

Complementary Quantum Mechanics

Homework Set 1: Quantum Mechanics Revision

This problem set reviews wavefunctions, expectation values and uncertainties, operators and commutators, superposition and measurement, and Dirac notation. Show the essential steps in each calculation.

Useful notation and relations

For a normalised state $|\psi\rangle$,

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle, \quad (\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2.$$

In the position representation,

$$\hat{p}_x = -i\hbar \frac{d}{dx}, \quad [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}.$$

For a complete orthonormal set $\{|\psi_n\rangle\}$,

$$\langle \psi_n | \psi_m \rangle = \delta_{nm}, \quad \sum_n |\psi_n\rangle \langle \psi_n| = \hat{I}.$$

A. Wavefunctions, expectation values and uncertainties

Problem 1. A polynomial wavefunction in an infinite square well

A particle of mass m is confined to an infinite square well of width L , with $0 \leq x \leq L$. At $t = 0$ its wavefunction is

$$\psi(x, 0) = \begin{cases} B x(x - L), & 0 \leq x \leq L, \\ 0, & \text{elsewhere.} \end{cases}$$

(a) Normalise the wavefunction and show that

$$B = \sqrt{\frac{30}{L^5}}.$$

(b) Calculate the expectation value of the energy and show that

$$\langle E \rangle = \frac{10}{\pi^2} E_1,$$

where the ground-state energy of the infinite square well is

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2} = \frac{h^2}{8mL^2}.$$

Problem 2. Ground state of the harmonic oscillator

A particle of mass m in a one-dimensional harmonic oscillator of angular frequency ω has the normalised ground-state wavefunction

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \exp\left(-\frac{\alpha x^2}{2}\right), \quad \alpha = \frac{m\omega}{\hbar}.$$

(a) Calculate

$$\langle x \rangle, \quad \langle x^2 \rangle, \quad \langle p_x \rangle, \quad \langle p_x^2 \rangle.$$

Hence determine the uncertainties Δx and Δp_x .

(b) Verify explicitly that the Heisenberg uncertainty relation is satisfied, and determine the value of $\Delta x \Delta p_x$ for this state.

You may use, for $\beta > 0$,

$$\int_{-\infty}^{\infty} e^{-\beta x^2} dx = \sqrt{\frac{\pi}{\beta}}, \quad \int_{-\infty}^{\infty} x^2 e^{-\beta x^2} dx = \frac{\sqrt{\pi}}{2\beta^{3/2}}.$$

B. Operators and commutators

Problem 3. Hermiticity of the position operator

Show that the position operator $\hat{x}$ is Hermitian. State clearly the inner product you use.

Problem 4. Product rule for commutators

For arbitrary operators $\hat{A}$, $\hat{B}$ and $\hat{C}$, show that

$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}.$$

Problem 5. Commutator of the Hamiltonian with position

Consider a one-dimensional system with Hamiltonian

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + U(\hat{x}),$$

where $U(\hat{x})$ is an arbitrary function of the position operator. Using the result of Problem 4 and the canonical commutator $[\hat{x}, \hat{p}_x] = i\hbar$, show that

$$[\hat{H}, \hat{x}] = -\frac{i\hbar}{m} \hat{p}_x.$$

Problem 6. Basic commutators in three dimensions

Evaluate

$$[\hat{p}_x, \hat{x}], \quad [\hat{y}, \hat{p}_x], \quad [\hat{p}_x, \hat{p}_y].$$

Problem 7. Legendre differential operator

Consider the Legendre differential operator

$$\hat{L} = (1 - x^2) \frac{d^2}{dx^2} - 2x \frac{d}{dx}$$

acting on

$$\psi_1(x) = x, \quad \psi_2(x) = \frac{1}{2}(3x^2 - 1), \quad \psi_3(x) = \frac{1}{2}(5x^3 - 3x).$$

(a) Show that, for $n = 1, 2, 3$,

$$\hat{L}\psi_n(x) = -n(n+1)\psi_n(x).$$

(b) Show explicitly that the three functions are mutually orthogonal on the interval $[-1, 1]$:

$$\int_{-1}^1 \psi_n^*(x) \psi_m(x) dx = 0, \quad n \neq m.$$

C. Superposition and quantum measurement

Problem 8. Energy expectation value and uncertainty in a superposition

At $t = 0$, a particle is in the normalised state

$$|\Psi(0)\rangle = \frac{\sqrt{3}}{2}|\psi_1\rangle + \frac{i}{2}|\psi_2\rangle,$$

where $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthonormal energy eigenstates satisfying

$$\hat{H}|\psi_1\rangle = \varepsilon|\psi_1\rangle, \quad \hat{H}|\psi_2\rangle = 2\varepsilon|\psi_2\rangle.$$

- (a) Verify that $|\Psi(0)\rangle$ is normalised.
- (b) Determine the expectation value $\langle E \rangle$.
- (c) Determine $\langle E^2 \rangle$.
- (d) Hence determine the energy uncertainty ΔE .

Problem 9. Consecutive measurements in a two-state system

The Hamiltonian $\hat{H}$ of a two-state system has orthonormal eigenstates $|\psi_1\rangle$ and $|\psi_2\rangle$ with distinct eigenvalues E_1 and E_2 . Another Hermitian operator $\hat{B}$ has orthonormal eigenstates $|\phi_1\rangle$ and $|\phi_2\rangle$ with distinct eigenvalues b_1 and b_2 . The two bases are related by

$$|\psi_1\rangle = \frac{1}{\sqrt{13}}(2|\phi_1\rangle + 3|\phi_2\rangle), \quad |\psi_2\rangle = \frac{1}{\sqrt{13}}(3|\phi_1\rangle - 2|\phi_2\rangle).$$

- (a) Verify that $|\psi_1\rangle$ and $|\psi_2\rangle$ are normalised and mutually orthogonal.
- (b) Express $|\phi_1\rangle$ and $|\phi_2\rangle$ in terms of $|\psi_1\rangle$ and $|\psi_2\rangle$.
- (c) A sequence of three measurements is performed immediately one after another, so that time evolution between measurements can be neglected.
 - (i) In the first measurement, the energy E_1 is obtained. What is the state immediately after this measurement?

- (ii) In the second measurement, $\hat{B}$ is measured. What are the possible outcomes, their probabilities, and the corresponding post-measurement states?
- (iii) In the third measurement, the energy is measured again. Determine the probability of obtaining E_1 , taking into account both possible outcomes of the second measurement. Determine also the probability of obtaining E_2 .

Problem 10. Expansion in the eigenstates of an infinite square well

A particle of mass m is confined to an infinite square well of width L , $0 \leq x \leq L$. The normalised energy eigenfunctions and energy eigenvalues are

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad E_n = n^2 E_1, \quad E_1 = \frac{\pi^2 \hbar^2}{2mL^2},$$

with $n = 1, 2, 3, \dots$

The particle is initially described by

$$\Psi(x) = \begin{cases} Bx, & 0 \leq x \leq L/2, \\ B(L-x), & L/2 \leq x \leq L, \\ 0, & \text{elsewhere,} \end{cases} \quad B = \sqrt{\frac{12}{L^3}}.$$

- (a) Expand $\Psi(x)$ in the energy eigenbasis,

$$\Psi(x) = \sum_{n=1}^{\infty} c_n \psi_n(x),$$

and show that

$$|c_n|^2 = \begin{cases} 0, & n \text{ even,} \\ \frac{96}{n^4 \pi^4}, & n \text{ odd.} \end{cases}$$

- (b) Using the probabilities $|c_n|^2$, show that

$$\langle E \rangle = \frac{12}{\pi^2} E_1.$$

You may use

$$\int x \sin(ax) dx = -\frac{x \cos(ax)}{a} + \frac{\sin(ax)}{a^2}, \quad \sum_{k=0}^{\infty} \frac{1}{(2k+1)^2} = \frac{\pi^2}{8}.$$

D. Dirac notation and operator algebra

Problem 11. Classifying Dirac expressions

For each expression below, state whether it is well-defined. If it is, classify the result as a scalar, operator, ket, or bra. Here a is a scalar and $\hat{A}, \hat{B}$ are operators.

(a) $a \psi\rangle$	(b) $\langle\psi \hat{A} \psi\rangle$
(c) $\langle\psi \hat{A} \phi\rangle\langle\psi \phi\rangle$	(d) $ \psi\rangle\hat{A}$
(e) $\langle\psi \hat{B}$	(f) $ \psi\rangle\langle\psi $
(g) $ \psi\rangle\langle\psi \phi\rangle$	(h) $[\hat{A}, \hat{B}] \psi\rangle$

Problem 12. Inner products and normalisation

Consider

$$|u\rangle = |\phi_1\rangle + 2i|\phi_2\rangle, \quad |v\rangle = |\phi_1\rangle + 2|\phi_2\rangle + |\phi_3\rangle,$$

where $|\phi_1\rangle, |\phi_2\rangle$, and $|\phi_3\rangle$ form an orthonormal basis.

(a) Evaluate

$$\langle u | v \rangle, \quad \langle u | u \rangle, \quad \langle v | v \rangle, \quad \langle v | u \rangle.$$

(b) Construct the normalised ket corresponding to $|v\rangle$.

Problem 13. Eigenstates of a two-state Hamiltonian

A two-state system has Hamiltonian

$$\hat{H} = \alpha(|1\rangle\langle 2| + |2\rangle\langle 1|),$$

where α is a real constant and $|1\rangle, |2\rangle$ form an orthonormal basis.

(a) Show that $|1\rangle$ and $|2\rangle$ are not eigenstates of $\hat{H}$ by evaluating $\hat{H}|1\rangle$ and $\hat{H}|2\rangle$.

(b) Seek an eigenstate in the form

$$|\psi\rangle = a_1|1\rangle + a_2|2\rangle.$$

Determine the two normalised eigenstates and their corresponding eigenvalues.

Problem 14. Hermiticity in Dirac notation

Suppose that $|0\rangle, |1\rangle$, and $|2\rangle$ form an orthonormal basis. Determine whether each of the following operators is Hermitian. Justify your answer by taking the adjoint explicitly.

$$\hat{A} = |0\rangle\langle 1| - i|1\rangle\langle 0|.$$

$$\hat{B} = |0\rangle\langle 0| + i|1\rangle\langle 0| - i|0\rangle\langle 1| + |2\rangle\langle 2|.$$