MERIDIAN UNIVERSITY · DEPARTMENT OF PHYSICS

Quantum Mechanics I

Problem Set 4: Operator Algebra, Spin Dynamics & Perturbation Theory

Course: PHYS 401
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Student Name: ____________________
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Total Points: 100 Points
Format: Show all intermediate operator derivations.
Honor Code: Standard academic integrity rules apply.

Problem 1: Harmonic Oscillator Matrix Elements & Uncertainty [30 Points]

Consider a one-dimensional quantum harmonic oscillator of mass m and natural frequency ω. Recall the ladder (annihilation and creation) operators defined by:

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

which obey the canonical commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$. The energy eigenstates are denoted by $|n\rangle$ with $n = 0, 1, 2, \ldots$, where $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ and $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$.

(a) Express the position operator $\hat{x}$ and momentum operator $\hat{p}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$. Use these to evaluate the matrix elements $\langle n|\hat{x}^2|m\rangle$ and $\langle n|\hat{p}^2|m\rangle$ for arbitrary non-negative integers n and m. [12 Points]

(b) Calculate the expectation values $\langle \hat{x} \rangle$, $\langle \hat{x}^2 \rangle$, $\langle \hat{p} \rangle$, and $\langle \hat{p}^2 \rangle$ for a stationary state $|n\rangle$. Show that the product of uncertainties $\Delta x \Delta p$ satisfies:

$$\Delta x \Delta p = \left(n + \frac{1}{2}\right)\hbar$$

Verify that the ground state $|0\rangle$ saturates the Heisenberg Uncertainty Principle bound. [10 Points]

(c) A quantum particle at $t = 0$ is prepared in the coherent superposition state:

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

Calculate the time-dependent expectation value of position $\langle \hat{x} \rangle(t)$ for $t > 0$, and determine its amplitude and oscillation frequency. [8 Points]

Solution to Problem 1

Part (a): Operator Expressions and Matrix Elements
Inverting the definitions of $\hat{a}$ and $\hat{a}^\dagger$, we obtain:

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

Squaring the position operator $\hat{x}^2$:

$$\hat{x}^2 = \frac{\hbar}{2m\omega}\left(\hat{a} + \hat{a}^\dagger\right)^2 = \frac{\hbar}{2m\omega}\left(\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + (\hat{a}^\dagger)^2\right)$$

Using $\hat{a}\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1 = \hat{N} + 1$, where $\hat{N} = \hat{a}^\dagger\hat{a}$ is the number operator:

$$\hat{x}^2 = \frac{\hbar}{2m\omega}\left(\hat{a}^2 + 2\hat{N} + 1 + (\hat{a}^\dagger)^2\right)$$

Taking matrix elements between orthonormal states $\langle n|$ and $|m\rangle$:

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

Similarly, for the squared momentum operator $\hat{p}^2$:

$$\hat{p}^2 = -\frac{m\hbar\omega}{2}\left(\hat{a}^2 - (2\hat{N}+1) + (\hat{a}^\dagger)^2\right)$$

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

Part (b): Uncertainty Relation in State $|n\rangle$
For any stationary state $|n\rangle$, off-diagonal terms vanish, yielding $\langle\hat{x}\rangle_n = 0$ and $\langle\hat{p}\rangle_n = 0$. From the diagonal matrix elements ($n = m$):

$$\left\langle\hat{x}^2\right\rangle_n = \frac{\hbar}{2m\omega}(2n+1), \qquad \left\langle\hat{p}^2\right\rangle_n = \frac{m\hbar\omega}{2}(2n+1)$$

The standard deviations (uncertainties) are:

$$\Delta x = \sqrt{\frac{\hbar}{2m\omega}(2n+1)}, \qquad \Delta p = \sqrt{\frac{m\hbar\omega}{2}(2n+1)}$$

Multiplying the uncertainties:

$$\Delta x \Delta p = \sqrt{\frac{\hbar}{2m\omega}(2n+1)} \cdot \sqrt{\frac{m\hbar\omega}{2}(2n+1)} = \left(n + \frac{1}{2}\right)\hbar$$

For $n = 0$: $\Delta x \Delta p = \frac{\hbar}{2}$, saturating the Heisenberg Uncertainty Principle bound.
Part (c): Time Evolution of Position Expectation Value
State evolution: $|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(e^{-iE_0t/\hbar}|0\rangle + e^{-iE_1t/\hbar}|1\rangle\right)$, where $E_1 - E_0 = \hbar\omega$.

$$\langle\hat{x}\rangle(t) = \langle\psi(t)|\hat{x}|\psi(t)\rangle = \frac{1}{2}\left[e^{i\omega t}\langle 0|\hat{x}|1\rangle + e^{-i\omega t}\langle 1|\hat{x}|0\rangle\right] = \sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t)$$

The expectation value executes simple harmonic motion with amplitude $A = \sqrt{\frac{\hbar}{2m\omega}}$ and frequency ω.

Problem 2: Spin-1/2 Particle in a Rotating Magnetic Field [35 Points]

A spin-1/2 particle with gyromagnetic ratio γ is subject to a strong constant magnetic field along the z-axis, combined with a transverse rotating magnetic field of frequency ω:

$$\vec{B}(t) = B_0\hat{\mathbf{z}} + B_1\left(\cos(\omega t)\hat{\mathbf{x}} + \sin(\omega t)\hat{\mathbf{y}}\right)$$

where $B_0 \gg B_1 > 0$. The spin operators are $\hat{\mathbf{S}} = \frac{\hbar}{2}\vec{\sigma}$, where $\sigma_x, \sigma_y, \sigma_z$ are the Pauli spin matrices.

(a) Write down the explicit 2×2 matrix representation of the time-dependent Hamiltonian $\hat{H}(t) = -\gamma \hat{\mathbf{S}} \cdot \vec{B}(t)$ in the standard S_z basis $\{|+\rangle, |-\rangle\}$. Define the Larmor frequencies $\omega_0 = -\gamma B_0$ and $\omega_1 = -\gamma B_1$. **[10 Points]**

(b) Transform the state vector into the rotating frame: $|\psi_R(t)\rangle = e^{i\omega t \sigma_z/2} |\psi(t)\rangle$. Show that $|\psi_R(t)\rangle$ satisfies an effective time-independent Schrödinger equation:

$$i\hbar \frac{d}{dt} |\psi_R(t)\rangle = \hat{H}_{\text{eff}} |\psi_R(t)\rangle$$

and write down the explicit matrix form of $\hat{H}_{\text{eff}}$. **[13 Points]**

(c) Assuming the particle is initially in the spin-down state $|\psi(0)\rangle = |-\rangle$ at $t = 0$, derive Rabi's formula for the spin-flip probability $P_{-\to+}(t) = |\langle +|\psi(t)\rangle|^2$:

$$P_{-\to+}(t) = \frac{\omega_1^2}{\Omega_R^2} \sin^2\left(\frac{\Omega_R t}{2}\right)$$

where $\Omega_R = \sqrt{(\omega - \omega_0)^2 + \omega_1^2}$ is the generalized Rabi frequency. State the resonance condition. **[12 Points]**

Solution to Problem 2

Part (a): Hamiltonian Matrix
Using Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ and frequencies $\omega_0 = -\gamma B_0$, $\omega_1 = -\gamma B_1$:

$$\hat{H}(t) = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1(\cos\omega t - i\sin\omega t) \\ \omega_1(\cos\omega t + i\sin\omega t) & -\omega_0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix}$$

Part (b): Rotating Frame Transformation
Let $U(t) = e^{i\omega t\sigma_z/2} = \begin{pmatrix} e^{i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{pmatrix}$. Substituting $|\psi(t)\rangle = U^\dagger(t)|\psi_R(t)\rangle$ into Schrödinger's equation:

$$i\hbar|\dot{\psi_R}\rangle = \left(U\hat{H}U^\dagger - i\hbar U\dot{U}^\dagger\right)|\psi_R\rangle \equiv \hat{H}_{\text{eff}}|\psi_R\rangle$$

Evaluating terms:

$$U\hat{H}(t)U^\dagger = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1 \\ \omega_1 & -\omega_0 \end{pmatrix}, \qquad -i\hbar U\dot{U}^\dagger = -\frac{\hbar\omega}{2}\sigma_z$$

Adding these together yields the time-independent effective Hamiltonian:

$$\hat{H}_{\text{eff}} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 - \omega & \omega_1 \\ \omega_1 & -(\omega_0 - \omega) \end{pmatrix}$$

Part (c): Rabi Oscillations & Resonance
The eigenvalues of $\hat{H}_{\text{eff}}$ are $\lambda_\pm = \pm\frac{\hbar}{2}\Omega_R$, with $\Omega_R = \sqrt{(\omega_0 - \omega)^2 + \omega_1^2}$. Starting in state $|\psi(0)\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$:

$$|\psi_R(t)\rangle = \begin{pmatrix} -i\frac{\omega_1}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right) \\ \cos\left(\frac{\Omega_R t}{2}\right) + i\frac{\omega_0 - \omega}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right) \end{pmatrix}$$

The spin-flip transition probability is:

$$P_{-\to+}(t) = |\langle +|\psi_R(t)\rangle|^2 = \frac{\omega_1^2}{(\omega-\omega_0)^2+\omega_1^2}\sin^2\left(\frac{\Omega_R t}{2}\right)$$

Resonance Condition: Complete transition ($P_{\max} = 1$) occurs when $\omega = \omega_0$.

Problem 3: Delta-Function Perturbation in an Infinite Square Well [35 Points]

A particle of mass m moves in an unperturbed one-dimensional infinite square well potential:

$$V(x) = \begin{cases} 0 & 0 < x < a \\ \infty & \text{otherwise} \end{cases}$$

The unperturbed energy eigenstates and eigenvalues are given by:

$$\psi_n^{(0)}(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right), \qquad E_n^{(0)} = \frac{n^2\pi^2\hbar^2}{2ma^2}, \qquad n = 1,2,3,\ldots$$

A delta-function perturbation is placed at the center of the well:

$$\hat{H}' = \alpha\delta\left(x - \frac{a}{2}\right)$$

where $\alpha > 0$ represents the strength of the potential barrier.

(a) Calculate the first-order energy correction $E_n^{(1)}$ for all energy levels $n = 1,2,3,\ldots$. [12 Points]

(b) Explain physically and mathematically why $E_n^{(1)} = 0$ for all even values of n. [8 Points]

(c) Obtain the first-order correction to the ground state wave function $\psi_1^{(1)}(x)$. Calculate the explicit coefficient for the first non-vanishing term in the expansion series. [15 Points]

Solution to Problem 3

Part (a): First-Order Energy Shifts
In non-degenerate perturbation theory:

$$E_n^{(1)} = \left\langle \psi_n^{(0)} \middle| \hat{H}' \middle| \psi_n^{(0)} \right\rangle = \int_0^a \left[\psi_n^{(0)}(x)\right]^* \alpha\delta\left(x-\frac{a}{2}\right)\psi_n^{(0)}(x)\,dx = \alpha\left|\psi_n^{(0)}\left(\frac{a}{2}\right)\right|^2$$

Evaluating the wave function at $x = a/2$:

$$E_n^{(1)} = \frac{2\alpha}{a}\sin^2\left(\frac{n\pi}{2}\right) = \begin{cases} \frac{2\alpha}{a} & \text{for } n \text{ odd } (n = 1,3,5,\ldots) \\ 0 & \text{for } n \text{ even } (n = 2,4,6,\ldots) \end{cases}$$

Part (b): Vanishing Shift for Even n
Even quantum numbers n correspond to wave functions with nodes at the well center ($\sin(n\pi/2) = 0$). Since the particle density at $x = a/2$ is zero, the particle does not interact with the delta perturbation, leaving its energy unchanged to first order.
Part (c): First-Order Wave Function Correction
Using first-order perturbation theory:

$$\psi_1^{(1)}(x) = \sum_{m\neq 1} \frac{\left\langle \psi_m^{(0)} \middle| \hat{H}' \middle| \psi_1^{(0)} \right\rangle}{E_1^{(0)} - E_m^{(0)}}\psi_m^{(0)}(x)$$

Matrix element: $H'_{m1} = \frac{2\alpha}{a}\sin\left(\frac{m\pi}{2}\right)$. For odd $m = 3, 5, 7, \ldots$:

$$E_1^{(0)} - E_m^{(0)} = \frac{\pi^2\hbar^2}{2ma^2}(1 - m^2)$$

For the dominant lowest correction term $m = 3$:

$$c_3 = \frac{-2\alpha/a}{-4\pi^2\hbar^2/ma^2} = \frac{ma\alpha}{2\pi^2\hbar^2}$$

The corrected ground state wave function to leading non-trivial order is:

$$\psi_1(x) \approx \sqrt{\frac{2}{a}}\left[\sin\left(\frac{\pi x}{a}\right) + \frac{ma\alpha}{2\pi^2\hbar^2}\sin\left(\frac{3\pi x}{a}\right)\right]$$

1D Harmonic Oscillator Operators:

- $[\hat{a}, \hat{a}^\dagger] = 1, \quad \hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$
- $\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle, \quad \hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle$

Spin-1/2 Pauli Matrices:

- $\sigma_x = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right), \quad \sigma_y = \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right), \quad \sigma_z = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$
- $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k, \quad \{\sigma_i, \sigma_j\} = 2\delta_{ij}I$

Time-Independent Perturbation Theory:

- $E_n^{(1)} = \left\langle \psi_n^{(0)} \middle| \hat{H}' \middle| \psi_n^{(0)} \right\rangle$
- $\psi_n^{(1)} = \sum_{m \neq n} \frac{\left\langle \psi_m^{(0)} \middle| \hat{H}' \middle| \psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_m^{(0)}} \psi_m^{(0)}$

Dirac Delta Property:

- $\int_a^b f(x)\delta(x - x_0)dx = f(x_0)$ for $x_0 \in (a, b)$