes us from $|1,1\rangle$ to $|1,-1\rangle$, so we may occasionally have the ability to rotate one pure state to another.