PHYS 660 - Quantum Mechanics I

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Contents

Homework 1

Based on problems 1.1, 1.7, 1.10/1.11, 1.14,1.23 of Sakurai's book.

Problem 1
Prove that
$$[AB, CD] = -AC\{D, B\} + A\{C, B\}D - C\{D, A\}B + \{C, A\}DB$$

Solution. Left hand-side:
$$[AB, CD] = ABCD - CDAB$$

Right hand-side:
$$\begin{aligned}
-AC\{D, B\} &+ A\{C, B\}D - C\{D, A\}B + \{C, A\}DB \\
&= -AC(DB + BD) + A(CB + BC)D - C(DA + AD)B + (CA + AC)DB \\
&= -ACDB - ACBD + ACBD + ABCD - CDAB - CADB + CADB + ACDB \\
&= ABCD - CDAB.
\end{aligned}$$

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Problem 2
Consider a Hermitian operator A, (i.e. $A = A^\dagger$). Let $\{|a_i\rangle, i = 1, \ldots, N\}$ be a basis of eigenstates $|a_i\rangle$ of A, with eigenvalues a_i. Assume for simplicity that there is no degeneracy, namely all the a_i are different.

(a) Prove that
$$\prod_{i=1}^{N}(A - a_i) = 0$$

(b) For a given value of i, consider the operator
$$P_i = \prod_{j=1, j\neq i}^{N}\left(\frac{A - a_j}{a_i - a_j}\right)$$
What does P_i do when applied to an arbitrary state?

(c) Illustrate points **(a)** and **(b)** by using the operator S_z of a spin 1/2 system.

(d) Discuss how to modify the formulas if there is a degeneracy in the spectrum of A.

Solution. (a) Since the product is over a complete set, the operator $\prod_{i=1}^{N}(A-a_i) = 0$ will always encounter an element $|a_j\rangle$ such that $a_i = a_j$ in which case the result is zero. Thus, for any state $|\psi\rangle$, we have

$$\begin{aligned}
\prod_{i=1}^{N}(A - a_i)|\psi\rangle &= \prod_{i=1}^{N}(A - a_i)\sum_{j=1}^{N}|a_j\rangle\langle a_j|\psi\rangle \\
&= \sum_{j=1}^{N}\prod_{i=1}^{N}(a_j - a_i)|a_j\rangle\langle a_j|\psi\rangle \\
&= \sum_{j=1}^{N} 0 \\
&= 0.
\end{aligned}$$

(b) If the product instead is over all $a_i \neq a_j$, then the only surviving term in the sum is

$$\prod_{i=1}^{N}(a_j - a_i) |a_j\rangle \langle a_j|\psi\rangle$$

and dividing by the factors $(a_j - a_i)$ just gives the projection of $|\psi\rangle$ on the direction $|a_i\rangle$. Therefore, it is like a projection operator which projects the $|a_i\rangle$ component of $|\psi\rangle$.

(c) For the operator $A = S_z$ and $|a_i\rangle = \{|+\rangle, |-\rangle\}$, we have

$$\prod_{i=1}^{N}(A - a_i) = (S_z - |+\rangle)(S_z - |-\rangle) = \left(S_z - \frac{\hbar}{2}\right)\left(S_z + \frac{\hbar}{2}\right)$$

$$\prod_{j=1, j\neq i}^{N}\left(\frac{A - a_j}{a_i - a_j}\right) = \begin{cases} \left(\frac{S_z - |+\rangle}{|-\rangle - |+\rangle}\right) = \left(\frac{S_z - \hbar/2}{-\hbar}\right), & \text{for } a_j = |+\rangle \\ \left(\frac{S_z - |-\rangle}{|+\rangle - |-\rangle}\right) = \left(\frac{S_z + \hbar/2}{\hbar}\right), & \text{for } a_j = |-\rangle \,. \end{cases}$$

For the first equation, it is easy to see we get $S_z^2 - \frac{\hbar^2}{4} = 0$. For the second equation, we can work them out explicitly

$$\left(\frac{S_z - \hbar/2}{-\hbar}\right) = -\frac{1}{2}\left[\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} - \mathbb{I}\right] = \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}, \text{ projection on } |-\rangle$$

$$\left(\frac{S_z + \hbar/2}{\hbar}\right) = \frac{1}{2}\left[\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} + \mathbb{I}\right] = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}, \text{ projection on } |+\rangle$$

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Problem 3
Consider the following Hamiltonian of a two-state system

$$H = E(|1\rangle\langle 1| - |2\rangle\langle 2|) + \Delta(|1\rangle\langle 2| + |2\rangle\langle 1|)$$

where E, Δ have dimension of energy. Find the energy eigenvalues and the corresponding eigenstates as linear combinations of $|1\rangle, |2\rangle$.

Solution. We find the following inner products

$$\langle 1|H|1\rangle = \langle 1|E|1\rangle\langle 1|1\rangle = E$$

$$\langle 1|H|2\rangle = \langle 1|\Delta|1\rangle\langle 2|2\rangle = \Delta$$

$$\langle 2|H|1\rangle = \langle 2|\Delta|2\rangle\langle 1|1\rangle = \Delta$$

$$\langle 2|H|2\rangle = -\langle 2|E|2\rangle\langle 2|2\rangle = -E$$

H can be represented in matrix form as

$$H = \begin{pmatrix}E & \Delta\\ \Delta & -E\end{pmatrix}$$

The eigenvalues are then the solution to the following equation

$$\det(H - \lambda\mathbb{I}) = 0$$

$$\begin{vmatrix}E - \lambda & \Delta\\ \Delta & -E - \lambda\end{vmatrix} = (E - \lambda)(-E - \lambda) - \Delta^2 = \lambda^2 - E^2 - \Delta^2 = 0$$

$$\lambda_{\pm} = \pm\sqrt{E^2 + \Delta^2}$$

For the corresponding eigenvectors, we have

- For $\lambda_+ = \sqrt{E^2+\Delta^2}$:

$$\begin{cases}(E-\sqrt{E^2+\Delta^2})\alpha + \Delta\beta &= 0\\ \Delta\alpha + (-E-\sqrt{E^2+\Delta^2})\beta &= 0\end{cases}$$

$$\implies \beta = \frac{\sqrt{E^2+\Delta^2}-E}{\Delta}\alpha = \left(\sqrt{\left(\frac{E}{\Delta}\right)^2+1}-\frac{E}{\Delta}\right)\alpha$$

Thus, the normalized eigenvector $|+\rangle$ corresponding to λ_+ is

$$|+\rangle = \frac{1}{\sqrt{\left(\sqrt{\left(\frac{E}{\Delta}\right)^2+1}\right)^2+\left(\frac{E}{\Delta}\right)^2-2\frac{E}{\Delta}\sqrt{\left(\frac{E}{\Delta}\right)^2+1}}}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

$$= \frac{1}{\sqrt{2\left(\frac{E}{\Delta}\right)^2+1-\frac{2E}{\Delta}\sqrt{\left(\frac{E}{\Delta}\right)^2+1}}}\begin{pmatrix}1\\ \frac{\sqrt{E^2+\Delta^2}-E}{\Delta}\end{pmatrix}$$

- For $\lambda_- = -\sqrt{E^2+\Delta^2}$:

$$\begin{cases}(E+\sqrt{E^2+\Delta^2})\alpha + \Delta\beta &= 0\\ \Delta\alpha + (-E+\sqrt{E^2+\Delta^2})\beta &= 0\end{cases}$$

$$\implies \beta = \frac{-\sqrt{E^2+\Delta^2}-E}{\Delta}\alpha = \left(-\sqrt{\left(\frac{E}{\Delta}\right)^2+1}-\frac{E}{\Delta}\right)\alpha$$

Thus, the normalized eigenvector $|-\rangle$ corresponding to λ_- is

$$|-\rangle = \frac{1}{\sqrt{\left(\sqrt{\left(\frac{E}{\Delta}\right)^2+1}\right)^2+\left(\frac{E}{\Delta}\right)^2+2\frac{E}{\Delta}\sqrt{\left(\frac{E}{\Delta}\right)^2+1}}}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

$$= \frac{1}{\sqrt{2\left(\frac{E}{\Delta}\right)^2+1+\frac{2E}{\Delta}\sqrt{\left(\frac{E}{\Delta}\right)^2+1}}}\begin{pmatrix}1\\ \frac{-\sqrt{E^2+\Delta^2}-E}{\Delta}\end{pmatrix}$$

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Problem 4
Consider the following Hamiltonian of a three-state system

$$H = \frac{\epsilon}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

where ϵ has dimension of energy. Find the energy eigenvalues and the corresponding eigenstates.

Solution. Finding the eigenvalues of the given matrix

$$\det(H - \lambda\mathbb{I}) = 0$$

$$\implies \begin{pmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{pmatrix} = -\lambda(\lambda^2 - 1) + \lambda = \lambda(2 - \lambda^2) = 0$$

$$\implies \lambda_1 = -\sqrt{2},\ \lambda_2 = 0,\ \lambda_3 = \sqrt{2}.$$

Finding the eigenvectors

- For $\lambda_1 = -\sqrt{2}$:

$$\begin{pmatrix} \sqrt{2} & 1 & 0 \\ 1 & \sqrt{2} & 1 \\ 0 & 1 & \sqrt{2} \end{pmatrix} |\lambda_1\rangle = 0 \implies |\lambda_1\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

- For $\lambda_2 = 0$:

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} |\lambda_2\rangle = 0 \implies |\lambda_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

- For $\lambda_3 = \sqrt{2}$:

$$\begin{pmatrix} -\sqrt{2} & 1 & 0 \\ 1 & -\sqrt{2} & 1 \\ 0 & 1 & -\sqrt{2} \end{pmatrix} |\lambda_3\rangle = 0 \implies |\lambda_3\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}.$$

Finally, the corresponding eigenstates of the Hamiltonian of our three-state system are

$$E_1 = -\epsilon,\ |E_1\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

$$E_2 = 0,\ |E_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

$$E_3 = \epsilon,\ |E_3\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}.$$

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Problem 5
Consider the following observables in a three-state system:

$$A = \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix}, \quad B = \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix},$$

where a, b are real numbers.

(a) The spectrum of A is degenerate. How about the spectrum of B?.

(b) Show that A and B commute.

(c) Find a new orthonormal basis where both A and B are diagonal. Do A and B form a complete set of observables for this system?

Solution. (a) The eigenvalues of A are obviously $\pm a$, with $-a$ twice. Finding the eigenvalues of B, we have

$$\det(B - \lambda\mathbb{I}) = 0$$

$$\implies \begin{pmatrix} b-\lambda & 0 & 0 \\ 0 & -\lambda & -ib \\ 0 & ib & -\lambda \end{pmatrix} = (\lambda - b)(\lambda^2 - b^2) = (\lambda - b)^2(\lambda + b) = 0$$

$$\implies \lambda_{1,2} = b, \ \lambda_3 = -b$$

Since we have degenerate eigenvalues, then the spectrum of B is also degenerate.

(b)

$$\begin{aligned} [A, B] = AB - BA &= \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix} \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix} - \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix} \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix} \\ &= \begin{pmatrix} ab & 0 & 0 \\ 0 & 0 & iab \\ 0 & -iab & 0 \end{pmatrix} - \begin{pmatrix} ab & 0 & 0 \\ 0 & 0 & iab \\ 0 & -iab & 0 \end{pmatrix} \\ &= 0 \end{aligned}$$

(c) Notice that A and B are Hermitian. Since A and B are Hermitian and $[A, B] = 0$, then there exists a basis where both A and B are both diagonal. To find these, write the eigenvector components as $u_i, \ i = 1, 2, 3$. Clearly, the basis states $|1\rangle$, $|2\rangle$, and $|3\rangle$ are eigenvectors of A with eigenvalues a, $-a$, and $-a$ respectively. We can notice that $|1\rangle$ is a common eigenvector for both A and B. We just need to work out the 2×2 block basis for $|2\rangle$ and $|3\rangle$. Indeed, both of these states have eigenvalues a for A, so one linear combinations should have eigenvalue b for B, and orthogonal combination with eigenvalue $-b$.

Let the eigenvector components be u_2 and u_3. Then, for eigenvalue b, we have

$$-ibu_3 = bu_2 \quad \text{and} \quad ibu_2 = bu_3$$

both of which imply $u_3 = iu_2$. For eigenvalue $-b$, we have

$$-ibu_3 = -bu_2 \quad \text{and} \quad ibu_2 = -bu_3$$

both of which imply $u_3 = -iu_2$.

Choosing u_2 to be real, then we have the set of simultaneous eigenstates

$$\lambda_{A1} = a, \ \lambda_{B1} = b : \ |1\rangle$$

$$\lambda_{A2} = -a,\ \lambda_{B2} = b:\ \frac{1}{\sqrt{2}}(|2\rangle + i\,|3\rangle)$$

$$\lambda_{A3} = -a,\ \lambda_{B3} = -b:\ \frac{1}{\sqrt{2}}(|2\rangle - i\,|3\rangle).$$

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Homework 2

Based on problems 1.12, 1.13, 1.18c, 1.30,1.32, 1.33 of Sakurai's book.

Problem 1
A spin $\frac{1}{2}$ system is in the state $|\uparrow\rangle_{\hat{n}}$, namely in a spin up eigenstate in an arbitrary direction defined by the unit vector $\hat{n} = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))$.

(a) If the component S_z is measured, find the possible results of the measurement and their probabilities.

(b) Evaluate the dispersion σ_x, given by

$$\sigma_x^2 = {}_{\hat{n}}\left\langle \uparrow \middle| \left(S_x - \bar{S}_x\right)^2 \middle| \uparrow \right\rangle_{\hat{n}},$$

where $\bar{S}_x = {}_{\hat{n}}\langle\uparrow|S_x|\uparrow\rangle_{\hat{n}}$.

(c) Check your answers for the cases $\theta = 0, \pi$ and $\theta = \pi/2$, $\phi = 0$.

Solution. (a) Given an arbitrary direction defined by the unit vector $\hat{n} = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))$, we can represent $|\uparrow\rangle_{\hat{n}}$ as

$$|\uparrow\rangle_{\hat{n}} = \cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|\downarrow\rangle.$$

Measuring S_x will give us the eigenvalues of S_x which are $\pm\frac{\hbar}{2}$. The probabilities are as follows

- **Probability of getting $+\frac{\hbar}{2}$:**

$$\begin{aligned}
|\langle S_x|\uparrow\rangle_{\hat{n}}|^2 &= \left|\left(\frac{1}{\sqrt{2}}\langle\uparrow| + \frac{1}{\sqrt{2}}\langle\downarrow|\right)\left(\cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|\downarrow\rangle\right)\right|^2 \\
&= \frac{1}{2}\left|(\langle\uparrow| + \langle\downarrow|)\left(\cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|\downarrow\rangle\right)\right|^2 \\
&= \frac{1}{2}\left|\cos\left(\frac{\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}\right|^2 \\
&= \frac{1}{2}\left(\cos\left(\frac{\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}\right)\left(\cos\left(\frac{\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\right) \\
&= \frac{1}{2}\left[\cos^2\left(\frac{\theta}{2}\right) + \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(e^{i\varphi} + e^{-i\varphi}\right) + \sin^2\left(\frac{\theta}{2}\right)\right] \\
&= \frac{1}{2}\left[1 + \sin(\theta)\cos(\varphi)\right].
\end{aligned}$$

- **Probability of getting $-\frac{\hbar}{2}$:**

  Since this is a two-state system, then

$$|\langle S_x|\downarrow\rangle_{\hat{n}}|^2 = 1 - |\langle S_x|\uparrow\rangle_{\hat{n}}|^2 = \frac{1}{2}\left[1 - \sin(\theta)\cos(\varphi)\right].$$

(b) We have that

$$\begin{aligned}
\sigma_x^2 &= {}_{\hat{n}}\left\langle\uparrow\middle|\left(S_x-\bar{S}_x\right)^2\middle|\uparrow\right\rangle_{\hat{n}} \\
&= {}_{\hat{n}}\langle\uparrow|S_x^2-2S_x\bar{S}_x+\bar{S}_x^2|\uparrow\rangle_{\hat{n}} \\
&= {}_{\hat{n}}\langle\uparrow|S_x^2|\uparrow\rangle_{\hat{n}} - 2\,{}_{\hat{n}}\langle\uparrow|S_x|\uparrow\rangle_{\hat{n}}\,{}_{\hat{n}}\langle\uparrow|S_x|\uparrow\rangle_{\hat{n}} + {}_{\hat{n}}\langle\uparrow|S_x|\uparrow\rangle_{\hat{n}}^2\,{}_{\hat{n}}\langle\uparrow|\uparrow\rangle_{\hat{n}} \\
&= {}_{\hat{n}}\langle\uparrow|S_x^2|\uparrow\rangle_{\hat{n}} - 2\,{}_{\hat{n}}\langle\uparrow|S_x|\uparrow\rangle_{\hat{n}}^2 + {}_{\hat{n}}\langle\uparrow|S_x|\uparrow\rangle_{\hat{n}}^2 \\
&= {}_{\hat{n}}\langle\uparrow|S_x^2|\uparrow\rangle_{\hat{n}} - {}_{\hat{n}}\langle\uparrow|S_x|\uparrow\rangle_{\hat{n}}^2 \\
&= \left(\cos\left(\frac{\theta}{2}\right)\langle\uparrow| + \sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\langle\downarrow|\right)S_x^2\left(\cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|\downarrow\rangle\right) \\
&\quad - \left[\left(\cos\left(\frac{\theta}{2}\right)\langle\uparrow| + \sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\langle\downarrow|\right)S_x\left(\cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|\downarrow\rangle\right)\right]^2 \\
&= \frac{\hbar^2}{4}\left(\cos\left(\frac{\theta}{2}\right)\langle\uparrow| + \sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\langle\downarrow|\right)\mathbb{I}\left(\cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|\downarrow\rangle\right) \\
&\quad - \frac{\hbar^2}{4}\left[\left(\cos\left(\frac{\theta}{2}\right)\langle\uparrow| + \sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\langle\downarrow|\right)\sigma_x\left(\cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|\downarrow\rangle\right)\right]^2 \\
&= \frac{\hbar^2}{4}\left(\cos^2\left(\frac{\theta}{2}\right) + \sin^2\left(\frac{\theta}{2}\right)\right) \\
&\quad - \frac{\hbar^2}{4}\left[\left(\cos\left(\frac{\theta}{2}\right)\langle\uparrow| + \sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\langle\downarrow|\right)\left(\sin\left(\frac{\theta}{2}\right)e^{i\varphi}|\uparrow\rangle + \cos\left(\frac{\theta}{2}\right)|\downarrow\rangle\right)\right]^2 \\
&= \frac{\hbar^2}{4}\left(\cos^2\left(\frac{\theta}{2}\right) + \sin^2\left(\frac{\theta}{2}\right)\right) - \frac{\hbar^2}{4}\left[\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(e^{i\varphi}+e^{-i\varphi}\right)\right]^2 \\
&= \frac{\hbar^2}{4}\left[1 - \left[\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(e^{i\varphi}+e^{-i\varphi}\right)\right]^2\right] \\
&= \frac{\hbar^2}{4}\left[1 - \left(\sin(\theta)\cos(\varphi)\right)^2\right] \\
&= \frac{\hbar^2}{4}\left[1 - \sin^2(\theta)\cos^2(\varphi)\right].
\end{aligned}$$

(c)
- **For $\theta = 0$ or $\theta = \pi$:** We measure $+\frac{\hbar}{2}$ with probability $\frac{1}{2}$ and $-\frac{\hbar}{2}$ with probability $\frac{1}{2}$ and the dispersion has a value of $\frac{\hbar^2}{4}$.
- **For $\theta = \frac{\pi}{2}$ and $\phi = 0$:** We measure $+\frac{\hbar}{2}$ with probability 1 and $-\frac{\hbar}{2}$ with probability 0 and the dispersion has a value of 0, which implies that there are no other possible values to measure.

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Problem 2
Continuing from Problem 1, a series of Stern-Gerlach experiments are done to measure different components of the spin in succession. The beams are directed along direction $\hat{x}$ and the experiments are done as follows:

- The first device accepts only $s_z = \hbar/2$ states, (i.e. those with $s_z = -\hbar/2$ are blocked) thus creating a polarized beam for the next devices.
- The second device accepts only states with $s_{\hat{n}} = \hbar/2$, where $\hat{n}$ is a unit vector perpendicular to $\hat{x}$.
- The third device accepts only $s_z = -\hbar/2$.

(a) What is the ratio of the intensities of the final $s_z = -\hbar/2$ beam and the initial $s_z = \hbar/2$ polarized beam?

(b) How should the orientation of the second device, namely the vector $\hat{n}$, should be chosen to maximize the ratio computed in (a).

Solution. (a) Denote the first device by s_{z+}, the second device by $s_{\hat{n}}$, and the third device by s_{z-}. The ratio of intensities of the final beam and the initial polarized beam is given by

$$\frac{I_f}{I_i} = \left|\langle s_{\hat{n}}|s_{z-}\rangle\right|^2 \left|\langle s_{z+}|s_{\hat{n}}\rangle\right|^2 .$$

In other words, the ratio of intensities will be given by the amplitude remaining after the second and third devices.

We have

$$\begin{aligned} |s_{z+}\rangle &= |\uparrow\rangle \,, \\ |s_{z-}\rangle &= |\downarrow\rangle \,, \\ |s_{\hat{n}}\rangle &= \cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|\downarrow\rangle \,, \end{aligned}$$

then, replacing in the ratio of intensities, we get

$$\begin{aligned} \frac{I_f}{I_i} &= \left|\langle s_{\hat{n}}|s_{z-}\rangle\right|^2 \left|\langle s_{z+}|s_{\hat{n}}\rangle\right|^2 \\ &= \langle s_{\hat{n}}|s_{z-}\rangle \langle s_{z-}|s_{\hat{n}}\rangle \langle s_{z+}|s_{\hat{n}}\rangle \langle s_{\hat{n}}|s_{z+}\rangle \\ &= \left[\left(\cos\left(\frac{\theta}{2}\right)\langle\uparrow| + \sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\langle\downarrow|\right)|\downarrow\rangle\right]\left[\langle\downarrow|\left(\cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|\downarrow\rangle\right)\right] \\ &\quad \left[\langle\uparrow|\left(\cos\left(\frac{\theta}{2}\right)|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|\downarrow\rangle\right)\right]\left[\left(\cos\left(\frac{\theta}{2}\right)\langle\uparrow| + \sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\langle\downarrow|\right)|\uparrow\rangle\right] \\ &= \left[\sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\right]\left[\sin\left(\frac{\theta}{2}\right)e^{i\varphi}\right]\left[\cos\left(\frac{\theta}{2}\right)\right]\left[\cos\left(\frac{\theta}{2}\right)\right] \\ &= \sin^2\left(\frac{\theta}{2}\right)\cos^2\left(\frac{\theta}{2}\right) \\ &= \frac{\sin^2(\theta)}{4}. \end{aligned}$$

(b) To maximize the ratio of intensities, the argument of the sine function should be $\frac{\pi}{2}$. The second device should be chosen to be at a 90° angle with respect to the first device, which also ends up being the same angle from the third device. In other words, the second device should be angles right in between the $|\uparrow\rangle$ and $|\downarrow\rangle$ states, in order to get the maximum intensity of $\frac{1}{4}$.

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Problem 3
Consider a particle in a state with a Gaussian wave-function

$$\langle x|\psi\rangle = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{ikx-\frac{1}{4\sigma^2}(x-x_0)^2}. \tag{1}$$

(a) Compute $\langle\psi|\hat{x}|\psi\rangle$, $\langle\psi|\hat{p}|\psi\rangle$, $\left\langle\psi\middle|(\Delta x)^2\middle|\psi\right\rangle$, and $\left\langle\psi\middle|(\Delta p)^2\middle|\psi\right\rangle$.

(b) Check that such state has minimal uncertainty, namely

$$\sqrt{\langle\psi|(\Delta x)^2|\psi\rangle}\sqrt{\langle\psi|(\Delta p)^2|\psi\rangle} = \frac{\hbar}{2}.$$

(c) Show that for this state

$$\langle x|\Delta x|\psi\rangle = i\lambda\,\langle x|\Delta p|\psi\rangle$$

where $\lambda \in \mathbb{R}$. How does this relate to the minimal uncertainty property? **Hint:** Recall the solution of the uncertainty principle based on defining an operator $\mathcal{O} = \Delta x + i\mu\Delta p$ and computing $\left\langle\psi\middle|\mathcal{O}^\dagger\mathcal{O}\middle|\psi\right\rangle \geq 0$.

Solution. (a) In the position basis, $\hat{x} = x$, and we have

$$\begin{aligned}
\langle\psi|\hat{x}|\psi\rangle &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-ikx} e^{ikx} x e^{-\frac{(x-x_0)^2}{2\sigma^2}}\,\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} x e^{-\frac{(x-x_0)^2}{2\sigma^2}}\,\mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \left(\sqrt{2\sigma^2}t + x_0\right) e^{-t^2}\sqrt{2\sigma^2}\,\mathrm{d}t \\
&= \frac{1}{\sqrt{\pi}} \left[\sqrt{2\sigma^2}\int_{-\infty}^{\infty} te^{-t^2}\,\mathrm{d}t + x_0\int_{-\infty}^{\infty} e^{-t^2}\,\mathrm{d}t\right] \\
&= \frac{1}{\sqrt{\pi}} \left[0 + x_0\sqrt{\pi}\,\mathrm{d}t\right] \\
&= x_0,
\end{aligned}$$

where the final jump was due to two things: the first integral is odd over an even domain and so evaluates to zero, and the second integral is equal to $\sqrt{\pi}$. Our solution makes sense as the Gaussian wave-function is centered at the mean $\mu = x_0$.

In the momentum basis, $\hat{p} = -i\hbar\frac{\partial}{\partial x}$, and we have

$$\begin{aligned}
\langle\psi|\hat{p}|\psi\rangle &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-ikx} e^{-\frac{(x-x_0)^2}{4\sigma^2}} \left(-i\hbar\frac{\partial}{\partial x}\right)\left(e^{ikx}e^{-\frac{(x-x_0)^2}{4\sigma^2}}\right) \mathrm{d}x \\
&= -\frac{i\hbar}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{-ikx} e^{-\frac{(x-x_0)^2}{4\sigma^2}} \frac{\partial}{\partial x}\left(e^{ikx}e^{-\frac{(x-x_0)^2}{4\sigma^2}}\right) \mathrm{d}x \\
&= -\frac{i\hbar}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{-ikx} e^{-\frac{(x-x_0)^2}{4\sigma^2}} \left(ik - \frac{2(x-x_0)}{4\sigma^2}\right) e^{ikx}e^{-\frac{(x-x_0)^2}{4\sigma^2}} \mathrm{d}x \\
&= -\frac{i\hbar}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \left(ik - \frac{2(x-x_0)}{4\sigma^2}\right) e^{-\frac{(x-x_0)^2}{2\sigma^2}} \mathrm{d}x \\
&= -\frac{i\hbar}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \left(ik - \frac{2t}{4\sigma^2}\right) e^{-\frac{t^2}{2\sigma^2}} \mathrm{d}t \\
&= -\frac{i\hbar}{\sqrt{2\pi\sigma^2}} \left[ik\int_{-\infty}^{\infty} e^{-\frac{t^2}{2\sigma^2}} \mathrm{d}t - \frac{1}{2\sigma^2}\int_{-\infty}^{\infty} te^{-\frac{t^2}{2\sigma^2}} \mathrm{d}t\right] \\
&= -\frac{i\hbar}{\sqrt{2\pi\sigma^2}} \left[ik\sqrt{2\pi\sigma^2} - 0\right] \\
&= \hbar k.
\end{aligned}$$

Computing the variance of position, we get

$$\begin{aligned}
\langle\psi\big|(\Delta x)^2\big|\psi\rangle &= \langle\psi\big|(\hat{x} - \langle x\rangle)^2\big|\psi\rangle \\
&= \langle\psi\big|x^2\big|\psi\rangle - \langle x\rangle^2 \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} x^2 e^{-\frac{(x-x_0)^2}{2\sigma^2}} \mathrm{d}x - x_0^2 \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} (t+x_0)^2 e^{-\frac{t^2}{2\sigma^2}} \mathrm{d}t - x_0^2 \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \left[-\frac{t}{\sigma^2}(t+x_0)^2 e^{-\frac{t^2}{2\sigma^2}}\Big|_{-\infty}^{\infty} - \frac{2t^2}{\sigma^4}(t+x_0)e^{-\frac{t^2}{2\sigma^2}}\Big|_{-\infty}^{\infty} + \frac{2t^3}{\sigma^6}e^{-\frac{t^2}{2\sigma^2}}\Big|_{-\infty}^{\infty}\right] - x_0^2 \\
&= \frac{1}{\sqrt{2\pi\sigma^2}}\sqrt{2\pi\sigma^2}\left(x_0^2 + \sigma^2\right) - x_0^2 \\
&= \left(x_0^2 + \sigma^2\right) - x_0^2 \\
&= \sigma^2.
\end{aligned}$$

Computing the variance of momentum, we get

$$
\begin{aligned}
\langle\psi|(\Delta p)^2|\psi\rangle &= \langle\psi|(\hat{p}-\langle p\rangle)^2|\psi\rangle \\
&= \langle\psi|p^2|\psi\rangle - \langle p\rangle^2 \\
&= -\frac{\hbar^2}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty}\left(e^{-ikx-\frac{(x-x_0)^2}{4\sigma^2}}\right)\frac{\partial^2}{\partial x^2}\left(e^{ikx-\frac{(x-x_0)^2}{4\sigma^2}}\right)\mathrm{d}x - (\hbar k)^2 \\
&= -\frac{\hbar^2}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty}\left(e^{-ikx-\frac{(x-x_0)^2}{4\sigma^2}}\right)\left(ik-\frac{2(x-x_0)}{4\sigma^2}\right)^2 e^{ikx-\frac{(x-x_0)^2}{4\sigma^2}}\,\mathrm{d}x - (\hbar k)^2 \\
&= -\frac{\hbar^2}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty}\left(ik-\frac{2(x-x_0)}{4\sigma^2}\right)^2 e^{-\frac{(x-x_0)^2}{2\sigma^2}}\,\mathrm{d}x - (\hbar k)^2 \\
&= -\frac{\hbar^2}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty}\left(-k^2-\frac{ik(x-x_0)}{\sigma^2}-\frac{(x-x_0)^2}{4\sigma^4}\right) e^{-\frac{(x-x_0)^2}{2\sigma^2}}\,\mathrm{d}x - (\hbar k)^2 \\
&= -\frac{\hbar^2}{\sqrt{2\pi\sigma^2}}\left(-\frac{\sqrt{\pi}\left(4k^2\sigma^2+1\right)}{2\sqrt{2\sigma^2}}\right) - (\hbar k)^2 \\
&= \frac{\hbar^2\left(4k^2\sigma^2+1\right)}{4\sigma^2} - (\hbar k)^2 \\
&= \hbar^2 k^2 + \frac{\hbar^2}{4\sigma^2} - (\hbar k)^2 \\
&= \frac{\hbar^2}{4\sigma^2}.
\end{aligned}
$$

(b) The uncertainty is

$$
\sqrt{\langle\psi|(\Delta x)^2|\psi\rangle}\sqrt{\langle\psi|(\Delta p)^2|\psi\rangle} = \sqrt{\sigma^2}\sqrt{\frac{\hbar^2}{4\sigma^2}} = \frac{\hbar}{2},
$$

and it fulfils the minimal uncertainty, as needed. This was expected as the condition of a Gaussian wave-functions for position and momentum creates the minimum uncertainty state.

(c) We have

$$
\begin{aligned}
\langle x|\Delta p|\psi\rangle &= \langle x|\hat{p}-\langle p\rangle|\psi\rangle \\
&= \langle x|\hat{p}|\psi\rangle - \langle x|\langle p\rangle|\psi\rangle \\
&= \hat{p}\,\langle x|\psi\rangle - \langle p\rangle\,\langle x|\psi\rangle \\
&= [\hat{p}-\langle p\rangle]\,\langle x|\psi\rangle \\
&= \left[-i\hbar\frac{\partial}{\partial x}-\langle p\rangle\right]\langle x|\psi\rangle \\
&= \left[-i\hbar\left(ik-\frac{2(x-x_0)}{4\sigma^2}\right)-\hbar k\right]\langle x|\psi\rangle \\
&= \left[\hbar k+\frac{i\hbar(x-x_0)}{2\sigma^2}-\hbar k\right]\langle x|\psi\rangle \\
&= \left[\frac{i\hbar(x-x_0)}{2\sigma^2}\right]\langle x|\psi\rangle \\
&= \left[\frac{i\hbar}{2\sigma^2}\right](\hat{x}-\langle x\rangle)\,\langle x|\psi\rangle \\
&= \left[\frac{i\hbar}{2\sigma^2}\right]\langle x|\hat{x}-\langle x\rangle|\psi\rangle \\
&= \left[\frac{i\hbar}{2\sigma^2}\right]\langle x|\Delta x|\psi\rangle\,.
\end{aligned}
$$

Thus,

$$\langle x|\Delta x|\psi\rangle = i\lambda\,\langle x|\Delta p|\psi\rangle = -\frac{2i\sigma^2}{\hbar}\,\langle x|\Delta p|\psi\rangle \implies \lambda = -\frac{2\sigma^2}{\hbar}.$$

If we rearrange the terms, we get

$$\sqrt{\langle\psi|(\Delta x)^2|\psi\rangle}\sqrt{\langle\psi|(\Delta p)^2|\psi\rangle} = \frac{\hbar}{2} = -\frac{\sigma^2}{\lambda}.$$

■

Problem 4
Continuing from Problem 3,

(a) Check the momentum wave function $\tilde{\psi}(p) = \langle p|\psi\rangle$ for the state $|\psi\rangle$.

(b) Using $\tilde{\psi}(p) = \langle p|\psi\rangle$, compute $\langle\psi|\hat{p}|\psi\rangle$, $\langle\psi|(\Delta p)^2|\psi\rangle$ and check that you obtain the same results as in Problem 3.

Solution. (a) We have that

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}} = \langle p|x\rangle^* .$$

Checking the momentum wave function, we get

$$\begin{aligned}
\tilde{\psi}(p) &= \langle p|\psi\rangle \\
&= \int_{-\infty}^{\infty} \langle p|x\rangle \langle x|\psi\rangle \, \mathrm{d}x \\
&= \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{ipx}{\hbar}}\right) \left(\frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{ikx - \frac{1}{4\sigma^2}(x-x_0)^2}\right) \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} \int_{-\infty}^{\infty} \left(e^{-\frac{ipx}{\hbar}}\right) \left(e^{ikx - \frac{1}{4\sigma^2}(x-x_0)^2}\right) \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} \int_{-\infty}^{\infty} \left(e^{ix\left(k-\frac{p}{\hbar}\right) - \frac{1}{4\sigma^2}(x-x_0)^2}\right) \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{ix_0\left(k-\frac{p}{\hbar}\right)} \int_{-\infty}^{\infty} \left(e^{i(x-x_0)\left(k-\frac{p}{\hbar}\right) - \frac{1}{4\sigma^2}(x-x_0)^2}\right) \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{ix_0\left(k-\frac{p}{\hbar}\right)} 2\sqrt{\pi\sigma^2} e^{-\sigma^2\left(\frac{p}{\hbar}-k\right)^2} \\
&= \sqrt{\frac{2\sigma}{\hbar}} \frac{1}{(2\pi)^{\frac{1}{4}}} e^{ix_0\left(k-\frac{p}{\hbar}\right)} e^{-\sigma^2\left(\frac{p}{\hbar}-k\right)^2} \\
&= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{4}} e^{ix_0\left(k-\frac{p}{\hbar}\right)} e^{-\sigma^2\left(\frac{p}{\hbar}-k\right)^2}.
\end{aligned}$$

(b) We have

$$
\begin{aligned}
\langle\psi|\hat{p}|\psi\rangle &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle\psi|p\rangle \langle p|\hat{p}|p'\rangle \langle p'|\psi\rangle \,\mathrm{d}p\,\mathrm{d}p' \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \tilde{\psi}^*(p)\, p\delta(p-p')\, \tilde{\psi}(p')\,\mathrm{d}p\,\mathrm{d}p' \\
&= \int_{-\infty}^{\infty} \tilde{\psi}^*(p) p \tilde{\psi}(p)\,\mathrm{d}p \\
&= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \left(e^{-ix_0\left(k-\frac{p}{\hbar}\right)} e^{-\sigma^2\left(\frac{p}{\hbar}-k\right)^2}\right) p \left(e^{ix_0\left(k-\frac{p}{\hbar}\right)} e^{-\sigma^2\left(\frac{p}{\hbar}-k\right)^2}\right) \mathrm{d}p \\
&= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \left(e^{-\sigma^2\left(\frac{p}{\hbar}-k\right)^2}\right) p \left(e^{-\sigma^2\left(\frac{p}{\hbar}-k\right)^2}\right) \mathrm{d}p \\
&= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} p e^{-2\sigma^2\left(\frac{p}{\hbar}-k\right)^2}\,\mathrm{d}p \\
&= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{2}} \frac{\sqrt{\pi}\hbar^2 k}{\sqrt{2\sigma^2}} \\
&= \hbar k.
\end{aligned}
$$

Now,

$$
\begin{aligned}
\left\langle\psi\middle|\hat{p}^2\middle|\psi\right\rangle &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle\psi|p\rangle \left\langle p\middle|\hat{p}^2\middle|p'\right\rangle \langle p'|\psi\rangle \,\mathrm{d}p\,\mathrm{d}p' \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \tilde{\psi}^*(p)\, p^2\delta(p-p')\, \tilde{\psi}(p')\,\mathrm{d}p\,\mathrm{d}p' \\
&= \int_{-\infty}^{\infty} \tilde{\psi}^*(p) p^2 \tilde{\psi}(p)\,\mathrm{d}p \\
&= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \left(e^{-ix_0\left(k-\frac{p}{\hbar}\right)} e^{-\sigma^2\left(\frac{p}{\hbar}-k\right)^2}\right) p^2 \left(e^{ix_0\left(k-\frac{p}{\hbar}\right)} e^{-\sigma^2\left(\frac{p}{\hbar}-k\right)^2}\right) \mathrm{d}p \\
&= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \left(e^{-\sigma^2\left(\frac{p}{\hbar}-k\right)^2}\right) p^2 \left(e^{-\sigma^2\left(\frac{p}{\hbar}-k\right)^2}\right) \mathrm{d}p \\
&= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} p^2 e^{-2\sigma^2\left(\frac{p}{\hbar}-k\right)^2}\,\mathrm{d}p \\
&= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{\frac{1}{2}} \frac{\sqrt{\pi}\hbar^3\left(4k^2\sigma^2+1\right)}{2^{\frac{5}{2}}\sigma^3} \\
&= \frac{\hbar^2\left(4k^2\sigma^2+1\right)}{4\sigma^2} \\
&= \hbar^2k^2 + \frac{\hbar^2}{4\sigma^2}.
\end{aligned}
$$

Checking, we have

$$
\langle\psi|\Delta p|\psi\rangle = \left\langle\psi\middle|\hat{p}^2\middle|\psi\right\rangle - \langle\psi|\hat{p}|\psi\rangle^2 = \hbar^2k^2 + \frac{\hbar^2}{4\sigma^2} - \hbar^2k^2 = \frac{\hbar^2}{4\sigma^2}.
$$

■

Problem 5
Given the translation operator
$$U(a) = e^{-i\frac{\hat{p}a}{\hbar}}.$$

(a) Use the fundamental commutation relation
$$[\hat{p}, \hat{x}] = -i\hbar$$
to compute the commutator $[\hat{x}, U(a)]$.

(b) Given a state $|\psi\rangle$ such that $\langle\psi|\hat{x}|\psi\rangle = \bar{x}$, what is the mean value of $\hat{x}$ in the state $|\phi\rangle = U(a)\,|\psi\rangle$?

Solution. (a) We are given
$$[\hat{p}, \hat{x}] = -i\hbar,$$
which implies, by the properties of the commutator, that
$$[\hat{x}, \hat{p}] = i\hbar.$$

Notice that
$$\begin{aligned} U(a) &= e^{-i\frac{\hat{p}a}{\hbar}} \\ &= \sum_{k=0}^{\infty} \frac{\left(-i\frac{\hat{p}a}{\hbar}\right)^k}{k!} \\ &= \sum_{k=0}^{\infty} \frac{\left(-i\frac{a}{\hbar}\right)^k}{k!}\hat{p}^k. \end{aligned}$$

If we can find a relation for the commutator between the position operator and the kth degree of the momentum operator, we can then solve what is needed. In other words, we need to find a general formula for $[\hat{x}, \hat{p}^k]$.

Consider the following argument

- **For** $k = 1$**:**
$$[\hat{x}, \hat{p}^1] = i\hbar,$$
which is given to us.
- **For** $k = 2$**:**
$$\begin{aligned} [\hat{x}, \hat{p}^2] &= [\hat{x}, \hat{p}\hat{p}] \\ &= \hat{p}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{p} \\ &= i\hbar\hat{p} + i\hbar\hat{p} \\ &= 2i\hbar\hat{p}. \end{aligned}$$
- **For** $k = 3$**:**
$$\begin{aligned} [\hat{x}, \hat{p}^3] &= [\hat{x}, (\hat{p})^2\hat{p}] \\ &= \hat{p}^2[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}^2]\hat{p} \\ &= i\hbar\hat{p}^2 + 2i\hbar\hat{p}^2 \\ &= 3i\hbar\hat{p}^2. \end{aligned}$$
- **For** $k = n$**:** We will claim that it is represented by the following formula
$$[\hat{x}, \hat{p}^n] = i\hbar n\hat{p}^{n-1}.$$

We will prove it by mathematical induction. The case for $k = 1$ is given to us. Assume this is true for all k up to n. Let us show it is indeed true for $k = n + 1$ and that we get $[\hat{x}, \hat{p}^{n+1}] = i\hbar(n+1)\hat{p}^n$. Consider

$$\begin{aligned}
[\hat{x}, \hat{p}^{n+1}] &= [\hat{x}, \hat{p}^n \hat{p}] \\
&= \hat{p}^n [\hat{x}, \hat{p}] + [\hat{x}, \hat{p}^n]\hat{p} \\
&= i\hbar\hat{p}^n + i\hbar n\hat{p}^{n-1}\hat{p} \qquad (\text{since } [\hat{x}, \hat{p}^n] = i\hbar n \hat{p}^{n-1}) \\
&= i\hbar(n+1)\hat{p}^n,
\end{aligned}$$

and is, thus, proven.

Computing the needed commutator, we have

$$\begin{aligned}
[\hat{x}, U(a)] &= \left[\hat{x}, e^{-i\frac{\hat{p}a}{\hbar}}\right] \\
&= \left[\hat{x}, \sum_{k=0}^{\infty} \frac{\left(-i\frac{a}{\hbar}\right)^k}{k!}\hat{p}^k\right] \\
&= \sum_{k=0}^{\infty} \frac{\left(-i\frac{a}{\hbar}\right)^k}{k!}[\hat{x}, \hat{p}^k] \\
&= \sum_{k=0}^{\infty} \frac{\left(-i\frac{a}{\hbar}\right)^k}{k!}\left[i\hbar k\hat{p}^{k-1}\right] \\
&= \left(-i\frac{a}{\hbar}\right)(i\hbar)\sum_{k=0}^{\infty} \frac{\left(-i\frac{\hat{p}a}{\hbar}\right)^{k-1}}{(k-1)!} \\
&= a\sum_{k=0}^{\infty} \frac{\left(-i\frac{\hat{p}a}{\hbar}\right)^{k-1}}{(k-1)!} \\
&= aU(a).
\end{aligned}$$

(b) From part (a), we have

$$[\hat{x}, U(a)] = \hat{x}U(a) - U(a)\hat{x} = aU(a) \qquad \Longrightarrow \qquad \hat{x}U(a) = aU(a) + U(a)\hat{x}.$$

Also note that $U(a)$ represents the translation operator, which is unitary.

Given the state $|\phi\rangle = U(a)|\psi\rangle$, then $\langle\phi| = U^\dagger(a)\langle\psi|$. Taking the inner product of $\hat{x}$ in the $|\phi\rangle$ basis, we get

$$\begin{aligned}
\langle\phi|\hat{x}|\phi\rangle &= \left\langle\psi\middle|U^\dagger(a)\hat{x}U(a)\middle|\psi\right\rangle \\
&= \left\langle\psi\middle|U^\dagger(a)\left(aU(a) + U(a)\hat{x}\right)\middle|\psi\right\rangle \\
&= \left\langle\psi\middle|U^\dagger(a)aU(a)\middle|\psi\right\rangle + \left\langle\psi\middle|U^\dagger(a)U(a)\hat{x}\middle|\psi\right\rangle \\
&= a\left\langle\psi\middle|U^\dagger(a)U(a)\middle|\psi\right\rangle + \left\langle\psi\middle|U^\dagger(a)U(a)\hat{x}\middle|\psi\right\rangle \\
&= a\langle\psi|\psi\rangle + \langle\psi|\hat{x}|\psi\rangle \\
&= a + \bar{x}.
\end{aligned}$$

Thus, the mean value of $\hat{x}$ in the state $|\phi\rangle$ is the same as it is in the state $|\psi\rangle$ but shifted by a units.

■

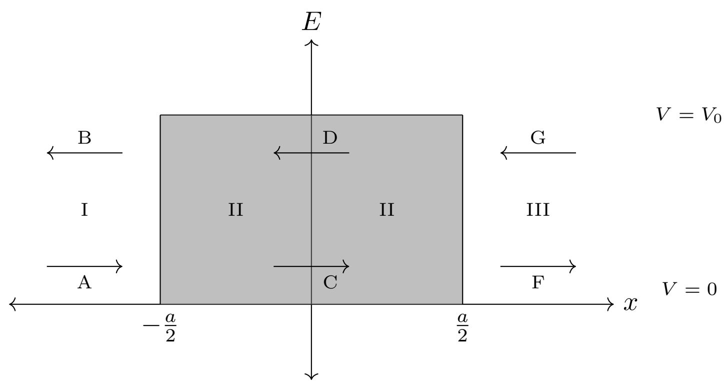
Homework 3

Problem 1
Consider an inverted square-well potential

$$V(x) = \begin{cases} V_0, & \text{if } |x| < \frac{a}{2}, \\ 0, & \text{if } |x| > \frac{a}{2}, \end{cases}$$

with $V_0 > 0$. Compute the scattering matrix S and the reflection and transmission coefficients. Consider both cases, $0 < E < V_0$ and $V_0 < E$. Check the unitarity and symmetries of S. Plot the transmission coefficient as a function of energy. Choose the parameters such that there are well-defined resonance peaks.

Solution. The system given looks like the following



The Hamiltonian of the system is given by

$$H = \frac{p^2}{2m} + V_0.$$

Notice that we have symmetry under parity inversion.
$\boxed{\text{For } 0 < E < V_0\text{:}}$

- **Region I**: The Schrodinger equation is given by

  $$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = E\psi.$$

  We are looking for a solution of the form

  $$\psi_I(x) = c\mathrm{e}^{ikx},$$

  where c is an arbitrary constant.

  By separation of variables, we have that our constant k should be

  $$k = \pm\frac{\sqrt{2mE}}{\hbar}.$$

  Thus, the solution to the Schrodinger equation is given by

  $$\psi_I(x) = A\mathrm{e}^{ikx} + B\mathrm{e}^{-ikx}.$$

- **Region II**: The Schrodinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V_0\psi=E\psi.$$

We are looking for a solution of the form

$$\psi_{II}(x)=c\mathrm{e}^{ik'x},$$

where c is an arbitrary constant.

Similarly, by separation of variables, we have that our constant k should be

$$k'=\pm\frac{\sqrt{2m(E-V_0)}}{\hbar},\quad (E-V_0<0).$$

This means that k' is an imaginary number. We could denote $k'=i\kappa$, where $\kappa=\frac{\sqrt{2m(V_0-E)}}{\hbar}$, but we will stick with the k' notation, keeping in mind that it is imaginary.

The solution to the Schrodinger equation is given by

$$\psi_{II}(x)=C\mathrm{e}^{ik'x}+D\mathrm{e}^{-ik'x}.$$

- **Region III**: Similar to Region I, the solution to the Schrodinger equation is given by

$$\psi_{III}(x)=F\mathrm{e}^{ikx}+G\mathrm{e}^{-ikx}.$$

For the second order partial differential equation to be defined, the wave function ψ and it's first derivative must be continuous. More formally, the wave function should be once-differentiable and belong to the first differentiability class, *i.e.* $\psi\in\mathcal{C}^1$. Thus, we must evaluate our wave function solutions and their derivatives at $x=\pm\frac{a}{2}$ and force continuity.
Applying boundary conditions at $x=-\frac{a}{2}$, we have

$$\begin{cases}\psi_I\left(-\frac{a}{2}\right)=\psi_{II}\left(-\frac{a}{2}\right)\\ \frac{\partial}{\partial x}\psi_I\left(x\right)\big|_{-\frac{a}{2}}=\frac{\partial}{\partial x}\psi_{II}\left(x\right)\big|_{-\frac{a}{2}}\end{cases}\implies\begin{cases}A\mathrm{e}^{-ik\frac{a}{2}}+B\mathrm{e}^{ik\frac{a}{2}}=C\mathrm{e}^{-ik'\frac{a}{2}}+D\mathrm{e}^{ik'\frac{a}{2}}\\ ikA\mathrm{e}^{-ik\frac{a}{2}}-ikB\mathrm{e}^{ik\frac{a}{2}}=ik'C\mathrm{e}^{-ik'\frac{a}{2}}-ik'D\mathrm{e}^{ik'\frac{a}{2}}\end{cases}$$

which gives us

$$\begin{pmatrix}\mathrm{e}^{-ik\frac{a}{2}} & \mathrm{e}^{ik\frac{a}{2}}\\ ik\mathrm{e}^{-ik\frac{a}{2}} & -ik\mathrm{e}^{ik\frac{a}{2}}\end{pmatrix}\begin{pmatrix}A\\ B\end{pmatrix}=\begin{pmatrix}\mathrm{e}^{-ik'\frac{a}{2}} & \mathrm{e}^{ik'\frac{a}{2}}\\ ik'\mathrm{e}^{-ik'\frac{a}{2}} & -ik'\mathrm{e}^{ik'\frac{a}{2}}\end{pmatrix}\begin{pmatrix}C\\ D\end{pmatrix}$$

Taking the inverse of the matrix on the right hand side, we get

$$\begin{aligned}\begin{pmatrix}C\\ D\end{pmatrix}&=\frac{1}{-2ik'}\begin{pmatrix}-ik'\mathrm{e}^{ik'\frac{a}{2}} & -\mathrm{e}^{ik'\frac{a}{2}}\\ -ik'\mathrm{e}^{-ik'\frac{a}{2}} & \mathrm{e}^{-ik'\frac{a}{2}}\end{pmatrix}\begin{pmatrix}\mathrm{e}^{-ik\frac{a}{2}} & \mathrm{e}^{ik\frac{a}{2}}\\ ik\mathrm{e}^{-ik\frac{a}{2}} & -ik\mathrm{e}^{ik\frac{a}{2}}\end{pmatrix}\begin{pmatrix}A\\ B\end{pmatrix}\\ &=\frac{1}{-2ik'}\begin{pmatrix}-ik'\mathrm{e}^{ik'\frac{a}{2}}\mathrm{e}^{-ik\frac{a}{2}}-ik\mathrm{e}^{ik'\frac{a}{2}}\mathrm{e}^{-ik\frac{a}{2}} & -ik'\mathrm{e}^{ik'\frac{a}{2}}\mathrm{e}^{ik\frac{a}{2}}+ik\mathrm{e}^{ik'\frac{a}{2}}\mathrm{e}^{ik\frac{a}{2}}\\ -ik'\mathrm{e}^{-ik'\frac{a}{2}}\mathrm{e}^{-ik\frac{a}{2}}+ik\mathrm{e}^{-ik'\frac{a}{2}}\mathrm{e}^{-ik\frac{a}{2}} & -ik'\mathrm{e}^{-ik'\frac{a}{2}}\mathrm{e}^{ik\frac{a}{2}}-ik\mathrm{e}^{-ik'\frac{a}{2}}\mathrm{e}^{ik\frac{a}{2}}\end{pmatrix}\begin{pmatrix}A\\ B\end{pmatrix}\\ &=\frac{1}{2k'}\begin{pmatrix}(k+k')\mathrm{e}^{-i(k-k')\frac{a}{2}} & (-k+k')\mathrm{e}^{i(k+k')\frac{a}{2}}\\ (-k+k')\mathrm{e}^{-i(k+k')\frac{a}{2}} & (k+k')\mathrm{e}^{i(k-k')\frac{a}{2}}\end{pmatrix}\begin{pmatrix}A\\ B\end{pmatrix}.\end{aligned}$$

The large factor is the transfer matrix given from region I to region II.
Applying boundary conditions at $x=\frac{a}{2}$, we have

$$\begin{cases}\psi_{II}\left(\frac{a}{2}\right)=\psi_{III}\left(\frac{a}{2}\right)\\ \frac{\partial}{\partial x}\psi_{II}\left(x\right)\big|_{\frac{a}{2}}=\frac{\partial}{\partial x}\psi_{III}\left(x\right)\big|_{\frac{a}{2}}\end{cases}\implies\begin{cases}C\mathrm{e}^{ik'\frac{a}{2}}+D\mathrm{e}^{-ik'\frac{a}{2}}=F\mathrm{e}^{ik\frac{a}{2}}+G\mathrm{e}^{-ik\frac{a}{2}}\\ ik'C\mathrm{e}^{ik'\frac{a}{2}}-ik'D\mathrm{e}^{-ik'\frac{a}{2}}=ikF\mathrm{e}^{ik\frac{a}{2}}-ikG\mathrm{e}^{-ik\frac{a}{2}}\end{cases}$$

which gives us

$$\begin{pmatrix} e^{ik'\frac{a}{2}} & e^{-ik'\frac{a}{2}} \\ ik'e^{ik'\frac{a}{2}} & -ik'e^{-ik'\frac{a}{2}} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} e^{ik\frac{a}{2}} & e^{-ik\frac{a}{2}} \\ ike^{ik\frac{a}{2}} & -ike^{-ik\frac{a}{2}} \end{pmatrix}\begin{pmatrix} F \\ G \end{pmatrix}$$

Taking the inverse of the matrix on the right hand side, we get

$$\begin{aligned}
\begin{pmatrix} F \\ G \end{pmatrix} &= \frac{1}{-2ik}\begin{pmatrix} -ike^{-ik\frac{a}{2}} & -e^{-ik\frac{a}{2}} \\ -ike^{ik\frac{a}{2}} & e^{ik\frac{a}{2}} \end{pmatrix}\begin{pmatrix} e^{ik'\frac{a}{2}} & e^{-ik'\frac{a}{2}} \\ ik'e^{ik'\frac{a}{2}} & -ik'e^{-ik'\frac{a}{2}} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix} \\
&= \frac{1}{-2ik}\begin{pmatrix} -ike^{-ik\frac{a}{2}}e^{ik'\frac{a}{2}} - ik'e^{-ik\frac{a}{2}}e^{ik'\frac{a}{2}} & -ike^{-ik\frac{a}{2}}e^{-ik'\frac{a}{2}} + ik'e^{-ik\frac{a}{2}}e^{-ik'\frac{a}{2}} \\ -ike^{ik\frac{a}{2}}e^{ik'\frac{a}{2}} + ik'e^{ik\frac{a}{2}}e^{ik'\frac{a}{2}} & -ike^{ik\frac{a}{2}}e^{-ik'\frac{a}{2}} - ik'e^{ik\frac{a}{2}}e^{-ik'\frac{a}{2}} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix} \\
&= \frac{1}{2k}\begin{pmatrix} (k+k')e^{-i(k-k')\frac{a}{2}} & (k-k')e^{-i(k+k')\frac{a}{2}} \\ (k-k')e^{i(k+k')\frac{a}{2}} & (k+k')e^{i(k-k')\frac{a}{2}} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix}.
\end{aligned}$$

The large factor is the transfer matrix given from region II to region III.
Thus, we have

$$\begin{aligned}
\begin{pmatrix} F \\ G \end{pmatrix} &= \frac{1}{4kk'}\begin{pmatrix} (k+k')e^{-i(k-k')\frac{a}{2}} & (k-k')e^{-i(k+k')\frac{a}{2}} \\ (k-k')e^{i(k+k')\frac{a}{2}} & (k+k')e^{i(k-k')\frac{a}{2}} \end{pmatrix}\begin{pmatrix} (k+k')e^{-i(k-k')\frac{a}{2}} & (-k+k')e^{i(k+k')\frac{a}{2}} \\ (-k+k')e^{-i(k+k')\frac{a}{2}} & (k+k')e^{i(k-k')\frac{a}{2}} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} \\
&= \frac{1}{4kk'}\begin{pmatrix} (k+k')^2e^{-i(k-k')a} - (k-k')^2e^{-i(k+k')a} & -(k+k')(k-k')e^{ik'a} + (k+k')(k-k')e^{-ik'a} \\ (k+k')(k-k')e^{ik'a} - (k+k')(k-k')e^{-ik'a} & -(k-k')^2e^{i(k+k')a} + (k+k')^2e^{i(k-k')a} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} \\
&= \frac{1}{4kk'}\begin{pmatrix} (k+k')^2e^{-i(k-k')a} - (k-k')^2e^{-i(k+k')a} & -(k+k')(k-k')\left(e^{ik'a} - e^{-ik'a}\right) \\ (k+k')(k-k')\left(e^{ik'a} - e^{-ik'a}\right) & -(k-k')^2e^{i(k+k')a} + (k+k')^2e^{i(k-k')a} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} \\
&= \frac{1}{4kk'}\begin{pmatrix} (k+k')^2e^{-i(k-k')a} - (k-k')^2e^{-i(k+k')a} & -2i(k+k')(k-k')\sin(k'a) \\ 2i(k+k')(k-k')\sin(k'a) & -(k-k')^2e^{i(k+k')a} + (k+k')^2e^{i(k-k')a} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix}
\end{aligned}$$

Define $k_\pm = k \pm k'$, which reduces our total transfer matrix to

$$\begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{4kk'}\begin{pmatrix} k_+^2e^{-ik_-a} - k_-^2e^{-ik_+a} & -2ik_+k_-\sin(k'a) \\ 2ik_+k_-\sin(k'a) & -k_-^2e^{ik_+a} + k_+^2e^{ik_-a} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix}$$

The scattering matrix is given by

$$S = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix}$$

such that

$$\begin{pmatrix} G \\ A \end{pmatrix} = S\begin{pmatrix} B \\ F \end{pmatrix}.$$

This means that

$$\begin{cases} F = t_{11}A + t_{12}B, \\ G = t_{21}A + t_{22}B, \end{cases} \implies \begin{cases} A = \frac{1}{t_{11}}F - \frac{t_{12}}{t_{11}}B, \\ G = \frac{t_{21}}{t_{11}}F + \frac{1}{t_{11}}\left(t_{11}t_{22} - t_{12}t_{21}\right)B, \end{cases}$$

where $t_{11}t_{22} - t_{12}t_{21}$ is the determinant of the transfer matrix, which is equal to 1. Thus,

$$\begin{cases} A = -\frac{t_{12}}{t_{11}}B + \frac{1}{t_{11}}F, \\ G = \frac{1}{t_{11}}B + \frac{t_{21}}{t_{11}}F. \end{cases}$$

Rewriting this, we have

$$\begin{pmatrix} G \\ A \end{pmatrix} = \frac{1}{t_{11}}\begin{pmatrix} 1 & t_{21} \\ -t_{12} & 1 \end{pmatrix}\begin{pmatrix} B \\ F \end{pmatrix}.$$

Therefore, the scattering matrix S is given by

$$\begin{aligned}
S = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} &= \frac{4kk'}{k_+^2 \mathrm{e}^{-ik_-a} - k_-^2 \mathrm{e}^{-ik_+a}} \begin{pmatrix} 1 & \frac{2ik_+k_-}{4kk'} \sin(k'a) \\ \frac{2ik_+k_-}{4kk'} \sin(k'a) & 1 \end{pmatrix} \\
&= \frac{2}{k_+^2 \mathrm{e}^{-ik_-a} - k_-^2 \mathrm{e}^{-ik_+a}} \begin{pmatrix} 2kk' & ik_+k_- \sin(k'a) \\ ik_+k_- \sin(k'a) & 2kk' \end{pmatrix} \\
&= \frac{2}{(k+k')^2 \mathrm{e}^{-i(k-k')a} - (k-k')^2 \mathrm{e}^{-i(k+k')a}} \begin{pmatrix} 2kk' & i(k+k')(k-k')\sin(k'a) \\ i(k+k')(k-k')\sin(k'a) & 2kk' \end{pmatrix} \\
&= \frac{2\mathrm{e}^{ika}}{(k^2+2kk'+k'^2)\mathrm{e}^{ik'a} - (k^2-2kk'+k'^2)\mathrm{e}^{-ik'a}} \begin{pmatrix} 2kk' & i(k^2-k'^2)\sin(k'a) \\ i(k^2-k'^2)\sin(k'a) & 2kk' \end{pmatrix} \\
&= \frac{2\mathrm{e}^{ika}}{(k^2+k'^2)\left(\mathrm{e}^{ik'a} - \mathrm{e}^{-ik'a}\right) + 2kk'\left(\mathrm{e}^{ik'a} + \mathrm{e}^{-ik'a}\right)} \begin{pmatrix} 2kk' & i(k^2-k'^2)\sin(k'a) \\ i(k^2-k'^2)\sin(k'a) & 2kk' \end{pmatrix} \\
&= \frac{\mathrm{e}^{ika}}{(k^2+k'^2)i\sin(k'a) + 2kk'\cos(k'a)} \begin{pmatrix} 2kk' & i(k^2-k'^2)\sin(k'a) \\ i(k^2-k'^2)\sin(k'a) & 2kk' \end{pmatrix} \\
&= \frac{\mathrm{e}^{ika}}{(k^2+k'^2)\sin(k'a) + 2ikk'\cos(k'a)} \begin{pmatrix} 2ikk' & -(k^2-k'^2)\sin(k'a) \\ -(k^2-k'^2)\sin(k'a) & 2ikk' \end{pmatrix}.
\end{aligned}$$

The transmission coefficient is given by

$$\begin{aligned}
T &= |s_{11}|^2 \\
&= \left| \frac{2ikk'\mathrm{e}^{ika}}{(k^2+k'^2)\sin(k'a) + 2ikk'\cos(k'a)} \right|^2 \\
&= \frac{4k^2k'^2}{(k^2+k'^2)^2\sin^2(k'a) + 4k^2k'^2\cos^2(k'a)} \\
&= \frac{4k^2k'^2}{(k^2-k'^2)^2\sin^2(k'a) + 4k^2k'^2} \\
&= \frac{1}{\frac{(k^2-k'^2)^2\sin^2(k'a)}{4k^2k'^2} + 1}.
\end{aligned}$$

The reflection coefficient is given by

$$\begin{aligned}
R &= |s_{21}|^2 \\
&= \left| \frac{-(k^2-k'^2)\sin(k'a)\mathrm{e}^{ika}}{(k^2+k'^2)\sin(k'a) + 2ikk'\cos(k'a)} \right|^2 \\
&= \frac{(k^2-k'^2)^2\sin^2(k'a)}{(k^2+k'^2)^2\sin^2(k'a) + 4k^2k'^2\cos^2(k'a)} \\
&= \frac{(k^2-k'^2)^2\sin^2(k'a)}{(k^2-k'^2)^2\sin^2(k'a) + 4k^2k'^2} \\
&= \frac{1}{1 + \frac{4k^2k'^2}{(k^2-k'^2)^2\sin^2(k'a)}}.
\end{aligned}$$

Checking the unitarity of S, we have

$$\begin{aligned}
SS^\dagger &= \frac{\mathrm{e}^{ika}\mathrm{e}^{-ika}}{(k^2+k'^2)^2\sin^2(k'a) + 4k^2k'^2\cos^2(k'a)} \begin{pmatrix} 4k^2k'^2 + (k^2-k'^2)^2\sin^2(k'a) & 0 \\ 0 & 4k^2k'^2 + (k^2-k'^2)^2\sin^2(k'a) \end{pmatrix} \\
&= \frac{1}{(k^2-k'^2)^2\sin^2(k'a) + 4k^2k'^2} \begin{pmatrix} 4k^2k'^2 + (k^2-k'^2)^2\sin^2(k'a) & 0 \\ 0 & 4k^2k'^2 + (k^2-k'^2)^2\sin^2(k'a) \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
&= \mathbb{I},
\end{aligned}$$

which means S is unitary. It is also clear that S is a symmetric matrix.
The symmetries of the scattering matrix are the following

- **Symmetry under parity inversion:** If we make the transformation

$$\psi(x) \mapsto \psi(-x),$$

which is equivalent to switching regions I and III, then S also describes a solution to the new system. In fact,

$$\begin{cases} \tilde{\psi}_I(x) = G\mathrm{e}^{ikx} + F\mathrm{e}^{-ikx} \\ \tilde{\psi}_{III}(x) = B\mathrm{e}^{ikx} + A\mathrm{e}^{-ikx} \end{cases}$$

which gives us

$$\begin{pmatrix} A \\ G \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} \begin{pmatrix} F \\ B \end{pmatrix} \implies \begin{pmatrix} G \\ A \end{pmatrix} = \begin{pmatrix} s_{22} & s_{21} \\ s_{12} & s_{11} \end{pmatrix} \begin{pmatrix} B \\ F \end{pmatrix}$$

This is satisfied when $s_{11} = s_{22}$ and $s_{12} = s_{21}$, which is true since S is symmetric. Thus, the scattering matrix S is symmetric under parity inversion.

- **Symmetry under time reversal:** If we make the transformation

$$t \mapsto -t,$$

which is equivalent to flipping the directions of the waves in regions I and III, then S also describes a solution to the new system. In fact,

$$\begin{cases} \psi_I^*(x) = B^*\mathrm{e}^{ikx} + A^*\mathrm{e}^{-ikx} \\ \psi_{III}^*(x) = G^*\mathrm{e}^{ikx} + F^*\mathrm{e}^{-ikx} \end{cases}$$

which gives us

$$\begin{pmatrix} A^* \\ G^* \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} \begin{pmatrix} F^* \\ B^* \end{pmatrix}$$

Additionally, if the potential $V(x)$ is real, then the system possesses time-reversal symmetry. Thus, the scattering matrix S is symmetric under parity inversion.

$\boxed{\text{For } V_0 < E\text{:}}$

In this case, practically everything works out the same, except that, in Region II, k' is real, and, in the scattering matrix, $k^2 \pm k'^2 \to k^2 \mp k'^2$.
Going back to the transmission coefficient T, we will use the small-angle approximation for sin to get $\sin(x) \approx x$, and thus

$$\begin{aligned} T &= \frac{1}{\frac{(k^2-k'^2)^2 \sin^2(k'a)}{4k^2k'^2} + 1} \\ &= \frac{1}{\frac{(k^2-k'^2)^2 a^2}{4k^2} + 1}. \end{aligned}$$

Replacing the values of k and k', we get

$$T = \frac{1}{\frac{mV_0^2}{2\hbar^2 E} a^2 + 1}.$$

The interesting points are when $\sin(k'a) = 0 \implies k'a = n\pi$ for integer values of n. Replacing k', we get

$$\frac{\sqrt{2m(E-V_0)}}{\hbar} a = n\pi \implies E = V_0 + \frac{(n\pi\hbar)^2}{2ma^2}.$$

Setting $\hbar = m = 1$ and some arbitrary values for V_0 and a, we plot the transmission coefficient T as a function of energy E, getting

■

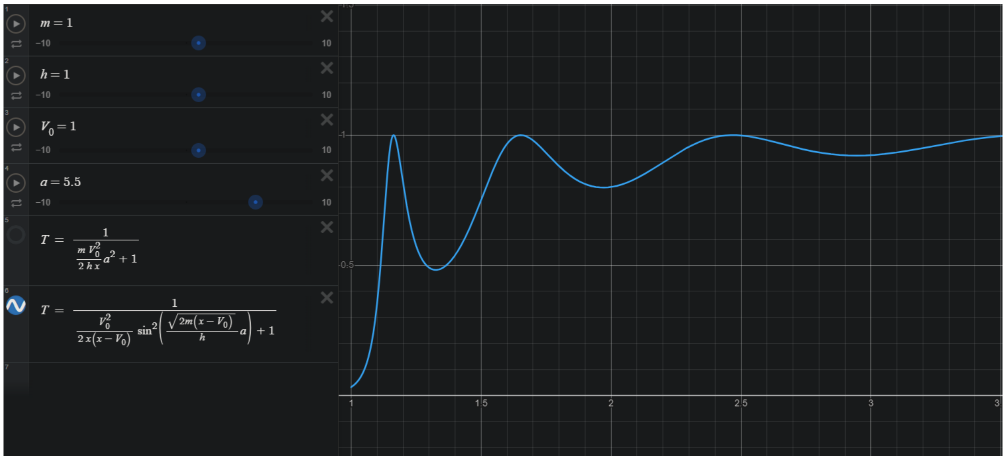


Figure 1: Transmission Coefficient T as a Function of Energy E.

Problem 2
Consider the spin $\frac{1}{2}$ Heisenberg chain and the operator $\hat{n} = \frac{1}{2}(1 + \sigma_z)$ that has expectation value 0 for a spin down and 1 for a spin up. It can be thought as the particle number in the interpretation where the vacuum are all spins down and a few spins are up.

(a) Compute the mean value of $\left\langle k \middle| n^{(i)} \middle| k \right\rangle$ for a given site i in the one particle state, assuming the spin chain has a finite length $N \gg 1$ for normalization purposes (but ignoring boundary effects).

(b) Compute the correlation

$$C_{ij} = \left\langle \psi \middle| n^{(i)} n^{(j)} \middle| \psi \right\rangle, \quad i < j$$

as a function of $|i - j|$ for the two particle state, *i.e.* $|\psi\rangle = |k_1, k_2\rangle$ in the infinite chain. Pay particular attention to the bound states and argue that the two particles are combined.

Solution. The Hamiltonian of a spin $\frac{1}{2}$ Heisenberg chain is given by

$$H = 2\lambda \sum_j \left(\mathbb{I}_{j,j+1} - \mathbb{P}_{j,j+1} \right),$$

where

$$\mathbb{P}_{j,j+1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

is the permutation matrix.

(a) We have

$$\begin{aligned} H\,|j\rangle &= 2\lambda(|j\rangle - |j-1\rangle + |j\rangle - |j+1\rangle) \\ &= 2\lambda(2\,|j\rangle - |j-1\rangle - |j+1\rangle) \end{aligned}$$

and

$$\begin{aligned} H\,|\psi\rangle &= \sum_j H\,|j\rangle \\ &= 2\lambda \sum_j (2\,|j\rangle - |j-1\rangle - |j+1\rangle) \\ &= \epsilon\,|\psi\rangle \end{aligned}$$

$$\implies \epsilon c_j = 2\lambda(2c_j - c_{j-1} - c_{j+1}).$$

Since the coefficients are constant, we try a solution of $c_j = \mathrm{e}^{jm}$, which gives us

$$\epsilon \mathrm{e}^{jm} = 2\lambda \mathrm{e}^{jm}\left(2 - \mathrm{e}^{-m} - \mathrm{e}^{m}\right)$$
$$\epsilon = 4\lambda - 2\lambda\left(\mathrm{e}^{m} + \mathrm{e}^{-m}\right).$$

The only way to stay finite is if we analytically continue $m \to ik$, which gives us

$$\begin{aligned}\epsilon &= 4\lambda - 2\lambda\left(\mathrm{e}^{ik} + \mathrm{e}^{-ik}\right)\\ &= 4\lambda - 4\lambda\cos(k)\\ &= 8\lambda\sin^2\left(\frac{k}{2}\right).\end{aligned}$$

We have that $|\epsilon\rangle = \sum_j e^{ikj}|j\rangle$, which gives us

$$\begin{aligned}\langle\epsilon|\epsilon\rangle &= \left(\sum_{j'} e^{-ikj'}\langle j'|\right)\left(\sum_j e^{ikj}|j\rangle\right)\\ &= \sum_{j,j'} e^{ik(j-j')}\langle j'|j\rangle\\ &= N.\end{aligned}$$

Normalizing, we get

$$|k\rangle = \frac{1}{\sqrt{N}}\sum_j e^{ikj}|j\rangle.$$

Computing the mean value, we have

$$\begin{aligned}\left\langle k\middle|n^{(i)}\middle|k\right\rangle &= \left(\frac{1}{\sqrt{N}}\sum_{j'} e^{-ikj'}\langle j'|\right)\frac{1}{2}(\mathbb{I}^{(i)} + \sigma_z^{(i)})\left(\frac{1}{\sqrt{N}}\sum_j e^{ikj}|j\rangle\right)\\ &= \frac{1}{2N}\sum_{j,j'} e^{ik(j-j')}\left\langle j'\middle|\mathbb{I}^{(i)} + \sigma_z^{(i)}\middle|j\right\rangle\\ &= \frac{1}{2N}\sum_{j,j'} e^{ik(j-j')}\left\langle j'\middle|\mathbb{I}^{(i)} + \sigma_z^{(i)}\middle|j\right\rangle\\ &= \frac{1}{N}\sum_{j,j'} e^{ik(j-j')}\langle j'|\delta_{ij}|j\rangle\\ &= \frac{1}{N}\sum_{j,j'} e^{ik(j-j')}\delta_{ij}\delta_{jj'}\\ &= \frac{1}{N}.\end{aligned}$$

(b) For the two-particle spin $\frac{1}{2}$ Heisenberg chain, we will denote the first particle by j_1 and the second by j_2 (to prevent confusion with the particle i and the imaginary unit i). We have

$$|\epsilon\rangle = \sum_{j_1,j_2} A_{j_1,j_2}|j_1,j_2\rangle,$$

where

$$A_{j_1,j_2} = \mathrm{e}^{i\frac{\theta}{2}}\mathrm{e}^{ik_1j_1}\mathrm{e}^{ik_2j_2} + \mathrm{e}^{-i\frac{\theta}{2}}\mathrm{e}^{ik_2j_1}\mathrm{e}^{ik_1j_2}$$

Calculating, we have

$$
\begin{aligned}
\langle\epsilon|\epsilon\rangle &= \left(\sum_{j_1',j_2'} A^*_{j_1',j_2'}\langle j_1',j_2'|\right)\left(\sum_{j_1,j_2} A_{j_1,j_2}|j_1,j_2\rangle\right)\\
&= \sum_{j_1,j_2,j_1',j_2'} A^*_{j_1',j_2'}A_{j_1,j_2}\langle j_1',j_2'|j_1,j_2\rangle\\
&= \sum_{j_1,j_2,j_1',j_2'}\left(\mathrm{e}^{-i\frac{\theta}{2}}\mathrm{e}^{-ik_1j_1'}\mathrm{e}^{-ik_2j_2'}+\mathrm{e}^{i\frac{\theta}{2}}\mathrm{e}^{-ik_2j_1'}\mathrm{e}^{-ik_1j_2'}\right)\left(\mathrm{e}^{i\frac{\theta}{2}}\mathrm{e}^{ik_1j_1}\mathrm{e}^{ik_2j_2}+\mathrm{e}^{-i\frac{\theta}{2}}\mathrm{e}^{ik_2j_1}\mathrm{e}^{ik_1j_2}\right)\langle j_1',j_2'|j_1,j_2\rangle\\
&= \sum_{j_1,j_2,j_1',j_2'}\Big(\mathrm{e}^{ik_1(j_1-j_1')}\mathrm{e}^{ik_2(j_2-j_2')}+\mathrm{e}^{-i\theta}\mathrm{e}^{ik_1(j_2-j_1')}\mathrm{e}^{ik_2(j_1-j_2')}\\
&\qquad+\mathrm{e}^{i\theta}\mathrm{e}^{ik_2(j_2-j_1')}\mathrm{e}^{ik_1(j_1-j_2')}+\mathrm{e}^{ik_2(j_1-j_1')}\mathrm{e}^{ik_1(j_2-j_2')}\Big)\langle j_1',j_2'|j_1,j_2\rangle\,.
\end{aligned}
$$

We have that $j_1<j_2$ and $j_1'<j_2'$, in addition to $\langle j_1',j_2'|j_1,j_2\rangle=\delta_{j_1,j_1'}\delta_{j_2,j_2'}$, which gives us

$$
\begin{aligned}
\langle\epsilon|\epsilon\rangle &= \sum_{j_1<j_2}\left(2+\mathrm{e}^{-i\theta}\mathrm{e}^{ik_1(j_2-j_1)}\mathrm{e}^{ik_2(j_1-j_2)}+\mathrm{e}^{i\theta}\mathrm{e}^{ik_2(j_2-j_1)}\mathrm{e}^{ik_1(j_1-j_2)}\right)\\
&= \sum_{j_1<j_2}\left(2+\mathrm{e}^{i\theta}\mathrm{e}^{ik_1(j_1-j_2)}\mathrm{e}^{ik_2(j_2-j_1)}+\mathrm{e}^{-i\theta}\mathrm{e}^{-ik_1(j_1-j_2)}\mathrm{e}^{-ik_2(j_2-j_1)}\right)\\
&= \sum_{j_1<j_2}\left[2+2\cos(\theta+k_1(j_1-j_2)+k_2(j_2-j_1))\right]\\
&= \sum_{j_1<j_2}\left[2+2\cos(\theta+(k_1-k_2)(j_1-j_2))\right].
\end{aligned}
$$

Then, $|\psi\rangle=|k_1,k_2\rangle=\frac{1}{\sqrt{\langle\epsilon|\epsilon\rangle}}|\epsilon\rangle$.

Calculating the correlation C_{j_1,j_2}, we have

$$
\begin{aligned}
C_{j_1,j_2} &= \left\langle\psi\middle|n^{(i)}n^{(j)}\middle|\psi\right\rangle\\
&= \frac{1}{\sqrt{\langle\epsilon|\epsilon\rangle}}\left\langle\epsilon\middle|n^{(i)}n^{(j)}\middle|\epsilon\right\rangle\\
&= \frac{1}{\sqrt{\langle\epsilon|\epsilon\rangle}}\sum_{j_1<j_2,j_1'<j_2'}\Big(\mathrm{e}^{ik_1(j_1-j_1')}\mathrm{e}^{ik_2(j_2-j_2')}+\mathrm{e}^{-i\theta}\mathrm{e}^{ik_1(j_2-j_1')}\mathrm{e}^{ik_2(j_1-j_2')}\\
&\qquad+\mathrm{e}^{i\theta}\mathrm{e}^{ik_2(j_2-j_1')}\mathrm{e}^{ik_1(j_1-j_2')}+\mathrm{e}^{ik_2(j_1-j_1')}\mathrm{e}^{ik_1(j_2-j_2')}\Big)\left\langle j_1',j_2'\middle|n^{(i)}n^{(j)}\middle|j_1,j_2\right\rangle\\
&= \frac{1}{\sqrt{\langle\epsilon|\epsilon\rangle}}\sum_{j_1<j_2,j_1'<j_2'}\Big(\mathrm{e}^{ik_1(j_1-j_1')}\mathrm{e}^{ik_2(j_2-j_2')}+\mathrm{e}^{-i\theta}\mathrm{e}^{ik_1(j_2-j_1')}\mathrm{e}^{ik_2(j_1-j_2')}\\
&\qquad+\mathrm{e}^{i\theta}\mathrm{e}^{ik_2(j_2-j_1')}\mathrm{e}^{ik_1(j_1-j_2')}+\mathrm{e}^{ik_2(j_1-j_1')}\mathrm{e}^{ik_1(j_2-j_2')}\Big)\delta_{j_1j_1'}\delta_{j_2j_2'}\delta_{j_1'i}\delta_{j_2'j}\\
&= \frac{1}{\sqrt{\langle\epsilon|\epsilon\rangle}}\left[2+2\cos(\theta+(k_1-k_2)(j_1-j_2))\right].
\end{aligned}
$$

Returning to the needed notation as per the problem, we have

$$
C_{ij}=\frac{1+\cos(\theta+(k_1-k_2)(i-j))}{\sum_{j_1<j_2}\left[1+\cos(\theta+(k_1-k_2)(j_1-j_2))\right]}.
$$

We define

$$
\begin{cases}\kappa=k_1+k_2\\ q=\frac{k_2-k_1}{2}\end{cases}
$$

and, thus, get

$$C_{ij} = \frac{1+\cos(\theta - 2q(i-j))}{\sum_{j_1<j_2}\left[1+\cos(\theta - 2q(j_1-j_2))\right]}.$$

This creates a bound state when the wave function of j_2 is far away from j_1. For bound states, we have $\theta = i\alpha$, $\alpha \to -\infty$ and $q = i\eta$, $\eta = -2\ln(\cos(\kappa)) > 0$, which gives us

$$\begin{aligned}
C_{ij} &= \frac{1+\cosh(\alpha - 2\eta(i-j))}{\sum_{j_1<j_2}\left[1+\cosh(\alpha - 2\eta(j_1-j_2))\right]} \\
&= \frac{2+\mathrm{e}^{\alpha+2\eta(j-i)}+\mathrm{e}^{-\alpha-2\eta(j-i)}}{\sum_{j_1<j_2}\left[2+\mathrm{e}^{\alpha+2\eta(j_2-j_1)}+\mathrm{e}^{-\alpha-2\eta(j_2-j_1)}\right]} \\
&= \frac{2\mathrm{e}^{\alpha}+\mathrm{e}^{2\alpha+2\eta(j-i)}+\mathrm{e}^{-2\eta(j-i)}}{\sum_{j_1<j_2}\left[2\mathrm{e}^{\alpha}+\mathrm{e}^{2\alpha+2\eta(j_2-j_1)}+\mathrm{e}^{-2\eta(j_2-j_1)}\right]} \\
&\to \frac{\mathrm{e}^{-2\eta(j-i)}}{\sum_{j_1<j_2}\mathrm{e}^{-2\eta(j_2-j_1)}} \quad \text{as } \alpha \to -\infty
\end{aligned}$$

Since we are assuming that the chain is infinitely long, then there is no need to normalize to the states. Thus, we can just write

$$C_{ij} = 1+\cos(\theta + 2q(i-j)).$$

For bound states

$$C_{ij} = \mathrm{e}^{-2\eta(j-1)}.$$

$\blacksquare$

Problem 3
Consider a particle in the one dimensional potential $V(x) = \lambda x^4$ such that the Hamiltonian is

$$H = \frac{p^2}{2m} + \lambda x^4.$$

(a) Write the corresponding Schrodinger equation for the (possible) wave function of energy E. Rescale the variable x by a constant a, namely define $z = ax$ and find a to eliminate λ from the equation (after appropriately rescaling E).

(b) Solve the resulting equation numerically for different values of E. [Use the boundary condition $\psi(0) = 1$, $\psi'(0) = 0$]. By considering the behavior of ψ at infinity, determine the lowest eigenvalue of the energy. After that, compute two other eigenvalues.

(c) Consider the wave function

$$\psi = A\mathrm{e}^{-\alpha x^2}.$$

Choose A such that the wave function $\psi(x)$ is normalized and then compute $E(\alpha) = \langle\psi|H|\psi\rangle$. Minimize $E(\alpha)$ with respect to α and compare the minimum value of $E(\alpha)$ with the result of the previous point to see how good the approximation is.

Note: This problem requires the use of a compute algebra program such as Mathematica, Maple, Matlab etc. (or the coding the integration in some computer language such as C, Fortran etc.). It is more difficult and requires some extra research but playing with the numerics is always useful to understand what one is doing analytically.

Solution. (a) Writing the corresponding Schrodinger equation, we have

$$\left\langle x\middle|\hat{H}\middle|\psi\right\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \lambda x^4\psi(x) = E\psi(x).$$

Letting $z = ax \implies x = \frac{z}{a}$, and denoting $\phi(z) = \psi\left(\frac{z}{a}\right)$ and we get

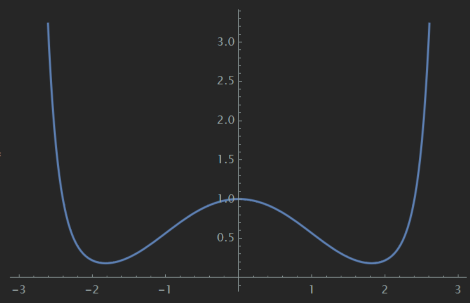
$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\left(\frac{z}{a}\right)^2}\psi\left(\frac{z}{a}\right) + \lambda\left(\frac{z}{a}\right)^4\psi\left(\frac{z}{a}\right) &= E\psi\left(\frac{z}{a}\right)\\
-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\phi(z) + \lambda\frac{z^4}{a^6}\phi(z) &= \frac{E}{a^2}\phi(z)\\
-\frac{\partial^2\phi(z)}{\partial z^2} + \frac{2m\lambda}{a^6\hbar^2}z^4\phi(z) &= \frac{2mE}{a^2\hbar^2}\phi(z).
\end{aligned}$$

Now, to eliminate λ, we set $\lambda = \frac{a^6\hbar^2}{2m} \implies a^2 = \left(\frac{2m\lambda}{\hbar^2}\right)^{\frac{1}{3}} \implies \epsilon = \left(\frac{2m}{\hbar^2}\right)^{\frac{2}{3}}\frac{E}{\lambda^{\frac{1}{3}}}$, and we get

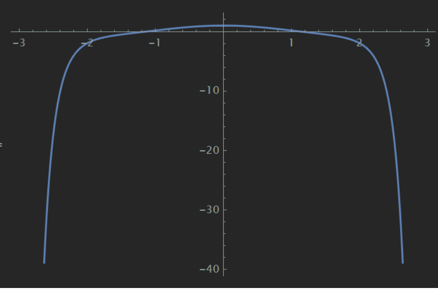
$$-\frac{\partial^2\phi(z)}{\partial z^2} + z^4\phi(z) = \epsilon\phi(z).$$

(b) We are given the boundary conditions $\psi(0) = 1$ and $\psi'(0) = 0$, which, after our transformation to z, we have $\phi(0) = 1$ and $\phi'(0) = 0$. Plugging our second-order IVP differential equation into Mathematica, we first change ϵ in a way that helps us see the change of our solution to the ODE. We then pick arbitrary starting and ending energies and search for the energy eigenvalue in between these two bounds. This effectively is solving for when the solution to the ODE coincides with the x-axes, up to a certain degree of precision.

```
In[1]:= epsilon = 1
        s = NDSolve[{-phi''[z] + z^4*phi[z] == epsilon * phi[z], phi[0] == 1, phi'[0] == 0}, phi, {z, -3, 3}]
        Plot[Evaluate[phi[z] /. %], {z, -3, 3}]

Out[1]= 1

Out[2]= {{phi → InterpolatingFunction[ Domain: {{-3., 3.}} Output: scalar ]}}

Out[3]=
```




```
In[4]:= epsilon = 2;
        NDSolve[{-D[D[phi[z], z], z] + z^4 * phi[z] == epsilon*phi[z], phi[0] == 1, phi'[0] == 0}, phi[z], {z, -3, 3}]
        Plot[Evaluate[phi[z] /. %], {z, -3, 3}]

Out[5]= {{phi[z] → InterpolatingFunction[ Domain: {{-3., 3.}} Output: scalar ][z]}}

Out[6]=
```




```
In[7]:= e1 = 1.0;
        e2 = 2.0;
        precision = 0.000001;
        While[e2 - e1 > precision,
         avg = (e1 + e2) / 2;
         sol = NDSolve[{-phi''[z] + z^4*phi[z] == avg*phi[z], phi[0] == 1, phi'[0] == 0}, phi, {z, -4, 4}];
         If[Part[phi[4] /. sol, 1] > 0, e1 = avg];
         If[Part[phi[4] /. sol, 1] < 0, e2 = avg];
        ]
        NumberForm[e1, 7]
        NumberForm[e2, 7]

Out[11]//NumberForm=
        1.060362

Out[12]//NumberForm=
        1.060363
```

Thus, the numerical result for our lowest energy eigenvalue is $\epsilon = 1.060362$. By the same method, and by searching using trial-and-error, we get the next two energy eigenvalues, which are $\epsilon_1 = 16.26183$ and $\epsilon_2 = 37.923$.

(c) Given $\psi(x) = A\mathrm{e}^{-\alpha x^2}$, we find A such that ψ is normalized

$$\begin{aligned}\langle\psi|\psi\rangle &= \int_{-\infty}^{\infty} \psi^*\psi \,\mathrm{d}x \\ &= |A|^2 \int_{-\infty}^{\infty} \mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x \\ &= \sqrt{\frac{\pi}{2\alpha}}|A|^2 \\ &= 1 \\ \implies A &= \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}}.\end{aligned}$$

Thus, we can write

$$\psi(x) = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\alpha x^2}.$$

Computing $\left\langle\psi\middle|\hat{H}\middle|\psi\right\rangle$, we have

$$\begin{aligned}E(\alpha) = \left\langle\psi\middle|\hat{H}\middle|\psi\right\rangle &= \sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty}\psi^*\left(\frac{\hat{p}^2}{2m}+\lambda\hat{x}^4\right)\psi\,\mathrm{d}x \\ &= \sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{-\alpha x^2}\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\lambda x^4\right)\mathrm{e}^{-\alpha x^2}\,\mathrm{d}x \\ &= \sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{-\alpha x^2}\left(\frac{-\hbar^2}{2m}\left(-2\alpha+4\alpha^2x^2\right)+\lambda x^4\right)\mathrm{e}^{-\alpha x^2}\,\mathrm{d}x \\ &= \sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty}\left(\frac{-\hbar^2}{2m}\left(-2\alpha+4\alpha^2x^2\right)+\lambda x^4\right)\mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x \\ &= \sqrt{\frac{2\alpha}{\pi}}\left[\frac{\hbar^2}{m}\int_{-\infty}^{\infty}\alpha\mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x - \frac{2\hbar^2}{m}\int_{-\infty}^{\infty}\alpha^2x^2\mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x + \int_{-\infty}^{\infty}\lambda x^4\mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x\right] \\ &= \sqrt{\frac{2\alpha}{\pi}}\left[\frac{\hbar^2}{m}\left(\sqrt{\frac{\pi\alpha}{2}}\right) - \frac{2\hbar^2}{m}\left(\frac{\sqrt{\pi\alpha}}{4\sqrt{2}}\right) + \left(\frac{3\lambda\sqrt{\pi}}{16\alpha^2\sqrt{2\alpha}}\right)\right] \\ &= \frac{\alpha\hbar^2}{2m} + \frac{3\lambda}{16\alpha^2}.\end{aligned}$$

To minimize $E(\alpha)$, we take the derivative of E with respect to α and set it to zero, and we get

$$\frac{\mathrm{d}E}{\mathrm{d}\alpha} = \frac{\hbar^2}{2m} - \frac{3\lambda}{8\alpha^3} = 0$$

$$\implies \alpha = \left(\frac{3m\lambda}{4\hbar^2}\right)^{\frac{1}{3}}.$$

Thus, the energy E is minimum when

$$\begin{aligned}E_{\min} &= \left(\frac{3m\lambda}{4\hbar^2}\right)^{\frac{1}{3}}\frac{\hbar^2}{2m} + \frac{3\lambda}{16}\left(\frac{4\hbar^2}{3m\lambda}\right)^{\frac{2}{3}} \\ &= \frac{9\lambda}{16}\left(\frac{4\hbar^2}{3m\lambda}\right)^{\frac{2}{3}}.\end{aligned}$$

Now, if we replace $E_{\min}$ into ϵ, we get

$$\begin{aligned}
\epsilon &= \left(\frac{2m}{\hbar^2}\right)^{\frac{2}{3}} \frac{E}{\lambda^{\frac{1}{3}}} \\
&= \left(\frac{2m}{\hbar^2}\right)^{\frac{2}{3}} \frac{1}{\lambda^{\frac{1}{3}}} \frac{9\lambda}{16} \left(\frac{4\hbar^2}{3m\lambda}\right)^{\frac{2}{3}} \\
&= \frac{9}{4}\left(\frac{1}{3}\right)^{\frac{2}{3}} \\
&\approx 1.08168,
\end{aligned}$$

which matches the value we got numerically in part (b).

■

Homework 4

Based on problems 2.3, 2.13, 2.18, 2.15, 2.23 of Sakurai's book.

Problem 1
An electron is subject to a uniform, time-independent magnetic field $\vec{B} = B\hat{z}$ in the z direction. At $t = 0$, the electron is in an eigenstate of $\vec{S} \cdot \hat{n}$ with eigenvalue $\frac{\hbar}{2}$. Here $\hat{n}$ is an arbitrary unit vector with polar angles (θ, ϕ). (Similar to previous homework)

(a) Find the state of the electron at any subsequent time t.

(b) At a given time t, what are the possible results of measuring S_x, and their probabilities? Repeat the same for S_z and S_y.

(c) Compute the mean value of S_x, S_y, and S_z as a function of time.

Solution. (a) We have that $\hat{n} = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))$. Then

$$S_{\hat{n}} = \vec{S} \cdot \hat{n} = \frac{\hbar}{2} \begin{pmatrix} \cos(\theta) & \sin(\theta)\mathrm{e}^{-i\phi} \\ \sin(\theta)\mathrm{e}^{i\phi} & -\cos(\theta) \end{pmatrix}.$$

The state with eigenvalue $\frac{\hbar}{2}$ is

$$\frac{\hbar}{2} \begin{pmatrix} \cos(\theta) - 1 & \sin(\theta)\mathrm{e}^{-i\phi} \\ \sin(\theta)\mathrm{e}^{i\phi} & -\cos(\theta) - 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \implies \begin{cases} (\cos(\theta) - 1)\alpha + \sin(\theta)\mathrm{e}^{-i\phi}\beta = 0 \\ \sin(\theta)\mathrm{e}^{i\phi}\alpha - (\cos(\theta) + 1)\beta = 0 \end{cases}$$
$$\implies \alpha = \frac{\sin(\theta)\mathrm{e}^{-i\phi}}{1 - \cos(\theta)}\beta.$$

Let $\beta = 1 - \cos(\theta)$, then $\alpha = \sin(\theta)\mathrm{e}^{-i\phi}$. The initial state of $S_{\hat{n}}$ corresponding to the eigenvalue $\frac{\hbar}{2}$ at $t = 0$ is

$$|\alpha, t_0 = 0, 0\rangle = \sin(\theta)\mathrm{e}^{-i\phi} |{\uparrow}\rangle + (1 - \cos(\theta)) |{\downarrow}\rangle .$$

Normalizing, we get

$$\begin{aligned} \left|\sin(\theta)\mathrm{e}^{-i\phi}\right|^2 + |1 - \cos(\theta)|^2 &= \sin^2(\theta) + (1 - \cos(\theta))^2 \\ &= \sin^2(\theta) + 1 - 2\cos(\theta) + \cos^2(\theta) \\ &= 2 - 2\cos(\theta) \\ &= 4\sin^2\left(\frac{\theta}{2}\right). \end{aligned}$$

Then,

$$\begin{aligned} |\alpha, t_0 = 0, 0\rangle &= \frac{1}{2\sin\left(\frac{\theta}{2}\right)} \left[\sin(\theta)\mathrm{e}^{-i\phi} |{\uparrow}\rangle + (1 - \cos(\theta)) |{\downarrow}\rangle\right] \\ &= \frac{1}{2\sin\left(\frac{\theta}{2}\right)} \left[2\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\phi} |{\uparrow}\rangle + 2\sin^2\left(\frac{\theta}{2}\right) |{\downarrow}\rangle\right] \\ &= \cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\phi} |{\uparrow}\rangle + \sin\left(\frac{\theta}{2}\right) |{\downarrow}\rangle \\ &= \cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}} |{\uparrow}\rangle + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}} |{\downarrow}\rangle . \end{aligned}$$

The magnetic field is given as $\vec{B} = B\hat{z}$, which yields the unitary operator $U(t, 0) = \mathrm{e}^{\frac{-i\omega\hat{S}_z t}{\hbar}}$, where $\omega = \frac{eB}{mc}$.

So, at any time t, the state of our system is

$$\begin{aligned}
|\alpha, t_0 = 0, t\rangle &= U(t,0)\,|\alpha, t_0 = 0, 0\rangle \\
&= \mathrm{e}^{\frac{-i\omega \hat{S}_z t}{\hbar}}\,|\alpha, t_0 = 0, 0\rangle \\
&= \mathrm{e}^{\frac{-i\omega \hat{S}_z t}{\hbar}}\left[\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\,|{\uparrow}\rangle + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\,|{\downarrow}\rangle\right] \\
&= \cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}\,|{\uparrow}\rangle + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\,|{\downarrow}\rangle,
\end{aligned}$$

where the last step is due to $\hat{S}_z\,|{\uparrow}\rangle = \frac{\hbar}{2}$ and $\hat{S}_z\,|{\downarrow}\rangle = -\frac{\hbar}{2}$. Additionally, the state for any time t is normalized since

$$\left|\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}\right|^2 + \left|\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\right|^2 = 1.$$

(b) We have

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- **For S_x:** Finding the eigenvalues, we have

$$\begin{aligned}
|S_x - \lambda \mathbb{I}| &= 0 \\
\begin{vmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{vmatrix} &= 0 \\
\lambda^2 - \frac{\hbar^2}{4} &= 0 \\
\lambda &= \pm\frac{\hbar}{2}.
\end{aligned}$$

The eigenvectors are given by

$$\begin{pmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \implies -\lambda\alpha + \frac{\hbar}{2}\beta = 0 \implies \beta = \frac{2\lambda}{\hbar}\alpha.$$

  - **For $\lambda = \frac{\hbar}{2}$:** We have $\beta = \alpha$. Since α is arbitrary, we can set $\alpha = 1 \implies \beta = 1$. Then, we have

$$|S_{x\uparrow}\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |{\uparrow}\rangle + |{\downarrow}\rangle.$$

  Normalizing the state, we get

$$|S_{x\uparrow}\rangle = \frac{1}{\sqrt{2}}\left(|{\uparrow}\rangle + |{\downarrow}\rangle\right).$$

The probability of measuring $\frac{\hbar}{2}$ is

$$\begin{aligned}
P_{x\uparrow} &= \left|\langle S_{x\uparrow}|\alpha, t_0 = 0, t\rangle\right|^2 \\
&= \left|\left(\frac{1}{\sqrt{2}}\langle\uparrow| + \frac{1}{\sqrt{2}}\langle\downarrow|\right)\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}|\downarrow\rangle\right)\right|^2 \\
&= \frac{1}{2}\left|\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}} + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\right|^2 \\
&= \frac{1}{2}\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}} + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\right)\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}} + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}\right) \\
&= \frac{1}{2}\left(\cos^2\left(\frac{\theta}{2}\right) + \sin^2\left(\frac{\theta}{2}\right) + \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\phi}\mathrm{e}^{i\omega t} + \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\phi}\mathrm{e}^{-i\omega t}\right) \\
&= \frac{1}{2}\left(1 + \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(\mathrm{e}^{i\phi}\mathrm{e}^{i\omega t} + \mathrm{e}^{-i\phi}\mathrm{e}^{-i\omega t}\right)\right) \\
&= \frac{1}{2}\left(1 + 2\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\cos(\phi + \omega t)\right) \\
&= \frac{1}{2}\left(1 + \sin(\theta)\cos(\phi + \omega t)\right).
\end{aligned}$$

– **For $\lambda = -\frac{\hbar}{2}$:** We have $\beta = -\alpha$. Since α is arbitrary, we can set $\alpha = 1 \implies \beta = -1$. Then, we have

$$|S_{x\downarrow}\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\uparrow\rangle - |\downarrow\rangle.$$

Normalizing the state, we get

$$|S_{x\downarrow}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle - |\downarrow\rangle\right).$$

The probability of measuring $-\frac{\hbar}{2}$ is

$$\begin{aligned}
P_{x\downarrow} &= \left|\langle S_{x\downarrow}|\alpha, t_0 = 0, t\rangle\right|^2 \\
&= \left|\left(\frac{1}{\sqrt{2}}\langle\uparrow| - \frac{1}{\sqrt{2}}\langle\downarrow|\right)\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}|\downarrow\rangle\right)\right|^2 \\
&= \frac{1}{2}\left|\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}} - \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\right|^2 \\
&= \frac{1}{2}\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}} - \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\right)\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}} - \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}\right) \\
&= \frac{1}{2}\left(\cos^2\left(\frac{\theta}{2}\right) + \sin^2\left(\frac{\theta}{2}\right) - \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\phi}\mathrm{e}^{i\omega t} - \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\phi}\mathrm{e}^{-i\omega t}\right) \\
&= \frac{1}{2}\left(1 - \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(\mathrm{e}^{i\phi}\mathrm{e}^{i\omega t} + \mathrm{e}^{-i\phi}\mathrm{e}^{-i\omega t}\right)\right) \\
&= \frac{1}{2}\left(1 - 2\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\cos(\phi + \omega t)\right) \\
&= \frac{1}{2}\left(1 - \sin(\theta)\cos(\phi + \omega t)\right).
\end{aligned}$$

- **For S_y:** Finding the eigenvalues, we have

$$\begin{aligned}|S_y - \lambda \mathbb{I}| &= 0\\ \begin{vmatrix}-\lambda & -\frac{i\hbar}{2}\\ \frac{i\hbar}{2} & -\lambda\end{vmatrix} &= 0\\ \lambda^2 - \frac{\hbar^2}{4} &= 0\\ \lambda &= \pm\frac{\hbar}{2}.\end{aligned}$$

The eigenvectors are given by

$$\begin{pmatrix}-\lambda & -\frac{i\hbar}{2}\\ \frac{i\hbar}{2} & -\lambda\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \begin{pmatrix}0\\ 0\end{pmatrix} \implies -\lambda\alpha - \frac{i\hbar}{2}\beta = 0 \implies \beta = \frac{2i\lambda}{\hbar}\alpha.$$

  - **For $\lambda = \frac{\hbar}{2}$:** We have $\beta = i\alpha$. Since α is arbitrary, we can set $\alpha = 1 \implies \beta = i$. Then, we have

$$|S_{y\uparrow}\rangle = \begin{pmatrix}1\\ i\end{pmatrix} = \begin{pmatrix}1\\ 0\end{pmatrix} + i\begin{pmatrix}0\\ 1\end{pmatrix} = |{\uparrow}\rangle + i\,|{\downarrow}\rangle\,.$$

Normalizing the state, we get

$$|S_{y\uparrow}\rangle = \frac{1}{\sqrt{2}}\left(|{\uparrow}\rangle + i\,|{\downarrow}\rangle\right).$$

The probability of measuring $\frac{\hbar}{2}$ is

$$\begin{aligned}P_{y\uparrow} &= \left|\langle S_{y\uparrow}|\alpha, t_0 = 0, t\rangle\right|^2\\ &= \left|\left(\frac{1}{\sqrt{2}}\langle{\uparrow}| - \frac{i}{\sqrt{2}}\langle{\downarrow}|\right)\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}\,|{\uparrow}\rangle + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\,|{\downarrow}\rangle\right)\right|^2\\ &= \frac{1}{2}\left|\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}} - i\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\right|^2\\ &= \frac{1}{2}\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}} - i\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\right)\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}} + i\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}\right)\\ &= \frac{1}{2}\left(\cos^2\left(\frac{\theta}{2}\right) + \sin^2\left(\frac{\theta}{2}\right) - i\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\phi}\mathrm{e}^{i\omega t} + i\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\phi}\mathrm{e}^{-i\omega t}\right)\\ &= \frac{1}{2}\left(1 - i\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(\mathrm{e}^{i\phi}\mathrm{e}^{i\omega t} - \mathrm{e}^{-i\phi}\mathrm{e}^{-i\omega t}\right)\right)\\ &= \frac{1}{2}\left(1 + 2\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\sin(\phi + \omega t)\right)\\ &= \frac{1}{2}\left(1 + \sin(\theta)\sin(\phi + \omega t)\right).\end{aligned}$$

  - **For $\lambda = -\frac{\hbar}{2}$:** We have $\beta = -i\alpha$. Since α is arbitrary, we can set $\alpha = 1 \implies \beta = -i$. Then, we have

$$|S_{y\downarrow}\rangle = \begin{pmatrix}1\\ -i\end{pmatrix} = \begin{pmatrix}1\\ 0\end{pmatrix} - i\begin{pmatrix}0\\ 1\end{pmatrix} = |{\uparrow}\rangle - i\,|{\downarrow}\rangle\,.$$

Normalizing the state, we get

$$|S_{y\downarrow}\rangle = \frac{1}{\sqrt{2}}\left(|{\uparrow}\rangle - i\,|{\downarrow}\rangle\right).$$

The probability of measuring $-\frac{\hbar}{2}$ is

$$\begin{aligned}
P_{y\downarrow} &= |\langle S_{y\downarrow}|\alpha, t_0 = 0, t\rangle|^2 \\
&= \left|\left(\frac{1}{\sqrt{2}}\langle\uparrow| + \frac{i}{\sqrt{2}}\langle\downarrow|\right)\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}|\downarrow\rangle\right)\right|^2 \\
&= \frac{1}{2}\left|\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}} + i\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\right|^2 \\
&= \frac{1}{2}\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}} + i\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\right)\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}} - i\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}\right) \\
&= \frac{1}{2}\left(\cos^2\left(\frac{\theta}{2}\right) + \sin^2\left(\frac{\theta}{2}\right) + i\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\phi}\mathrm{e}^{i\omega t} - i\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\phi}\mathrm{e}^{-i\omega t}\right) \\
&= \frac{1}{2}\left(1 + i\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(\mathrm{e}^{i\phi}\mathrm{e}^{i\omega t} - \mathrm{e}^{-i\phi}\mathrm{e}^{-i\omega t}\right)\right) \\
&= \frac{1}{2}\left(1 - 2\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\sin(\phi + \omega t)\right) \\
&= \frac{1}{2}\left(1 - \sin(\theta)\sin(\phi + \omega t)\right).
\end{aligned}$$

- **For S_z:** Finding the eigenvalues, we have

$$\begin{aligned}
|S_z - \lambda\mathbb{I}| &= 0 \\
\begin{vmatrix} \frac{\hbar}{2} - \lambda & 0 \\ 0 & -\frac{\hbar}{2} - \lambda \end{vmatrix} &= 0 \\
-\left(\frac{\hbar}{2} - \lambda\right)\left(\frac{\hbar}{2} + \lambda\right) &= 0 \\
\lambda &= \pm\frac{\hbar}{2}.
\end{aligned}$$

The eigenvectors are given by

$$\begin{pmatrix} \frac{\hbar}{2} - \lambda & 0 \\ 0 & -\frac{\hbar}{2} - \lambda \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \implies \left(\frac{\hbar}{2} - \lambda\right)\alpha = 0 \text{ and } \left(\frac{\hbar}{2} + \lambda\right)\beta = 0.$$

  - **For $\lambda = \frac{\hbar}{2}$:** We have $0\alpha = 0$ and $\hbar\beta = 0$. Since α is arbitrary, we can set $\alpha = 1$ and then $\beta = 0$. Then, we have

$$|S_{z\uparrow}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\uparrow\rangle.$$

The state is already normalized.
The probability of measuring $\frac{\hbar}{2}$ is

$$\begin{aligned}
P_{z\uparrow} &= |\langle S_{z\uparrow}|\alpha, t_0 = 0, t\rangle|^2 \\
&= \left|\langle\uparrow|\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}|\downarrow\rangle\right)\right|^2 \\
&= \left|\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}\right|^2 \\
&= \cos^2\left(\frac{\theta}{2}\right).
\end{aligned}$$

  - **For $\lambda = -\frac{\hbar}{2}$:** We have $\hbar\alpha = 0$ and $0\beta = 0$. Since β is arbitrary, we can set $\beta = 1$ and then $\alpha = 0$. Then, we have

$$|S_{x\downarrow}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\downarrow\rangle.$$

The state is already normalized.
The probability of measuring $-\frac{\hbar}{2}$ is

$$\begin{aligned}
P_{z\downarrow} &= \left|\langle S_{z\downarrow}|\alpha, t_0 = 0, t\rangle\right|^2 \\
&= \left|\langle\downarrow|\left(\cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-i\frac{\phi}{2}}\mathrm{e}^{\frac{-i\omega t}{2}}\left|\uparrow\right\rangle + \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\left|\downarrow\right\rangle\right)\right|^2 \\
&= \left|\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{i\frac{\phi}{2}}\mathrm{e}^{\frac{i\omega t}{2}}\right|^2 \\
&= \sin^2\left(\frac{\theta}{2}\right).
\end{aligned}$$

(c) Formally, the expectation value is given by

$$\langle x\rangle = \sum_x xP(x).$$

- **For S_x:** We have

$$\begin{aligned}
\langle S_x\rangle &= \left(\frac{\hbar}{2}\right)P_{x\uparrow} + \left(-\frac{\hbar}{2}\right)P_{x\downarrow} \\
&= \frac{\hbar}{4}\left[(1+\sin(\theta)\cos(\phi+\omega t)) - (1-\sin(\theta)\cos(\phi+\omega t))\right] \\
&= \frac{\hbar}{2}\sin(\theta)\cos(\phi+\omega t).
\end{aligned}$$

- **For S_y:** We have

$$\begin{aligned}
\langle S_y\rangle &= \left(\frac{\hbar}{2}\right)P_{y\uparrow} + \left(-\frac{\hbar}{2}\right)P_{y\downarrow} \\
&= \frac{\hbar}{4}\left[(1+\sin(\theta)\sin(\phi+\omega t)) - (1-\sin(\theta)\sin(\phi+\omega t))\right] \\
&= \frac{\hbar}{2}\sin(\theta)\sin(\phi+\omega t).
\end{aligned}$$

- **For S_z:** We have

$$\begin{aligned}
\langle S_z\rangle &= \left(\frac{\hbar}{2}\right)P_{z\uparrow} + \left(-\frac{\hbar}{2}\right)P_{z\downarrow} \\
&= \frac{\hbar}{2}\left[\cos^2\left(\frac{\theta}{2}\right) - \sin^2\left(\frac{\theta}{2}\right)\right] \\
&= \frac{\hbar}{2}\cos(\theta).
\end{aligned}$$

■

Problem 2
Consider a one-dimensional harmonic oscillator with frequency ω. Using the algebraic method (*i.e.* operators a, $a^\dagger$) compute

(a) $\langle m|x|n\rangle$, $\langle m|p|n\rangle$, $\langle m|xp+px|n\rangle$, $\langle m|x^2|n\rangle$, $\langle m|p^2|n\rangle$, where $|n\rangle$ and $|m\rangle$ are eigenstates of energy.

(b) $\langle \alpha|x|\alpha\rangle$, $\langle \alpha|p|\alpha\rangle$, $\langle \alpha|x^2|\alpha\rangle$, $\langle \alpha|p^2|\alpha\rangle$, where $|\alpha\rangle$ is a coherent state.

(c) Use the previous result to show that coherent states have minimum uncertainty.

Solution. We know that

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^\dagger + \hat{a}\right), \qquad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a}^\dagger - \hat{a}\right)$$

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n|0\rangle, \qquad \hat{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle, \qquad \hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle,$$

(a) • Computing $\langle m|\hat{x}|n\rangle$, we have

$$\begin{aligned}
\langle m|\hat{x}|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left\langle m\middle|\hat{a}^\dagger + \hat{a}\middle|n\right\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\left\langle m\middle|\hat{a}^\dagger\middle|n\right\rangle + \langle m|\hat{a}|n\rangle\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\langle m|n+1\rangle + \sqrt{n}\,\langle m|n-1\rangle\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\delta_{m,n+1} + \sqrt{n}\delta_{m,n-1}\right).
\end{aligned}$$

• Computing $\langle m|\hat{p}|n\rangle$, we have

$$\begin{aligned}
\langle m|\hat{p}|n\rangle &= i\sqrt{\frac{\hbar m\omega}{2}}\left\langle m\middle|\hat{a}^\dagger - \hat{a}\middle|n\right\rangle \\
&= i\sqrt{\frac{\hbar m\omega}{2}}\left(\left\langle m\middle|\hat{a}^\dagger\middle|n\right\rangle - \langle m|\hat{a}|n\rangle\right) \\
&= i\sqrt{\frac{\hbar m\omega}{2}}\left(\sqrt{n+1}\,\langle m|n+1\rangle - \sqrt{n}\,\langle m|n-1\rangle\right) \\
&= i\sqrt{\frac{\hbar m\omega}{2}}\left(\sqrt{n+1}\delta_{m,n+1} - \sqrt{n}\delta_{m,n-1}\right).
\end{aligned}$$

- Computing $\langle m|\hat{x}\hat{p}+\hat{p}\hat{x}|n\rangle$, we have

$$\begin{aligned}
\langle m|\hat{x}\hat{p}+\hat{p}\hat{x}|n\rangle &= \langle m|\hat{x}\hat{p}|n\rangle + \langle m|\hat{p}\hat{x}|n\rangle \\
&= i\sqrt{\frac{\hbar m\omega}{2}}\left\langle m\middle|\hat{x}\left(\hat{a}^\dagger-\hat{a}\right)\middle|n\right\rangle + \sqrt{\frac{\hbar}{2m\omega}}\left\langle m\middle|\hat{p}\left(\hat{a}^\dagger+\hat{a}\right)\middle|n\right\rangle \\
&= i\sqrt{\frac{\hbar m\omega}{2}}\left[\left\langle m\middle|\hat{x}\hat{a}^\dagger\middle|n\right\rangle - \langle m|\hat{x}\hat{a}|n\rangle\right] + \sqrt{\frac{\hbar}{2m\omega}}\left[\left\langle m\middle|\hat{p}\hat{a}^\dagger\middle|n\right\rangle + \langle m|\hat{p}\hat{a}|n\rangle\right] \\
&= i\sqrt{\frac{\hbar m\omega}{2}}\left[\sqrt{n+1}\,\langle m|\hat{x}|n+1\rangle - \sqrt{n}\,\langle m|\hat{x}|n-1\rangle\right] \\
&\quad + \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n+1}\,\langle m|\hat{p}|n+1\rangle + \sqrt{n}\,\langle m|\hat{p}|n-1\rangle\right] \\
&= i\sqrt{\frac{\hbar m\omega}{2}}\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n+1}\left\langle m\middle|\hat{a}^\dagger+\hat{a}\middle|n+1\right\rangle - \sqrt{n}\left\langle m\middle|\hat{a}^\dagger+\hat{a}\middle|n-1\right\rangle\right] \\
&\quad + \sqrt{\frac{\hbar}{2m\omega}}i\sqrt{\frac{\hbar m\omega}{2}}\left[\sqrt{n+1}\left\langle m\middle|\hat{a}^\dagger-\hat{a}\middle|n+1\right\rangle + \sqrt{n}\left\langle m\middle|\hat{a}^\dagger-\hat{a}\middle|n-1\right\rangle\right] \\
&= \frac{i\hbar}{2}\left[\sqrt{n+1}\left(\left\langle m\middle|\hat{a}^\dagger\middle|n+1\right\rangle + \langle m|\hat{a}|n+1\rangle\right) - \sqrt{n}\left(\left\langle m\middle|\hat{a}^\dagger\middle|n-1\right\rangle + \langle m|\hat{a}|n-1\rangle\right)\right] \\
&\quad + \frac{i\hbar}{2}\left[\sqrt{n+1}\left(\left\langle m\middle|\hat{a}^\dagger\middle|n+1\right\rangle - \langle m|\hat{a}|n+1\rangle\right) + \sqrt{n}\left(\left\langle m\middle|\hat{a}^\dagger\middle|n-1\right\rangle - \langle m|\hat{a}|n-1\rangle\right)\right] \\
&= \frac{i\hbar}{2}\left[\sqrt{n+1}\left(\sqrt{n+2}\,\langle m|n+2\rangle + \sqrt{n+1}\,\langle m|n\rangle\right) - \sqrt{n}\left(\sqrt{n}\,\langle m|n\rangle + \sqrt{n-1}\,\langle m|n-2\rangle\right)\right] \\
&\quad + \frac{i\hbar}{2}\left[\sqrt{n+1}\left(\sqrt{n+2}\,\langle m|n+2\rangle - \sqrt{n+1}\,\langle m|n\rangle\right) + \sqrt{n}\left(\sqrt{n}\,\langle m|n\rangle - \sqrt{n-1}\,\langle m|n-2\rangle\right)\right] \\
&= \frac{i\hbar}{2}\left[\sqrt{(n+1)(n+2)}\delta_{m,n+2} + (n+1)\delta_{m,n} - n\delta_{m,n} - \sqrt{n(n-1)}\delta_{m,n-2}\right] \\
&\quad + \frac{i\hbar}{2}\left[\sqrt{(n+1)(n+2)}\delta_{m,n+2} - (n+1)\delta_{m,n} + n\delta_{m,n} - \sqrt{n(n-1)}\delta_{m,n-2}\right] \\
&= i\hbar\left[\sqrt{(n+1)(n+2)}\delta_{m,n+2} - \sqrt{n(n-1)}\delta_{m,n-2}\right].
\end{aligned}$$

We could have also used the property $\hat{x}\hat{p}+\hat{p}\hat{x} = 2\hat{x}\hat{p} - [\hat{x}\hat{p}] = 2\hat{x}\hat{p} - i\hbar$.

- Computing $\left\langle m\middle|\hat{x}^2\middle|n\right\rangle$, we have

$$\begin{aligned}
\left\langle m\middle|\hat{x}^2\middle|n\right\rangle &= \frac{\hbar}{2m\omega}\left\langle m\middle|\left(\hat{a}^\dagger+\hat{a}\right)\left(\hat{a}^\dagger+\hat{a}\right)\middle|n\right\rangle \\
&= \frac{\hbar}{2m\omega}\langle m|\left(\hat{a}^\dagger+\hat{a}\right)\left(\sqrt{n+1}\,|n+1\rangle + \sqrt{n}\,|n-1\rangle\right) \\
&= \frac{\hbar}{2m\omega}\langle m|\left(\sqrt{n+2}\sqrt{n+1}\,|n+2\rangle + \sqrt{n}\sqrt{n}\,|n\rangle + \sqrt{n+1}\sqrt{n+1}\,|n\rangle + \sqrt{n}\sqrt{n-1}\,|n-2\rangle\right) \\
&= \frac{\hbar}{2m\omega}\left[\sqrt{(n+1)(n+2)}\delta_{m,n+2} + n\delta_{m,n} + (n+1)\delta_{m,n} + \sqrt{n(n-1)}\delta_{m,n-2}\right] \\
&= \frac{\hbar}{2m\omega}\left[\sqrt{(n+1)(n+2)}\delta_{m,n+2} + (2n+1)\delta_{m,n} + \sqrt{n(n-1)}\delta_{m,n-2}\right].
\end{aligned}$$

- Computing $\langle m|\hat{p}^2|n\rangle$, we have

$$\begin{aligned}
\langle m|\hat{p}^2|n\rangle &= -\frac{\hbar m\omega}{2}\langle m|\left(\hat{a}^\dagger-\hat{a}\right)\left(\hat{a}^\dagger-\hat{a}\right)|n\rangle \\
&= -\frac{\hbar m\omega}{2}\langle m|\left(\hat{a}^\dagger-\hat{a}\right)\left(\sqrt{n+1}\,|n+1\rangle-\sqrt{n}\,|n-1\rangle\right) \\
&= -\frac{\hbar m\omega}{2}\langle m|\left(\sqrt{n+2}\sqrt{n+1}\,|n+2\rangle-\sqrt{n}\sqrt{n}\,|n\rangle-\sqrt{n+1}\sqrt{n+1}\,|n\rangle+\sqrt{n}\sqrt{n-1}\,|n-2\rangle\right) \\
&= -\frac{\hbar m\omega}{2}\left[\sqrt{(n+1)(n+2)}\delta_{m,n+2}-n\delta_{m,n}-(n+1)\delta_{m,n}+\sqrt{n(n-1)}\delta_{m,n-2}\right] \\
&= -\frac{\hbar m\omega}{2}\left[\sqrt{(n+1)(n+2)}\delta_{m,n+2}-(2n+1)\delta_{m,n}+\sqrt{n(n-1)}\delta_{m,n-2}\right].
\end{aligned}$$

(b) Consider a normalized coherent state

$$|\alpha\rangle = \mathrm{e}^{-\frac{1}{2}|\alpha|^2}\mathrm{e}^{\alpha\hat{a}^\dagger}\,|0\rangle\,.$$

We have that $|\alpha\rangle$ is an eigenvector of $\hat{a}$: $\hat{a}\,|\alpha\rangle=\alpha\,|\alpha\rangle \iff \langle\alpha|\,\hat{a}^\dagger=\alpha^*\,\langle\alpha|$.
Additionally, we have

$$[\hat{a},\hat{a}^\dagger]=1,\qquad [\hat{a},\left(\hat{a}^\dagger\right)^n]=n\left(\hat{a}^\dagger\right)^{n-1}.$$

- Computing $\langle\alpha|\hat{x}|\alpha\rangle$, we have

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

- Computing $\langle\alpha|\hat{p}|\alpha\rangle$, we have

$$\begin{aligned}
\langle\alpha|\hat{p}|\alpha\rangle &= i\sqrt{\frac{m\hbar\omega}{2}}\langle\alpha|\hat{a}^\dagger-\hat{a}|\alpha\rangle \\
&= i\sqrt{\frac{m\hbar\omega}{2}}\left(\langle\alpha|\hat{a}^\dagger|\alpha\rangle-\langle\alpha|\hat{a}|\alpha\rangle\right) \\
&= i\sqrt{\frac{m\hbar\omega}{2}}\left(\alpha^*-\alpha\right).
\end{aligned}$$

- Computing $\langle\alpha|\hat{x}^2|\alpha\rangle$, we have

$$\begin{aligned}
\langle\alpha|\hat{x}^2|\alpha\rangle &= \frac{\hbar}{2m\omega}\langle\alpha|\left(\hat{a}^\dagger+\hat{a}\right)\left(\hat{a}^\dagger+\hat{a}\right)|\alpha\rangle \\
&= \frac{\hbar}{2m\omega}\left\langle\alpha\middle|\left(\hat{a}^\dagger\right)^2+\hat{a}^\dagger\hat{a}+\hat{a}\hat{a}^\dagger+\hat{a}^2\middle|\alpha\right\rangle \\
&= \frac{\hbar}{2m\omega}\left[\left\langle\alpha\middle|\left(\hat{a}^\dagger\right)^2\middle|\alpha\right\rangle+\langle\alpha|\hat{a}^\dagger\hat{a}+\hat{a}\hat{a}^\dagger|\alpha\rangle+\langle\alpha|\hat{a}^2|\alpha\rangle\right] \\
&= \frac{\hbar}{2m\omega}\left[\left\langle\alpha\middle|\left(\hat{a}^\dagger\right)^2\middle|\alpha\right\rangle+\langle\alpha|2\hat{a}^\dagger\hat{a}-[\hat{a}^\dagger,\hat{a}]|\alpha\rangle+\langle\alpha|\hat{a}^2|\alpha\rangle\right] \\
&= \frac{\hbar}{2m\omega}\left[\left\langle\alpha\middle|\left(\hat{a}^\dagger\right)^2\middle|\alpha\right\rangle+\langle\alpha|2\hat{a}^\dagger\hat{a}|\alpha\rangle-\langle\alpha|[\hat{a}^\dagger,\hat{a}]|\alpha\rangle+\langle\alpha|\hat{a}^2|\alpha\rangle\right] \\
&= \frac{\hbar}{2m\omega}\left[\left(\alpha^*\right)^2+2\alpha^*\alpha+1+\alpha^2\right] \\
&= \frac{\hbar}{2m\omega}\left[\left(\alpha^*+\alpha\right)^2+1\right].
\end{aligned}$$

- Computing $\langle\alpha|\hat{p}|\alpha\rangle$, we have

$$\begin{aligned}
\langle\alpha|\hat{p}^2|\alpha\rangle &= -\frac{m\hbar\omega}{2}\langle\alpha|\left(\hat{a}^\dagger - \hat{a}\right)\left(\hat{a}^\dagger - \hat{a}\right)|\alpha\rangle \\
&= -\frac{m\hbar\omega}{2}\left\langle\alpha\middle|\left(\hat{a}^\dagger\right)^2 - \hat{a}^\dagger\hat{a} - \hat{a}\hat{a}^\dagger + \hat{a}^2\middle|\alpha\right\rangle \\
&= -\frac{m\hbar\omega}{2}\left[\left\langle\alpha\middle|\left(\hat{a}^\dagger\right)^2\middle|\alpha\right\rangle - \langle\alpha|\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger|\alpha\rangle + \langle\alpha|\hat{a}^2|\alpha\rangle\right] \\
&= -\frac{m\hbar\omega}{2}\left[\left\langle\alpha\middle|\left(\hat{a}^\dagger\right)^2\middle|\alpha\right\rangle - \langle\alpha|2\hat{a}^\dagger\hat{a} - [\hat{a}^\dagger,\hat{a}]|\alpha\rangle + \langle\alpha|\hat{a}^2|\alpha\rangle\right] \\
&= -\frac{m\hbar\omega}{2}\left[\left\langle\alpha\middle|\left(\hat{a}^\dagger\right)^2\middle|\alpha\right\rangle - \langle\alpha|2\hat{a}^\dagger\hat{a}|\alpha\rangle + \langle\alpha|[\hat{a}^\dagger,\hat{a}]|\alpha\rangle + \langle\alpha|\hat{a}^2|\alpha\rangle\right] \\
&= -\frac{m\hbar\omega}{2}\left[\left(\alpha^*\right)^2 - 2\alpha^*\alpha - 1 + \alpha^2\right] \\
&= -\frac{m\hbar\omega}{2}\left[\left(\alpha^* - \alpha\right)^2 - 1\right].
\end{aligned}$$

(c) We need to show that coherent states have minimum uncertainty. In other words, we need to prove that

$$\Delta x \Delta p = \frac{\hbar}{2}.$$

- Calculating the uncertainty Δx, we have

$$\begin{aligned}
(\Delta x)^2 &= \langle\alpha|\hat{x}^2|\alpha\rangle - \langle\alpha|\hat{x}|\alpha\rangle^2 \\
&= \frac{\hbar}{2m\omega}\left[\left(\alpha^* + \alpha\right)^2 + 1\right] - \left(\sqrt{\frac{\hbar}{2m\omega}}\left(\alpha^* + \alpha\right)\right)^2 \\
&= \frac{\hbar}{2m\omega}\left[\left(\alpha^* + \alpha\right)^2 + 1\right] - \frac{\hbar}{2m\omega}\left(\alpha^* + \alpha\right)^2 \\
&= \frac{\hbar}{2m\omega} \\
&\implies \Delta x = \sqrt{\frac{\hbar}{2m\omega}}.
\end{aligned}$$

- Calculating the uncertainty Δp, we have

$$\begin{aligned}
(\Delta p)^2 &= \langle\alpha|\hat{p}^2|\alpha\rangle - \langle\alpha|\hat{p}|\alpha\rangle^2 \\
&= -\frac{m\hbar\omega}{2}\left[\left(\alpha^* - \alpha\right)^2 - 1\right] - \left(i\sqrt{\frac{m\hbar\omega}{2}}\left(\alpha^* - \alpha\right)\right)^2 \\
&= -\frac{m\hbar\omega}{2}\left[\left(\alpha^* - \alpha\right)^2 - 1\right] + \frac{m\hbar\omega}{2}\left(\alpha^* - \alpha\right)^2 \\
&= \frac{m\hbar\omega}{2} \\
&\implies \Delta p = \sqrt{\frac{m\hbar\omega}{2}}.
\end{aligned}$$

Thus,

$$\Delta x \Delta p = \left(\sqrt{\frac{\hbar}{2m\omega}}\right)\left(\sqrt{\frac{m\hbar\omega}{2}}\right) = \frac{\hbar}{2},$$

which is what we needed to prove.

$\blacksquare$

Problem 3
Continuing from Problem 2, consider $x_H(t)$, the position operator in the Heisenberg picture. Evaluate the correlation function

$$C(t) = \langle 0|x_H(t)x_H(0)|0\rangle \,,$$

where $|0\rangle$ is the ground state.

Solution. In the Heisenberg picture, the position operator $x_H(t)$ is given by

$$x_H(t) = \hat{U}^\dagger(t)\hat{x}_H(0)\hat{U}(t),$$

where $x_H(0) = \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^\dagger + \hat{a}\right)$, $\hat{U}(t) = \mathrm{e}^{-\frac{i\hat{H}t}{\hbar}}$, and $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$ with $\hat{H} = \hat{H}^\dagger$.
Additionally, we know that $\hat{a}\,|0\rangle = 0 \iff \langle 0|\,\hat{a}^\dagger = 0$.
We have

$$\begin{aligned}
C(t) &= \langle 0|\hat{x}_H(t)\hat{x}_H(0)|0\rangle \\
&= \left\langle 0\middle|\hat{U}^\dagger(t)\hat{x}_H(0)\hat{U}(t)\hat{x}_H(0)\middle|0\right\rangle \\
&= \frac{\hbar}{2m\omega}\left\langle 0\middle|\mathrm{e}^{\frac{i\hat{H}t}{\hbar}}\left(\hat{a}^\dagger + \hat{a}\right)\mathrm{e}^{-\frac{i\hat{H}t}{\hbar}}\left(\hat{a}^\dagger + \hat{a}\right)\middle|0\right\rangle \\
&= \frac{\hbar}{2m\omega}\left\langle 0\middle|\mathrm{e}^{\frac{i\hat{H}t}{\hbar}}\left(\hat{a}^\dagger + \hat{a}\right)\mathrm{e}^{-\frac{i\hat{H}t}{\hbar}}\hat{a}^\dagger\middle|0\right\rangle \\
&= \frac{\hbar\sqrt{1}}{2m\omega}\left\langle 0\middle|\mathrm{e}^{\frac{i\hat{H}t}{\hbar}}\left(\hat{a}^\dagger + \hat{a}\right)\mathrm{e}^{-\frac{i\hat{H}t}{\hbar}}\middle|1\right\rangle \\
&= \frac{\hbar}{2m\omega}\left\langle 0\middle|\mathrm{e}^{i\omega t\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)}\left(\hat{a}^\dagger + \hat{a}\right)\mathrm{e}^{-i\omega t\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)}\middle|1\right\rangle \\
&= \frac{\hbar}{2m\omega}\left\langle 0\middle|\mathrm{e}^{i\omega t\hat{a}^\dagger\hat{a}}\left(\hat{a}^\dagger + \hat{a}\right)\mathrm{e}^{-i\omega t\hat{a}^\dagger\hat{a}}\middle|1\right\rangle \\
&= \frac{\hbar}{2m\omega}\left\langle 0\middle|\left(\hat{a}^\dagger + \hat{a}\right)\mathrm{e}^{-i\omega t\left(\hat{a}^\dagger\hat{a}-\hat{a}\hat{a}^\dagger\right)}\middle|1\right\rangle \\
&= \frac{\hbar}{2m\omega}\left\langle 0\middle|\left(\hat{a}^\dagger + \hat{a}\right)\mathrm{e}^{-i\omega t[\hat{a}^\dagger,\hat{a}]}\middle|1\right\rangle \\
&= \frac{\hbar}{2m\omega}\left\langle 0\middle|\left(\hat{a}^\dagger + \hat{a}\right)\mathrm{e}^{i\omega t}\middle|1\right\rangle \\
&= \frac{\hbar}{2m\omega}\mathrm{e}^{i\omega t}\langle 0|\hat{a}|1\rangle \\
&= \frac{\hbar}{2m\omega}\mathrm{e}^{i\omega t}\langle 0|0\rangle \\
&= \frac{\hbar}{2m\omega}\mathrm{e}^{i\omega t}.
\end{aligned}$$

■

Problem 4
A particle of mass m in one dimension is bound to a fix center by an attractive δ-function potential

$$V(x) = -\lambda\delta(x), \quad (\lambda > 0).$$

At $t = 0$, the potential is suddenly switched off, that is, $V = 0$ for $t > 0$. At $t = 0$, the wave function is the one of the bound state since it cannot change instantaneously ($\partial_x \psi$ is finite for finite Hamiltonian). Compute the wave function for $t > 0$.

Solution. Given that the potential at $t = 0$ is $V(x) = -\lambda\delta(x)$ for $\lambda > 0$.

- **At $x = 0$:**
  The Schrodinger equation is given by
  $$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) - \lambda\delta(x)\psi(x) = E\psi(x).$$
  Integrating over space right around $x = 0$, *i.e.* within a range $(-\epsilon, \epsilon)$ and then taking the limit as $\epsilon \to 0$, we have
  $$\begin{aligned}
  -\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{\partial^2}{\partial x^2}\psi(x)\,\mathrm{d}x - \lambda\int_{-\epsilon}^{\epsilon}\delta(x)\psi(x)\,\mathrm{d}x &= E\int_{-\epsilon}^{\epsilon}\psi(x)\,\mathrm{d}x \\
  -\frac{\hbar^2}{2m}\left.\frac{\partial\psi(x)}{\partial x}\right|_{-\epsilon}^{\epsilon} - \lambda\psi(0) &= 0 \\
  -\frac{\hbar^2}{2m}\left(\frac{\partial\psi(0^+)}{\partial x} - \frac{\partial\psi(0^-)}{\partial x}\right) - \lambda\psi(0) &= 0 \\
  \frac{\partial\psi(0^+)}{\partial x} - \frac{\partial\psi(0^-)}{\partial x} &= -\frac{2m\lambda}{\hbar^2}\psi(0).
  \end{aligned}$$

- **At $x \neq 0$:**
  The Schrodinger equation is given by
  $$\begin{aligned}
  -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) &= E\psi(x) \\
  \frac{\partial^2\psi(x)}{\partial x^2} &= -\frac{2mE}{\hbar^2}\psi(x).
  \end{aligned}$$
  Let $k^2 \equiv -\frac{2mE}{\hbar^2}$, then
  $$\frac{\partial^2\psi(x)}{\partial x^2} = k^2\psi(x) \implies \psi(x) = \begin{cases} A\mathrm{e}^{-kx}, & \text{if } x > 0 \\ B\mathrm{e}^{kx}, & \text{if } x < 0 \end{cases}$$
  - **Continuity at $x = 0$:**
    We have that
    $$\begin{gathered}
    \psi(0^+) = A = \psi(0^-) = B = \psi(0), \\
    \partial_x\psi(0^+) = -kA, \quad \partial_x\psi(0^+) = kB.
    \end{gathered}$$

Replacing in the Schrodinger equation, we have

$$\begin{aligned}
\frac{\partial\psi(0^+)}{\partial x} - \frac{\partial\psi(0^-)}{\partial x} &= -\frac{2m\lambda}{\hbar^2}\psi(0) \\
-kA - kB &= -\frac{2m\lambda}{\hbar^2}A \\
2kA &= \frac{2m\lambda}{\hbar^2}A \\
k &= \frac{m\lambda}{\hbar^2}.
\end{aligned}$$

Thus, the solution is

$$\psi(x,0) = A\mathrm{e}^{-\frac{m\lambda}{\hbar^2}|x|}.$$

To find A, we use the normalization condition, and hence

$$\begin{aligned}
\int_{-\infty}^{\infty} |\psi(x)|^2 \,\mathrm{d}x &= 1 \\
2\int_{0}^{\infty} |A|^2 \mathrm{e}^{-\frac{2m\lambda}{\hbar^2}x} \,\mathrm{d}x &= 1 \\
2|A|^2 \left(-\frac{\hbar^2}{2m\lambda}\right) \mathrm{e}^{-\frac{2m\lambda}{\hbar^2}x}\Big|_0^{\infty} &= 1 \\
2|A|^2 \left(\frac{\hbar^2}{2m\lambda}\right) &= 1 \\
|A|^2 \left(\frac{\hbar^2}{m\lambda}\right) &= 1 \\
|A|^2 &= \frac{m\lambda}{\hbar^2} \\
A &= \sqrt{\frac{m\lambda}{\hbar^2}}.
\end{aligned}$$

Thus,

$$\psi(x,0) = \sqrt{\frac{m\lambda}{\hbar^2}}\mathrm{e}^{-\frac{m\lambda}{\hbar^2}|x|}.$$

Let $\frac{m\lambda}{\hbar^2} \equiv \frac{1}{x_0}$, then

$$\psi(x,0) = \frac{1}{\sqrt{x_0}}\mathrm{e}^{-\frac{|x|}{x_0}}.$$

Now, we need to find $\psi(x,t)$ when $\hat{H} = \frac{\hat{p}^2}{2m}$. We will use the propagator, given by

$$K(x,t,x',t_0) = \sum_{a'} \langle x|a'\rangle \langle a'|x'\rangle \,\mathrm{e}^{-\frac{iE_{a'}(t-t_0)}{\hbar}} = \sqrt{\frac{m}{2i\pi\hbar t}}\mathrm{e}^{-\frac{1}{2}\frac{m(x-x')^2}{i\hbar t}}.$$

Then, we have

$$\begin{aligned}
\psi(x,t) &= \int_{-\infty}^{+\infty} K(x,t,x',0)\psi(x',0)\,\mathrm{d}x' \\
&= \sqrt{\frac{m}{2i\pi\hbar t}}\sqrt{\frac{m\lambda}{\hbar^2}} \int_{-\infty}^{\infty} \mathrm{e}^{\frac{im(x-x')^2}{2\hbar t}} \mathrm{e}^{-\frac{m\lambda}{\hbar^2}|x'|} \,\mathrm{d}x' \\
&= m\sqrt{\frac{2\lambda}{i\pi\hbar^2 t}} \int_{0}^{\infty} \mathrm{e}^{-\frac{1}{2}\frac{m(x-x')^2}{i\hbar t}} \mathrm{e}^{-\frac{m\lambda}{\hbar^2}x'} \,\mathrm{d}x' \\
&= m\sqrt{\frac{2\lambda}{i\pi\hbar^2 t}} \int_{0}^{\infty} \mathrm{e}^{-\frac{1}{2}\frac{m(x^2-2xx'+x'^2)}{i\hbar t}} \mathrm{e}^{-\frac{m\lambda}{\hbar^2}x'} \,\mathrm{d}x' \\
&= m\sqrt{\frac{2\lambda}{i\pi\hbar^2 t}} \int_{0}^{\infty} \mathrm{e}^{\frac{imx^2}{2\hbar t}} \mathrm{e}^{-\frac{imx}{\hbar t}x'} \mathrm{e}^{\frac{im}{2\hbar t}x'^2} \mathrm{e}^{-\frac{m\lambda}{\hbar^2}x'} \,\mathrm{d}x' \\
&= m\sqrt{\frac{2\lambda}{i\pi\hbar^2 t}}\mathrm{e}^{\frac{imx^2}{2\hbar t}} \int_{0}^{\infty} \mathrm{e}^{-\frac{m}{2i\hbar t}x'^2} \mathrm{e}^{\left(\frac{mx}{i\hbar t}-\frac{m\lambda}{\hbar^2}\right)x'} \,\mathrm{d}x'.
\end{aligned}$$

This is an integral solution of our equation for any time t. An analytic closed form solution in terms of error functions exists. We obtained this solution via a symbolic integral calculator, which gave

$$
\begin{aligned}
-\frac{\sqrt{\pi}\hbar t \mathrm{e}^{-\frac{mx\lambda}{\hbar^2}}}{4\sqrt{m}} \Bigg[& \operatorname{erf}\left(\frac{\sqrt{m}((i+1)t\lambda+(i-1)\hbar x)}{2\hbar^{\frac{3}{2}}\sqrt{t}}\right) \\
& + \mathrm{e}^{\frac{2mx\lambda}{\hbar^2}}\left(\operatorname{erf}\left(\frac{\sqrt{m}((i+1)t\lambda-(i-1)\hbar x)}{2\hbar^{\frac{3}{2}}\sqrt{t}}\right)+\operatorname{erf}\left(\frac{\sqrt{-i}\sqrt{m}(it\lambda+\hbar x)}{\sqrt{2t}\hbar^{\frac{3}{2}}}\right)-2\right) \\
& + \operatorname{erf}\left(\frac{\sqrt{-im}(it\lambda-\hbar x)}{\sqrt{2t}\hbar^{\frac{3}{2}}}\right)-2\Bigg]\left((i-1)\sin\left(\frac{mt\lambda^2}{2h^3}\right)+(i+1)\cos\left(\frac{mt\lambda^2}{2h^3}\right)\right).
\end{aligned}
$$

$\blacksquare$

Homework 5

Based on problems 3.12, 3.15, 3.18, 3.20 of Sakurai's book.

Problem 1
An angular momentum eigenstate $|\ell, \ell_z = \ell\rangle$ is rotated by an infinitesimal angle $\alpha \ll 1$ about the y-axis. If, in the new state, we measure $\hat{\ell}_z$, what is the probability of obtaining $\ell_z = \ell$? Find the answer up to terms of order α^2.
Note: Perform the calculation *without* using the explicit form of the $d^{(j)}_{\ell_z', \ell_z}$ matrix.

Solution. The quantum rotation operator $\hat{D}$ is given by

$$\hat{D}(\hat{\mathbf{n}}, \theta) = \mathrm{e}^{-i\theta \frac{\hat{\mathbf{n}}\cdot\mathbf{J}}{\hbar}} = \mathrm{e}^{-i\theta \hat{\mathbf{n}}\cdot\mathbf{j}}.$$

A rotation by an infinitesimal angle $\alpha \ll 1$ is given by the rotation operator

$$\begin{aligned}\hat{D}(\hat{\mathbf{y}}, \alpha) &= \mathrm{e}^{-i\alpha\hat{\ell}_y} \\ &= \sum_{n=0}^{\infty} \frac{(-i\alpha)^n}{n!}\hat{\ell}_y^n \\ &= \mathbb{I} - i\alpha\hat{\ell}_y - \frac{\alpha^2}{2}\hat{\ell}_y^2 + \mathcal{O}(\alpha^3).\end{aligned}$$

Now, we will rewrite the operator above in terms of $\hat{\ell}_\pm = \hat{\ell}_x \pm i\hat{\ell}_y \implies \hat{\ell}_y = \frac{\hat{\ell}_+ - \hat{\ell}_-}{2i}$. Additionally, we will use the following facts

$$\begin{aligned}\hat{\ell}_\pm |\ell, \ell_z\rangle &= \sqrt{\ell(\ell+1) - \ell_z(\ell_z \pm 1)}\, |\ell, \ell_z \pm 1\rangle, \\ \hat{\ell}^2 |\ell, \ell_z\rangle &= \ell(\ell+1)\, |\ell, \ell_z\rangle, \\ \hat{\ell}_z |\ell, \ell_z\rangle &= \ell_z\, |\ell, \ell_z\rangle.\end{aligned}$$

Additionally,

$$\hat{\ell}_+ |\ell, \ell_z = \ell\rangle = \sqrt{\ell(\ell+1) - \ell(\ell+1)}\, |\ell, \ell+1\rangle = 0.$$

Replacing in the Taylor expansion of the exponential, we have

$$\begin{aligned}\hat{D}(\hat{\mathbf{y}}, \alpha) &= \mathbb{I} - i\alpha\hat{\ell}_y - \frac{\alpha^2}{2}\hat{\ell}_y^2 + \mathcal{O}(\alpha^3) \\ &= \mathbb{I} - i\alpha\left(\frac{\hat{\ell}_+ - \hat{\ell}_-}{2i}\right) - \frac{\alpha^2}{2}\left(\frac{\hat{\ell}_+ - \hat{\ell}_-}{2i}\right)^2 + \mathcal{O}(\alpha^3) \\ &= \mathbb{I} - \frac{\alpha}{2}\left(\hat{\ell}_+ - \hat{\ell}_-\right) + \frac{\alpha^2}{8}\left(\hat{\ell}_+ - \hat{\ell}_-\right)^2 + \mathcal{O}(\alpha^3) \\ &= \mathbb{I} - \frac{\alpha}{2}\left(\hat{\ell}_+ - \hat{\ell}_-\right) + \frac{\alpha^2}{8}\left(\hat{\ell}_+^2 - \hat{\ell}_+\hat{\ell}_- - \hat{\ell}_-\hat{\ell}_+ + \hat{\ell}_-^2\right) + \mathcal{O}(\alpha^3).\end{aligned}$$

Applying this operator to the state $|\ell, \ell_z\rangle$, we have

$$\begin{aligned}
\hat{D}(\hat{\mathbf{y}}, \alpha) |\ell, \ell_z\rangle &= \left[\mathbb{I} - \frac{\alpha}{2}\left(\hat{\ell}_+ - \hat{\ell}_-\right) + \frac{\alpha^2}{8}\left(\hat{\ell}_+^2 - \hat{\ell}_+\hat{\ell}_- - \hat{\ell}_-\hat{\ell}_+ + \hat{\ell}_-^2\right) + \mathcal{O}(\alpha^3)\right] |\ell, \ell_z\rangle \\
&= \left[\mathbb{I} - \frac{\alpha}{2}\hat{\ell}_+ + \frac{\alpha}{2}\hat{\ell}_- + \frac{\alpha^2}{8}\hat{\ell}_+^2 - \frac{\alpha^2}{8}\hat{\ell}_+\hat{\ell}_- - \frac{\alpha^2}{8}\hat{\ell}_-\hat{\ell}_+ + \frac{\alpha^2}{8}\hat{\ell}_-^2 + \mathcal{O}(\alpha^3)\right] |\ell, \ell_z\rangle \\
&= |\ell, \ell_z\rangle - \frac{\alpha}{2}\hat{\ell}_+ |\ell, \ell_z\rangle + \frac{\alpha}{2}\hat{\ell}_- |\ell, \ell_z\rangle + \frac{\alpha^2}{8}\hat{\ell}_+^2 |\ell, \ell_z\rangle - \frac{\alpha^2}{8}\hat{\ell}_+\hat{\ell}_- |\ell, \ell_z\rangle - \frac{\alpha^2}{8}\hat{\ell}_-\hat{\ell}_+ |\ell, \ell_z\rangle + \frac{\alpha^2}{8}\hat{\ell}_-^2 |\ell, \ell_z\rangle \\
&= |\ell, \ell_z\rangle - \frac{\alpha}{2}\sqrt{\ell(\ell+1) - \ell_z(\ell_z+1)}\, |\ell, \ell_z + 1\rangle + \frac{\alpha}{2}\sqrt{\ell(\ell+1) - \ell_z(\ell_z-1)}\, |\ell, \ell_z - 1\rangle \\
&\quad + \frac{\alpha^2}{8}\sqrt{\ell(\ell+1) - (\ell_z+1)(\ell_z+2)}\sqrt{\ell(\ell+1) - \ell_z(\ell_z+1)}\, |\ell, \ell_z + 2\rangle \\
&\quad - \frac{\alpha^2}{8}\sqrt{\ell(\ell+1) - \ell_z(\ell_z-1)}\sqrt{\ell(\ell+1) - \ell_z(\ell_z-1)}\, |\ell, \ell_z\rangle \\
&\quad - \frac{\alpha^2}{8}\sqrt{\ell(\ell+1) - \ell_z(\ell_z+1)}\sqrt{\ell(\ell+1) - \ell_z(\ell_z+1)}\, |\ell, \ell_z\rangle \\
&\quad + \frac{\alpha^2}{8}\sqrt{\ell(\ell+1) - (\ell_z-1)(\ell_z-2)}\sqrt{\ell(\ell+1) - \ell_z(\ell_z-1)}\, |\ell, \ell_z - 2\rangle \\
&= |\ell, \ell_z\rangle - \frac{\alpha}{2}\left[\sqrt{\ell(\ell+1) - \ell_z(\ell_z+1)}\, |\ell, \ell_z + 1\rangle - \sqrt{\ell(\ell+1) - \ell_z(\ell_z-1)}\, |\ell, \ell_z - 1\rangle\right] \\
&\quad + \frac{\alpha^2}{8}\left[\sqrt{\ell(\ell+1) - (\ell_z+1)(\ell_z+2)}\sqrt{\ell(\ell+1) - \ell_z(\ell_z+1)}\, |\ell, \ell_z + 2\rangle\right. \\
&\quad \left. -2\left[\ell^2 + \ell - \ell_z^2\right] |\ell, \ell_z\rangle + \sqrt{\ell(\ell+1) - (\ell_z-1)(\ell_z-2)}\sqrt{\ell(\ell+1) - \ell_z(\ell_z-1)}\, |\ell, \ell_z - 2\rangle\right].
\end{aligned}$$

Now, we apply the operator to the state when $\ell_z = \ell$, and knowing that $\ell_+ |\ell, \ell\rangle = 0$, then

$$\hat{D}(\hat{\mathbf{y}}, \alpha) |\ell, \ell\rangle = \left(1 - \frac{\alpha^2}{4}\ell\right) |\ell, \ell\rangle + \frac{\alpha}{2}\sqrt{2\ell}\, |\ell, \ell - 1\rangle + \frac{\alpha^2}{4}\sqrt{2\ell(\ell-1)}\, |\ell, \ell - 2\rangle .$$

Thus, the probability of obtaining $\ell_z = \ell$ after a rotation by α is

$$\begin{aligned}
P\left(\ell_z = \ell \mid \hat{D}(\hat{\mathbf{y}}, \alpha)\right) &= \left|\left\langle \ell, \ell \middle| \hat{D}(\hat{\mathbf{y}}, \alpha) \middle| \ell, \ell \right\rangle\right|^2 \\
&= \left| |\ell, \ell\rangle \left[\left(1 - \frac{\alpha^2}{4}\ell\right) |\ell, \ell\rangle + \frac{\alpha}{2}\sqrt{2\ell}\, |\ell, \ell - 1\rangle + \frac{\alpha^2}{4}\sqrt{2\ell(\ell-1)}\, |\ell, \ell - 2\rangle\right]\right|^2 \\
&= \left|\left(1 - \frac{\alpha^2}{4}\ell\right)\right|^2 \\
&= 1 - \frac{\alpha^2}{2}\ell + \frac{\alpha^4}{16}\ell^2 \\
&= 1 - \frac{\alpha^2}{2}\ell + \mathcal{O}(\alpha^4).
\end{aligned}$$

■

Problem 2
The wave function of a particle subjected to a spherically symmetric potential $V(r)$ is given by

$$\psi(\vec{r}) = (x + y + 3z)f(r).$$

(a) Is ψ an eigenfunction of L^2? If so, what is the value of ℓ? If not, what are the possible values of ℓ we may obtain when L^2 is measured?

(b) What are the probabilities for the particle to be found in various $\hat{\ell}_z$ eigenstates?

(c) Suppose it is known that $\psi(\vec{r})$ is an energy eigenfunction with eigenvalue E. Indicate how to find $V(r)$.

Solution. (a) We will first rewrite ψ in terms of spherical coordinates

$$\begin{aligned}\psi(\mathbf{r}) &= \left(r\sin(\theta)\cos(\varphi) + r\sin(\theta)\sin(\varphi) + 3r\cos(\theta)\right) f(r)\\ &= \left(\sin(\theta)\cos(\varphi) + \sin(\theta)\sin(\varphi) + 3\cos(\theta)\right) r f(r).\end{aligned}$$

We will now analyze the spherical harmonics of the wave-function we have. First, we can directly see it cannot be $\ell = 0$ since there is no constant term. Additionally, all terms depend on each variable, θ or φ, at most once, so it would be wise to check $\ell = 1$. From a lookup table of spherical harmonics, we have

$$\begin{aligned}Y_1^{-1}(\theta,\varphi) &= \frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin(\theta)\mathrm{e}^{-i\varphi} \implies \sin(\theta)\mathrm{e}^{-i\varphi} = 2\sqrt{\frac{2\pi}{3}}Y_1^{-1},\\ Y_1^{0}(\theta,\varphi) &= \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos(\theta) \implies \cos(\theta) = 2\sqrt{\frac{\pi}{3}}Y_1^{0},\\ Y_1^{1}(\theta,\varphi) &= -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin(\theta)\mathrm{e}^{i\varphi} \implies \sin(\theta)\mathrm{e}^{i\varphi} = -2\sqrt{\frac{2\pi}{3}}Y_1^{1}.\end{aligned}$$

Replacing in our wave-function, we have

$$\begin{aligned}\psi(\mathbf{r}) &= \left(\sin(\theta)\cos(\varphi) + \sin(\theta)\sin(\varphi) + 3\cos(\theta)\right) r f(r)\\ &= \left[\sin(\theta)\left(\frac{\mathrm{e}^{i\varphi}+\mathrm{e}^{-i\varphi}}{2}\right) + \sin(\theta)\left(\frac{\mathrm{e}^{i\varphi}-\mathrm{e}^{-i\varphi}}{2i}\right) + 3\left(2\sqrt{\frac{\pi}{3}}Y_1^0\right)\right] r f(r)\\ &= \left[\frac{1}{2}\left(\sin(\theta)\mathrm{e}^{i\varphi} + \sin(\theta)\mathrm{e}^{-i\varphi}\right) - \frac{i}{2}\left(\sin(\theta)\mathrm{e}^{i\varphi} - \sin(\theta)\mathrm{e}^{-i\varphi}\right) + 2\sqrt{3\pi}Y_1^0\right] r f(r)\\ &= \left[\frac{1}{2}\left(-2\sqrt{\frac{2\pi}{3}}Y_1^1 + 2\sqrt{\frac{2\pi}{3}}Y_1^{-1}\right) - \frac{i}{2}\left(-2\sqrt{\frac{2\pi}{3}}Y_1^1 - 2\sqrt{\frac{2\pi}{3}}Y_1^{-1}\right) + 2\sqrt{3\pi}Y_1^0\right] r f(r)\\ &= \left[-\sqrt{\frac{2\pi}{3}}Y_1^1 + \sqrt{\frac{2\pi}{3}}Y_1^{-1} + i\sqrt{\frac{2\pi}{3}}Y_1^1 + i\sqrt{\frac{2\pi}{3}}Y_1^{-1} + 2\sqrt{3\pi}Y_1^0\right] r f(r)\\ &= \left[(i-1)\sqrt{\frac{2\pi}{3}}Y_1^1 + 2\sqrt{3\pi}Y_1^0 + (i+1)\sqrt{\frac{2\pi}{3}}Y_1^{-1}\right] r f(r).\end{aligned}$$

Thus, $\psi(\mathbf{r})$ is an eigenfunction of L^2 with $\ell = 1$.

(b) Before calculating the probabilities, we must first normalize the wave-function. To do so, we have to use the orthogonality property of the complex spherical harmonics, given by

$$\int_0^{2\pi}\int_0^{\pi} Y_{\ell_1}^{\ell_{z,1}}\left(Y_{\ell_2}^{\ell_{z,2}}\right)^* \sin(\theta)\,\mathrm{d}\theta\,\mathrm{d}\varphi = \delta_{\ell_1,\ell_2}\delta_{\ell_{z,1},\ell_{z,2}}.$$

Thus, we have

$$
\begin{aligned}
\iiint \psi^*(\mathbf{r})\psi(\mathbf{r})\,\mathrm{d}\mathbf{r} &= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \psi^*(\mathbf{r})\psi(\mathbf{r}) r^2 \sin(\theta)\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\varphi \\
&= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \left[(-i-1)\sqrt{\frac{2\pi}{3}}\left(Y_1^1\right)^* + 2\sqrt{3\pi}\left(Y_1^0\right)^* + (-i+1)\sqrt{\frac{2\pi}{3}}\left(Y_1^{-1}\right)^*\right] \\
&\qquad \left[(i-1)\sqrt{\frac{2\pi}{3}}Y_1^1 + 2\sqrt{3\pi}Y_1^0 + (i+1)\sqrt{\frac{2\pi}{3}}Y_1^{-1}\right] r^4 f^2(r)\sin(\theta)\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\varphi \\
&= \left[(-i-1)(i-1)\frac{2\pi}{3} + 12\pi + (-i+1)(i+1)\frac{2\pi}{3}\right]\cdot\left(\int_0^{\infty} r^4 f^2(r)\,\mathrm{d}r\right) \\
&= \frac{44\pi}{3}\int_0^{\infty} r^4 f^2(r)\,\mathrm{d}r \\
&= 1 \\
&\implies \int_0^{\infty} r^4 f^2(r)\,\mathrm{d}r = \frac{3}{44\pi}.
\end{aligned}
$$

The normalized wave-function Ψ is then

$$
\begin{aligned}
\Psi(\theta,\varphi) &= \sqrt{\frac{3}{44\pi}}\left[(i-1)\sqrt{\frac{2\pi}{3}}Y_1^1 + 2\sqrt{3\pi}Y_1^0 + (i+1)\sqrt{\frac{2\pi}{3}}Y_1^{-1}\right] \\
&= \frac{i-1}{\sqrt{22}}Y_1^1 + \frac{3}{\sqrt{11}}Y_1^0 + \frac{i+1}{\sqrt{22}}Y_1^{-1}.
\end{aligned}
$$

Thus, the probabilities for the particle to be found in various $\hat{\ell}_z$ states are

- For $\ell_z = 1$:

$$
\begin{aligned}
\mathbb{P}(\ell_z = 1) &= \left|\int_0^{2\pi}\int_0^{\pi}\left(Y_1^1\right)^*\Psi(\theta,\varphi)\sin(\theta)\,\mathrm{d}\theta\,\mathrm{d}\varphi\right|^2 \\
&= \left|\frac{i-1}{\sqrt{22}}\right|^2 \\
&= \frac{1}{11}.
\end{aligned}
$$

- For $\ell_z = 0$:

$$
\begin{aligned}
\mathbb{P}(\ell_z = 0) &= \left|\int_0^{2\pi}\int_0^{\pi}\left(Y_1^0\right)^*\Psi(\theta,\varphi)\sin(\theta)\,\mathrm{d}\theta\,\mathrm{d}\varphi\right|^2 \\
&= \left|\frac{3}{\sqrt{11}}\right|^2 \\
&= \frac{9}{11}.
\end{aligned}
$$

- For $\ell_z = -1$:

$$
\begin{aligned}
\mathbb{P}(\ell_z = -1) &= \left|\int_0^{2\pi}\int_0^{\pi}\left(Y_1^{-1}\right)^*\Psi(\theta,\varphi)\sin(\theta)\,\mathrm{d}\theta\,\mathrm{d}\varphi\right|^2 \\
&= \left|\frac{i+1}{\sqrt{22}}\right|^2 \\
&= \frac{1}{11}.
\end{aligned}
$$

(c) We have the Hamiltonian operator $\hat{H}$ given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\mathbf{r}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}).$$

To find $V(\mathbf{r})$, we have to solve the eigenvalue problem given by

$$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r}).$$

This eigenvalue problem is easier to solve if we use the original Cartesian coordinate system form of $\psi(\mathbf{r})$. Solving, we have

$$\begin{aligned}
\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi(\mathbf{r}) &= E\psi(\mathbf{r}) \\
-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) &= E\psi(\mathbf{r}) \\
(V(\mathbf{r}) - E)\psi(\mathbf{r}) &= \frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) \\
V(\mathbf{r}) - E &= \frac{\hbar^2}{2m}\frac{1}{\psi(\mathbf{r})}\nabla^2\psi(\mathbf{r}) \\
V(\mathbf{r}) &= E + \frac{\hbar^2}{2m}\frac{1}{\psi(\mathbf{r})}\nabla^2\psi(\mathbf{r}) \\
&= E + \frac{\hbar^2}{2m}\frac{1}{(x+y+3z)f(r)}\nabla^2\left[(x+y+3z)f(r)\right].
\end{aligned}$$

We have

$$\begin{aligned}
\frac{\partial^2}{\partial x^2}\psi(\mathbf{r}) &= \frac{\partial^2}{\partial x^2}\left[(x+y+3z)f(r)\right] \\
&= \frac{\partial}{\partial x}\left[f(r) + (x+y+3z)\frac{\mathrm{d}f}{\mathrm{d}r}\frac{\mathrm{d}r}{\mathrm{d}x}\right] \\
&= \frac{\partial}{\partial x}\left[f(r) + (x+y+3z)\frac{\mathrm{d}f}{\mathrm{d}r}\frac{x}{r}\right] \\
&= \left[\frac{\mathrm{d}f}{\mathrm{d}r}\frac{x}{r} + \frac{\mathrm{d}f}{\mathrm{d}r}\frac{x}{r} + (x+y+3z)\left(\frac{\mathrm{d}^2 f}{\mathrm{d}r^2}\left(\frac{x}{r}\right)^2 + \frac{\mathrm{d}f}{\mathrm{d}r}\frac{1}{r} + \frac{\mathrm{d}f}{\mathrm{d}r}\left(-\frac{x}{r^2}\frac{x}{r}\right)\right)\right] \\
&= \left[\frac{2x}{r}\frac{\mathrm{d}f}{\mathrm{d}r} + (x+y+3z)\left(\frac{x^2}{r^2}\frac{\mathrm{d}^2 f}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}f}{\mathrm{d}r} - \frac{x^2}{r^3}\frac{\mathrm{d}f}{\mathrm{d}r}\right)\right].
\end{aligned}$$

Thus, after doing the same for y and z and adding the results together, we get

We have

$$
\begin{aligned}
\nabla^2\psi(\mathbf{r}) &= \left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(\mathbf{r}) \\
&= \left[\frac{2x}{r}\frac{\mathrm{d}f}{\mathrm{d}r}+(x+y+3z)\left(\frac{x^2}{r^2}\frac{\mathrm{d}^2 f}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}f}{\mathrm{d}r}-\frac{x^2}{r^3}\frac{\mathrm{d}f}{\mathrm{d}r}\right)\right] \\
&\quad+\left[\frac{2y}{r}\frac{\mathrm{d}f}{\mathrm{d}r}+(x+y+3z)\left(\frac{y^2}{r^2}\frac{\mathrm{d}^2 f}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}f}{\mathrm{d}r}-\frac{y^2}{r^3}\frac{\mathrm{d}f}{\mathrm{d}r}\right)\right] \\
&\quad+\left[\frac{6z}{r}\frac{\mathrm{d}f}{\mathrm{d}r}+(x+y+3z)\left(\frac{z^2}{r^2}\frac{\mathrm{d}^2 f}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}f}{\mathrm{d}r}-\frac{z^2}{r^3}\frac{\mathrm{d}f}{\mathrm{d}r}\right)\right] \\
&= (x+y+3z)\frac{2}{r}\frac{\mathrm{d}f}{\mathrm{d}r}+(x+y+3z)\left[\left(\frac{x^2+y^2+z^2}{r^2}\right)\frac{\mathrm{d}^2 f}{\mathrm{d}r^2}+\frac{3}{r}\frac{\mathrm{d}f}{\mathrm{d}r}-\left(\frac{x^2+y^2+z^2}{r^3}\right)\frac{\mathrm{d}f}{\mathrm{d}r}\right] \\
&= (x+y+3z)\left[\frac{2}{r}\frac{\mathrm{d}f}{\mathrm{d}r}+\frac{\mathrm{d}^2 f}{\mathrm{d}r^2}+\frac{3}{r}\frac{\mathrm{d}f}{\mathrm{d}r}-\frac{1}{r}\frac{\mathrm{d}f}{\mathrm{d}r}\right] \\
&= (x+y+3z)\left[\frac{4}{r}\frac{\mathrm{d}f}{\mathrm{d}r}+\frac{\mathrm{d}^2 f}{\mathrm{d}r^2}\right].
\end{aligned}
$$

Therefore, the potential V is given by

$$
\begin{aligned}
V(\mathbf{r}) &= E+\frac{\hbar^2}{2m}\frac{1}{(x+y+3z)f(r)}(x+y+3z)\left[\frac{4}{r}\frac{\mathrm{d}f}{\mathrm{d}r}+\frac{\mathrm{d}^2 f}{\mathrm{d}r^2}\right] \\
&= E+\frac{\hbar^2}{2m}\frac{1}{f(r)}\left[\frac{4}{r}\frac{\mathrm{d}f}{\mathrm{d}r}+\frac{\mathrm{d}^2 f}{\mathrm{d}r^2}\right].
\end{aligned}
$$

■

Problem 3
Consider an orbital angular momentum eigenstate $|\ell = 2, \ell_z = 0\rangle$. Suppose that this state is rotated by an angle β about the y-axis.
If we measure $\hat{\ell}_z$, what are the possible values we can obtain and what is the probability of measuring each of them?

Solution. If we measure $\hat{\ell}_z$, we can obtain $0, \pm 1, \pm 2$. The probability of obtaining each is given by

$$P(\ell_z) = |\langle 2, \ell_z|\mathcal{D}(R)|2, 0\rangle|^2 .$$

The quantum rotation operator $\hat{\mathcal{D}}(R)$ for a rotation by an angle β about the y-axis applied to the eigenstate $|\ell, \ell_z\rangle$ is given by

$$\hat{\mathcal{D}}(R)\,|\ell, \ell_z\rangle = \hat{\mathcal{D}}(\alpha = 0, \beta, \gamma = 0)\,|\ell, \ell_z\rangle = \sum_{m'} |\ell, m'\rangle\, \hat{\mathcal{D}}^{(\ell)}_{m',\ell_z}(\beta) = \sum_{m'} |\ell, m'\rangle \sqrt{\frac{4\pi}{5}} \left(Y_\ell^{m'}\right)^* (\beta, \ell_z).$$

For $\ell = 2$ and $\ell_z = 0$, we have

$$\begin{aligned}
\hat{\mathcal{D}}(R)\,|\ell, \ell_z\rangle &= \sum_{m'} |2, m'\rangle\, \hat{\mathcal{D}}^{(2)}_{m',0}(\beta) \\
&= \sum_{m'} |2, m'\rangle \sqrt{\frac{4\pi}{5}} \left(Y_2^{m'}\right)^* (\beta, 0).
\end{aligned}$$

Thus, the probability of measuring each is given by

$$\begin{aligned}
P(\ell_z) &= |\langle 2, \ell_z|\mathcal{D}(R)|2, 0\rangle|^2 \\
&= \left|\langle 2, \ell_z| \left(\sum_{m'} |2, m'\rangle \sqrt{\frac{4\pi}{5}} \left(Y_2^{\ell_z}\right)^* (\beta, 0)\right)\right|^2 \\
&= \left|\sqrt{\frac{4\pi}{5}} \left(Y_2^{\ell_z}\right)^* (\beta, 0)\, \delta_{m',\ell_z}\right|^2 \\
&= \left|\sqrt{\frac{4\pi}{5}} \left(Y_2^{\ell_z}\right)^* (\beta, 0)\right|^2 \\
&= \frac{4\pi}{5} \left|\left(Y_2^{\ell_z}\right)^* (\beta, 0)\right|^2 \\
&= \frac{4\pi}{5} \left|(-1)^{\ell_z} Y_2^{-\ell_z}(\beta, 0)\right|^2 \\
&= \frac{4\pi}{5} \left|Y_2^{-\ell_z}(\beta, 0)\right|^2 .
\end{aligned}$$

Therefore, the probability of measuring each possibility is

- For $\ell_z = 0$:

$$\begin{aligned}
P(0) &= \frac{4\pi}{5} \left|Y_2^0(\beta, 0)\right|^2 \\
&= \frac{4\pi}{5} \left|\frac{1}{4}\sqrt{\frac{5}{\pi}} (3\cos^2(\beta) - 1)\right|^2 \\
&= \frac{1}{4}(3\cos^2(\beta) - 1)^2.
\end{aligned}$$

- For $\ell_z = \pm 1$:

$$\begin{aligned} P(\pm 1) &= \frac{4\pi}{5}\left|Y_2^{\mp 1}(\beta, 0)\right|^2 \\ &= \frac{4\pi}{5}\left|\pm\frac{1}{2}\sqrt{\frac{15}{2\pi}}\mathrm{e}^{\mp i\varphi}\sin(\beta)\cos(\beta)\right|^2 \\ &= \frac{3}{2}\sin^2(\beta)\cos^2(\beta). \end{aligned}$$

- For $\ell_z = \pm 2$:

$$\begin{aligned} P(\pm 2) &= \frac{4\pi}{5}\left|Y_2^{\mp 2}(\beta, 0)\right|^2 \\ &= \frac{4\pi}{5}\left|\frac{1}{4}\sqrt{\frac{15}{2\pi}}\mathrm{e}^{\mp 2i\varphi}\sin^2(\beta)\right|^2 \\ &= \frac{3}{8}\sin^4(\beta). \end{aligned}$$

As a sanity check, we can show that the sum of the probabilities is equal to 1, but sanity is a privilege we do not have. ■

Problem 4
Given two particles in angular momentum eigenstates $\ell_1 = 1$ and $\ell_2 = 1$, the total possible angular momentum is $\ell_T = 0, 1, 2$.
Without using the table, write all eigenstates of the total angular momentum $|\ell_1, \ell_2; \ell_T, \ell_z\rangle$ as a linear combination of the states of the basis $|\ell_1, \ell_2; \ell_{1z}, \ell_{2z}\rangle$

Solution. Given that $\ell_1 = 1$ and $\ell_2 = 1$, then $\ell_T = 0, 1, 2$ and there are $(2\ell_1 + 1)(2\ell_2 + 1) = 9$ possible states. For the simplicity of notation, we will note the following: $|\ell_{1z} = a, \ell_{2z} = b\rangle = |a, b\rangle$.

- For $\ell_T = 2$ and $\ell_z = 2$:
  The only way to get $|\ell_T = 2, \ell_z = 2\rangle$ is if $\ell_{1z} = 1$ and $\ell_{2z} = 1$, which gives
  $$|\ell_T = 2, \ell_z = 2\rangle = |1, 1\rangle .$$
- For $\ell_T = 2$ and $\ell_z = -2$:
  The only way to get $|\ell_T = 2, \ell_z = -2\rangle$ is if $\ell_{1z} = -1$ and $\ell_{2z} = -1$, which gives
  $$|\ell_T = 2, \ell_z = -2\rangle = |-1, -1\rangle .$$

From the state $|\ell_T = 2, \ell_z = 2\rangle$, we can apply the angular momentum lowering operator $\hat{\ell}_-$ to find the other states. From this, we have
$$\hat{\ell}_\pm |\ell, \ell_z\rangle = \sqrt{\ell(\ell+1) - \ell_z(\ell_z \pm 1)}\, |\ell, \ell_z \pm 1\rangle .$$

- For $\ell_T = 2$ and $\ell_z = 1$:
  We apply the $\hat{\ell}_-$ operator to $|\ell_T = 2, \ell_z = 2\rangle$ and get
  $$\begin{aligned}
  \hat{\ell}_- |\ell_T = 2, \ell_z = 2\rangle &= \left(\hat{\ell}_{1-} + \hat{\ell}_{2-}\right) |1, 1\rangle \\
  \hat{\ell}_- |\ell_T = 2, \ell_z = 2\rangle &= \hat{\ell}_{1-} |1, 1\rangle + \hat{\ell}_{2-} |1, 1\rangle \\
  2\, |\ell_T = 2, \ell_z = 1\rangle &= \sqrt{2}\, |0, 1\rangle + \sqrt{2}\, |1, 0\rangle \\
  |\ell_T = 2, \ell_z = 1\rangle &= \frac{1}{\sqrt{2}} \left(|0, 1\rangle + |1, 0\rangle\right) .
  \end{aligned}$$
- For $\ell_T = 2$ and $\ell_z = 0$:
  We apply the $\hat{\ell}_-$ operator to $|\ell_T = 2, \ell_z = 1\rangle$ and get
  $$\begin{aligned}
  \hat{\ell}_- |\ell_T = 2, \ell_z = 1\rangle &= \left(\hat{\ell}_{1-} + \hat{\ell}_{2-}\right) \left(\frac{1}{\sqrt{2}} |0, 1\rangle + \frac{1}{\sqrt{2}} |1, 0\rangle\right) \\
  \hat{\ell}_- |\ell_T = 2, \ell_z = 1\rangle &= \frac{1}{\sqrt{2}} \hat{\ell}_{1-} |0, 1\rangle + \frac{1}{\sqrt{2}} \hat{\ell}_{1-} |1, 0\rangle + \frac{1}{\sqrt{2}} \hat{\ell}_{2-} |0, 1\rangle + \frac{1}{\sqrt{2}} \hat{\ell}_{2-} |1, 0\rangle \\
  \sqrt{6}\, |\ell_T = 2, \ell_z = 0\rangle &= \frac{1}{\sqrt{2}} \sqrt{2}\, |-1, 1\rangle + \frac{1}{\sqrt{2}} \sqrt{2}\, |0, 0\rangle + \frac{1}{\sqrt{2}} \sqrt{2}\, |0, 0\rangle + \frac{1}{\sqrt{2}} \sqrt{2}\, |1, -1\rangle \\
  |\ell_T = 2, \ell_z = 0\rangle &= \frac{1}{\sqrt{6}} \left(|1, -1\rangle + 2\, |0, 0\rangle + |-1, 1\rangle\right) .
  \end{aligned}$$
- For $\ell_T = 2$ and $\ell_z = -1$:
  We apply the $\hat{\ell}_-$ operator to $|\ell_T = 2, \ell_z = 0\rangle$ and get
  $$\begin{aligned}
  \hat{\ell}_- |\ell_T = 2, \ell_z = 0\rangle &= \left(\hat{\ell}_{1-} + \hat{\ell}_{2-}\right) \frac{1}{\sqrt{6}} \left(|-1, 1\rangle + 2\, |0, 0\rangle + |1, -1\rangle\right) \\
  \hat{\ell}_- |\ell_T = 2, \ell_z = 0\rangle &= \frac{1}{\sqrt{6}} \left[\hat{\ell}_{1-} \left(|-1, 1\rangle + 2\, |0, 0\rangle + |1, -1\rangle\right) + \hat{\ell}_{2-} \left(|-1, 1\rangle + 2\, |0, 0\rangle + |1, -1\rangle\right)\right] \\
  \sqrt{6}\, |\ell_T = 2, \ell_z = -1\rangle &= \frac{1}{\sqrt{6}} \left[2\sqrt{2}\, |-1, 0\rangle + \sqrt{2}\, |0, -1\rangle + \sqrt{2}\, |-1, 0\rangle + 2\sqrt{2}\, |0, -1\rangle\right] \\
  |\ell_T = 2, \ell_z = -1\rangle &= \frac{1}{\sqrt{2}} \left(|-1, 0\rangle + |0, -1\rangle\right) .
  \end{aligned}$$

- For $\ell_T = 2$ and $\ell_z = -2$:
  We apply the $\hat{\ell}_-$ operator to $|\ell_T = 2, \ell_z = 0\rangle$ and get

$$\begin{aligned}
\hat{\ell}_- |\ell_T = 2, \ell_z = 0\rangle &= \left(\hat{\ell}_{1-} + \hat{\ell}_{2-}\right) \frac{1}{\sqrt{6}} \left(|-1, 1\rangle + 2\,|0, 0\rangle + |1, -1\rangle\right) \\
\hat{\ell}_- |\ell_T = 2, \ell_z = 0\rangle &= \frac{1}{\sqrt{6}} \left[\hat{\ell}_{1-} \left(|-1, 1\rangle + 2\,|0, 0\rangle + |1, -1\rangle\right) + \hat{\ell}_{2-} \left(|-1, 1\rangle + 2\,|0, 0\rangle + |1, -1\rangle\right)\right] \\
\sqrt{6}\,|\ell_T = 2, \ell_z = -1\rangle &= \frac{1}{\sqrt{6}} \left[2\sqrt{2}\,|-1, 0\rangle + \sqrt{2}\,|0, -1\rangle + \sqrt{2}\,|-1, 0\rangle + 2\sqrt{2}\,|0, -1\rangle\right] \\
|\ell_T = 2, \ell_z = -1\rangle &= \frac{1}{\sqrt{2}} \left(|-1, 0\rangle + |0, -1\rangle\right).
\end{aligned}$$

- For $\ell_T = 1$ and $\ell_z = 1$:
  To do this, we can use the orthogonality property between different values of ℓ_T for the same value of ℓ_z. Taking a general case where

$$|\ell_T = 1, \ell_z = 1\rangle = A\,|1, 0\rangle + B\,|0, 1\rangle\,,$$

  where $|A|^2 + |B|^2 = 1$, we have

$$\begin{aligned}
\langle \ell_T = 2, \ell_z = 1 | \ell_T = 1, \ell_z = 1\rangle &= \langle \ell_T = 2, \ell_z = 1| \left(A\,|1, 0\rangle + B\,|0, 1\rangle\right) \\
\langle \ell_T = 2, \ell_z = 1 | \ell_T = 1, \ell_z = 1\rangle &= \frac{1}{\sqrt{2}} \left(\langle 0, 1| + \langle 1, 0|\right) \left(A\,|1, 0\rangle + B\,|0, 1\rangle\right) \\
0 &= \frac{1}{\sqrt{2}} (A + B) \\
\implies A &= -B = \frac{1}{\sqrt{2}}.
\end{aligned}$$

  Thus,

$$|\ell_T = 1, \ell_z = 1\rangle = \frac{1}{\sqrt{2}} \left(|1, 0\rangle - |0, 1\rangle\right).$$

- For $\ell_T = 1$ and $\ell_z = 0$:
  We apply the $\hat{\ell}_-$ operator to $|\ell_T = 1, \ell_z = 1\rangle$ and get

$$\begin{aligned}
\hat{\ell}_- |\ell_T = 1, \ell_z = 1\rangle &= \left(\hat{\ell}_{1-} + \hat{\ell}_{2-}\right) \frac{1}{\sqrt{2}} \left(|1, 0\rangle - |0, 1\rangle\right) \\
\hat{\ell}_- |\ell_T = 1, \ell_z = 1\rangle &= \frac{1}{\sqrt{2}} \left[\hat{\ell}_{1-} \left(|1, 0\rangle - |0, 1\rangle\right) + \hat{\ell}_{2-} \left(|1, 0\rangle - |0, 1\rangle\right)\right] \\
\sqrt{2}\,|\ell_T = 1, \ell_z = 0\rangle &= \frac{1}{\sqrt{2}} \left[\sqrt{2}\,|0, 0\rangle - \sqrt{2}\,|-1, 1\rangle + \sqrt{2}\,|1, -1\rangle - \sqrt{2}\,|0, 0\rangle\right] \\
|\ell_T = 1, \ell_z = 0\rangle &= \frac{1}{\sqrt{2}} \left(|1, -1\rangle - |-1, 1\rangle\right).
\end{aligned}$$

- For $\ell_T = 1$ and $\ell_z = -1$:
  We apply the $\hat{\ell}_-$ operator to $|\ell_T = 1, \ell_z = 0\rangle$ and get

$$\begin{aligned}
\hat{\ell}_- |\ell_T = 1, \ell_z = 0\rangle &= \left(\hat{\ell}_{1-} + \hat{\ell}_{2-}\right) \frac{1}{\sqrt{2}} \left(|1, -1\rangle - |-1, 1\rangle\right) \\
\hat{\ell}_- |\ell_T = 1, \ell_z = 0\rangle &= \frac{1}{\sqrt{2}} \left[\hat{\ell}_{1-} \left(|1, -1\rangle - |-1, 1\rangle\right) + \hat{\ell}_{2-} \left(|1, -1\rangle - |-1, 1\rangle\right)\right] \\
\sqrt{2}\,|\ell_T = 1, \ell_z = -1\rangle &= \frac{1}{\sqrt{2}} \left[\sqrt{2}\,|0, -1\rangle - \sqrt{2}\,|-1, 0\rangle\right] \\
|\ell_T = 1, \ell_z = -1\rangle &= \frac{1}{\sqrt{2}} \left(|0, -1\rangle - |-1, 0\rangle\right).
\end{aligned}$$

- For $\ell_T = 0$ and $\ell_z = 0$:

  To do this, we can use the orthogonality property such that this state has to be orthogonal to all the other states we calculated. Taking a general case where

$$|\ell_T = 0, \ell_z = 0\rangle = A\,|1,-1\rangle + B\,|0,0\rangle + C\,|-1,1\rangle\,,$$

  where $|A|^2 + |B|^2 + |C|^2 = 1$, we have

  - Orthogonality with $\langle \ell_T = 2, \ell_z = 0|$:

$$\begin{aligned}
\langle \ell_T = 2, \ell_z = 0|\ell_T = 0, \ell_z = 0\rangle &= \langle \ell_T = 2, \ell_z = 0|\left(A\,|1,-1\rangle + B\,|0,0\rangle + C\,|-1,1\rangle\right) \\
\langle \ell_T = 2, \ell_z = 0|\ell_T = 0, \ell_z = 0\rangle &= \frac{1}{\sqrt{6}}\left(\langle 1,-1| + 2\,\langle 0,0| + \langle -1,1|\right)\left(A\,|1,-1\rangle + B\,|0,0\rangle + C\,|-1,1\rangle\right) \\
0 &= \frac{1}{\sqrt{6}}\left(A + 2B + C\right) \\
&\implies A + 2B + C = 0.
\end{aligned}$$

  - Orthogonality with $\langle \ell_T = 1, \ell_z = 0|$:

$$\begin{aligned}
\langle \ell_T = 1, \ell_z = 0|\ell_T = 0, \ell_z = 0\rangle &= \langle \ell_T = 1, \ell_z = 0|\left(A\,|1,-1\rangle + B\,|0,0\rangle + C\,|-1,1\rangle\right) \\
\langle \ell_T = 1, \ell_z = 0|\ell_T = 0, \ell_z = 0\rangle &= \frac{1}{\sqrt{2}}\left(\langle 1,-1| - \langle -1,1|\right)\left(A\,|1,-1\rangle + B\,|0,0\rangle + C\,|-1,1\rangle\right) \\
0 &= \frac{1}{\sqrt{2}}\left(A - C\right) \\
&\implies A - C = 0 \\
&\implies A = C \\
&\implies A = -B.
\end{aligned}$$

  Thus, $A = B = C = \frac{1}{\sqrt{3}}$, and we have

$$|\ell_T = 0, \ell_z = 0\rangle = \frac{1}{\sqrt{3}}\left(|1,-1\rangle + |0,0\rangle + |-1,1\rangle\right).$$

■