Quantum Mechanics: Problems 1

1. An operator A is said to be *linear* if it satisfies

$$A(a\psi_1 + b\psi_2) = aA\psi_1 + bA\psi_2$$

for any wavefunctions ψ_1 and ψ_2 and any complex numbers a and b.

Which of the following operators are linear?

(a)	$k+$	(add k)	(b)	x	(multiply by x)
(c)	$\sqrt{}$	(square root)	(d)	$*$	(complex conjugate)
(e)	$\dfrac{d}{dx}$	(differentiate)	(f)	$i\,\dfrac{d}{dx}$	

2. A linear operator A is *Hermitian* if it satisfies

$$\langle\psi_1\,|\,A\,|\,\psi_2\rangle = \langle\psi_2\,|\,A\,|\,\psi_1\rangle^*.$$

For a particle moving along the x axis the 'matrix element' $\langle\psi_1\,|\,A\,|\,\psi_2\rangle$ is

$$\langle\psi_1\,|\,A\,|\,\psi_2\rangle = \int_{-\infty}^{\infty} \psi_1(x)^*\, A\,\psi_2(x)\, dx,$$

and for bounded motion the wavefunctions must satisfy $\psi_n(x) \to 0$ as $x \to \infty$. (Why?)

Which of the operators x, $\dfrac{d}{dx}$, $i\dfrac{d}{dx}$ and $\dfrac{d^2}{dx^2}$ are Hermitian?

3. For a particle confined to a one-dimensional box $0 \le x \le L$, the 'inner product' $\langle\psi_1\,|\,\psi_2\rangle$ of the two wavefunctions ψ_1 and ψ_2 is given by

$$\langle\psi_1\,|\,\psi_2\rangle = \int_0^L \psi_1(x)^*\psi_2(x)\, dx.$$

The functions are said to be *orthogonal* if $\langle\psi_1\,|\,\psi_2\rangle = 0$, *normalized* if $\langle\psi_1\,|\,\psi_1\rangle = \langle\psi_2\,|\,\psi_2\rangle = 1$, and *orthonormal* if both of these conditions are satisfied.

Show that the functions $\psi_1 = N_1 \sin(\pi x/L)$ and $\psi_2 = N_2 \sin(2\pi x/L)$ are orthogonal, and determine the constants N_1 and N_2 which normalize them.

4. Show that $\exp(+ipx/\hbar)$ is an eigenfunction of the momentum operator $p_x = -i\hbar\, d/dx$ with eigenvalue p, and that the kinetic energy operator $T = (1/2m)\, p_x^2$ has two independent eigenfunctions, $\psi_\pm(x) = \exp(\pm ipx/\hbar)$, with a common eigenvalue $E = p^2/2m$ (they are said to be *two-fold degenerate*). What is the physical interpretation of this result?

Show that $\sin(px/\hbar)$ is an eigenfunction of T but not of p_x.

5. Show that the function

$$\psi(x) = \begin{cases} Ce^{+ipx/\hbar} + De^{-ipx/\hbar}, & 0 \le x \le L, \\ 0, & x < 0,\ x > L, \end{cases}$$

satisfies the Schrödinger equation when the potential energy is

$$V(x) = \begin{cases} 0, & 0 \le x \le L, \\ \infty, & x < 0,\ x > L. \end{cases}$$

By imposing the boundary condition that $\psi(x)$ is continuous, show that the eigenfunctions of the Hamiltonian have the form $\psi(x) = \sin(px/\hbar)$ with $p = nh/2L$ $(n = 1, 2, \ldots)$.

6. The expectation value $\langle A \rangle$ of an operator A for a system in a stationary state described by a normalized wavefunction ψ_n is

$$\langle A \rangle = \langle \psi_n \,|\, A \,|\, \psi_n \rangle.$$

For a particle having the (normalized) wavefunction

$$\psi_n(x) = \begin{cases} \sqrt{\dfrac{2}{L}} \sin\left(\dfrac{n\pi x}{L}\right), & 0 \le x \le L, \\ 0, & x < 0,\ x > L, \end{cases}$$

where n is an integer, show that:

(a) $\langle x \rangle = \dfrac{L}{2}$ (b) $\langle x^2 \rangle = L^2 \left(\dfrac{1}{3} - \dfrac{1}{2n^2\pi^2} \right)$

(c) $\langle p_x \rangle = 0$ (d) $\langle p_x^2 \rangle = \dfrac{n^2 h^2}{4L^2}$

Hint: The easiest way to do part (c) is to use a symmetry argument, and the easiest way to do part (d) is to note that $\langle p_x^2 \rangle = (2m)\langle T \rangle = (2m)\langle H \rangle = 2mE$.

7. The uncertainty principle states that $\Delta x \Delta p_x \geq \frac{1}{2}\hbar$, where Δx and Δp_x are the root mean square deviations of x and p_x from their mean values:

$$\Delta x = \left(\langle x^2 \rangle - \langle x \rangle^2\right)^{\frac{1}{2}},$$

$$\Delta p_x = \left(\langle p_x^2 \rangle - \langle p_x \rangle^2\right)^{\frac{1}{2}}.$$

Use your answer to question 6 to show that the particle-in-a-box eigenstates $\psi_n(x) = \sqrt{2/L}\,\sin(n\pi x/L)$ satisfy the uncertainty principle.

8. Consider a particle moving in one dimension with a time-independent Hamiltonian H. The full wavefunction for the particle satisfies the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = H\,\Psi(x,t),$$

and for a normalized wavefunction $\Psi(x,t)$ the expectation value of an operator A is

$$\langle A \rangle = \langle \Psi \,|\, A \,|\, \Psi \rangle = \int_{-\infty}^{\infty} \Psi(x,t)^*\, A\, \Psi(x,t)\, dx.$$

Using these two equations, and the fact that H is Hermitian, show that $\langle A \rangle$ changes with time according to

$$\frac{d}{dt}\langle A \rangle = \frac{i}{\hbar}\langle [H, A] \rangle,$$

and hence that the energy $E = \langle H \rangle$ of the particle is a constant of the motion.

9. The classical equations of motion for the position x and momentum p_x of a particle moving in a potential $V(x)$ are

$$\frac{d}{dt}x = \frac{p_x}{m} \qquad \text{and} \qquad \frac{d}{dt}p_x = -V'(x)$$

(i.e., $p = mv$ and $F = ma$, respectively). Ehrenfest's theorem states that the quantum mechanical expectation values of the operators x and p_x evolve in the same way:

$$\frac{d}{dt}\langle x \rangle = \frac{\langle p_x \rangle}{m} \qquad \text{and} \qquad \frac{d}{dt}\langle p_x \rangle = -\langle V'(x) \rangle.$$

Prove this theorem by setting $H = (1/2m)\,p_x^2 + V(x)$ and applying the general result $d\langle A \rangle/dt = (i/\hbar)\langle [H, A] \rangle$ to the operators $A = x$ and $A = p_x$.

10. Write down (a) the Hamiltonian, (b) the general form of the eigenvalues, and (c) the explicit forms of the eigenfunctions corresponding to the two lowest eigenvalues for each of the following three systems:

(i) A particle of mass m in a one-dimensional box of length L.

(ii) Two non-interacting particles of mass m in a one-dimensional box of length L.

(iii) A particle of mass m in a cube of side L.