SCIENCE I: Assignment 5 - Quantum Mechanics

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Problem I: Pauli Matrices

The operators are the Pauli matrices: $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

(a) Commutation Relations

We evaluate $[\sigma_i, \sigma_j] = \sigma_i\sigma_j - \sigma_j\sigma_i$.

- $[\sigma_1, \sigma_2] = 2i\sigma_3$
- $[\sigma_2, \sigma_3] = 2i\sigma_1$
- $[\sigma_3, \sigma_1] = 2i\sigma_2$

The general relation is $[\sigma_i, \sigma_j] = 2i\sum_k \epsilon_{ijk}\sigma_k$, where ϵ_{ijk} is the Levi-Civita symbol.

(b) Eigenvalues and Eigenvectors

All three Pauli matrices have eigenvalues $\lambda = \pm\mathbf{1}$.

- $\sigma_\mathbf{1}$: Eigenvectors are $v_{+1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $v_{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$.
- $\sigma_\mathbf{2}$: Eigenvectors are $v_{+1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$ and $v_{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$.
- $\sigma_\mathbf{3}$: Eigenvectors are $v_{+1} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $v_{-1} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

(c) Probability Distribution

We choose an eigenstate of σ_2, for example, $|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$, which corresponds to the eigenvalue $+1$. We then calculate the probability of measuring the eigenvalues of σ_1 and σ_3 in this state. To do this, we express $|\psi\rangle$ in the eigenbases of σ_1 and σ_3. The probabilities are the squared magnitudes of the coefficients in that basis.

- **For** σ_1: $P(\lambda = +1) = 1/2$ and $P(\lambda = -1) = 1/2$.
- **For** σ_3: $P(\lambda = +1) = 1/2$ and $P(\lambda = -1) = 1/2$.

(d) Variances and Uncertainty Relation

In the state $|\psi\rangle$ from part (c), we evaluate the variances and the uncertainty relation.

- Expectation values: $\langle\sigma_1\rangle = 0$, $\langle\sigma_3\rangle = 0$.
- Variances: $(\Delta\sigma_1)^2 = \langle\sigma_1^2\rangle - \langle\sigma_1\rangle^2 = 1 - 0 = 1$. Similarly, $(\Delta\sigma_3)^2 = 1$.
- Uncertainty Relation Product: $(\Delta\sigma_1)^2(\Delta\sigma_3)^2 = (1)(1) = 1$.
- Commutator Term: $\frac{1}{4}|\langle[\sigma_1, \sigma_3]\rangle|^2 = \frac{1}{4}|\langle -2i\sigma_2\rangle|^2 = \frac{1}{4}|-2i\langle\sigma_2\rangle|^2 = \frac{1}{4}|-2i(1)|^2 = 1$.

The uncertainty principle is satisfied, as $1 \geq 1$.

Problem II: Infinite 1D Potential Well

An electron is in the state $|\psi\rangle = \frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{2}}|\phi_2\rangle$ at $t = 0$, where $|\phi_1\rangle$ and $|\phi_2\rangle$ are the two lowest energy eigenstates in an infinite well of length L.

(a) Average Energy and Variance

The energy eigenvalues are $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$.

- **Average Energy** $\langle E\rangle$: $\langle E\rangle = \frac{1}{2}E_1 + \frac{1}{2}E_2 = \frac{5\pi^2\hbar^2}{4mL^2}$.
- **Variance** $(\Delta E)^2$: $(\Delta E)^2 = \langle E^2\rangle - \langle E\rangle^2 = \frac{1}{4}(E_2 - E_1)^2 = \frac{9\pi^4\hbar^4}{16m^2L^4}$.

Since the state is a superposition of energy eigenstates, the average energy and its variance are constant in time.

(b) Probability Density at x=L/2

At $t = 0$, the wavefunction is $\Psi(x, 0) = \frac{1}{\sqrt{L}}(\sin(\frac{\pi x}{L}) + \sin(\frac{2\pi x}{L}))$. At $x = L/2$, $\sin(\pi x/L) = \sin(\pi/2) = 1$ and $\sin(2\pi x/L) = \sin(\pi) = 0$. So, $\Psi(L/2, 0) = \frac{1}{\sqrt{L}}(1+0) = \frac{1}{\sqrt{L}}$. The probability density is $|\Psi(L/2, 0)|^2 = \mathbf{\frac{1}{L}}$.

(c) Average Position and Variance

The time-dependent wave function is $\Psi(x, t) = \frac{1}{\sqrt{2}}(\phi_1 e^{-iE_1t/\hbar} + \phi_2 e^{-iE_2t/\hbar})$.

- **Average Position** $\langle X\rangle$: The expectation value of position, $\langle X\rangle_t = \int \Psi^* x \Psi dx$, is time-dependent due to the interference between the ϕ_1 and ϕ_2 states. It oscillates around the center of the well, $L/2$.

$$\langle X\rangle_t = \frac{L}{2} - \frac{16L}{9\pi^2}\cos\left(\frac{(E_2 - E_1)t}{\hbar}\right)$$

- **Variance** $(\Delta X)^2$: This is also time-dependent.

(d) Average Momentum

The average momentum $\langle p\rangle = \int \Psi^*(-i\hbar\frac{\partial}{\partial x})\Psi dx$. For any single energy eigenstate, the average momentum is zero. However, for this superposition state, it is time-dependent and non-zero.

$$\langle p\rangle_t = \frac{8\hbar}{3L}\sin\left(\frac{(E_2 - E_1)t}{\hbar}\right)$$