

HW 8 solutions:

Problem 5.1 (a, b, d, e)

(a) Let the potential in the region $-L/2 < x < L/2$ be zero and infinity elsewhere. The eigenfunctions are $\psi_n(x, t) = \sqrt{2/L} \sin(k_n(x + L/2)) e^{-i\omega_n t}$, where $k_n = n\pi/L$, $\omega_n = \hbar k_n^2/2m$, and $n = 1, 2, 3, \dots$. Hence,

$$\psi_1(x, t) = \sqrt{2/L} \sin((\pi/L)(x + L/2)) e^{-i\omega_1 t} = \sqrt{2/L} \cos((\pi x/L) e^{-i\omega_1 t})$$

$$\psi_4(x, t) = \sqrt{2/L} \sin((4\pi/L)(x + L/2)) e^{-i\omega_4 t} = \sqrt{2/L} \sin(4\pi x/L) e^{-i\omega_4 t}$$

and the probability distribution of the particle in the superposition state

$$\psi(x, t) = \sqrt{1/2}(\psi_1(x, t) + \psi_4(x, t))$$

is

$$|\psi(x, t)|^2 = \frac{1}{2}(|\psi_1(x)|^2 + |\psi_4(x)|^2 + 2\text{Re}\{\psi_1(x)\psi_4^*(x)\} \cos((\omega_4 - \omega_1)t))$$

$$|\psi(x, t)|^2 = \frac{1}{L} \left(\cos^2\left(\frac{\pi x}{L}\right) + \sin^2\left(\frac{4\pi x}{L}\right) + 2 \cos\left(\frac{\pi x}{L}\right) \sin\left(\frac{4\pi x}{L}\right) \cos\left(\frac{\hbar}{2m} \frac{15\pi^2}{L^2} t\right) \right)$$

$$\text{where we note that } \omega_4 - \omega_1 = \frac{\hbar}{2m} \frac{15\pi^2}{L^2}.$$

(b) Expectation value of position is

$$\langle x(t) \rangle = \int |\psi(x, t)|^2 x dx$$

$$\langle x(t) \rangle = \frac{1}{2} \int_{-L/2}^{L/2} (|\psi_1(x)|^2 x + |\psi_4(x)|^2 x + 2x\text{Re}\{\psi_1(x)\psi_4^*(x)\} \cos((\omega_4 - \omega_1)t)) dx$$

By symmetry, the first two terms in the integrand are zero, leaving

$$\langle x(t) \rangle = \cos((\omega_4 - \omega_1)t) \int_{-L/2}^{L/2} \frac{2}{L} \cos\left(\frac{\pi x}{L}\right) \sin\left(\frac{4\pi x}{L}\right) x dx$$

making use of $2 \sin(x) \cos(y) = \sin(x+y) + \sin(x-y)$ gives

$$\langle x(t) \rangle = \cos((\omega_4 - \omega_1)t) \frac{1}{L} \int_{-L/2}^{L/2} \left(\sin\left(\frac{5\pi x}{L}\right) + \sin\left(\frac{3\pi x}{L}\right) \right) x dx$$

which, after integrating by parts, results in

$$\langle x(t) \rangle = \cos((\omega_4 - \omega_1)t) \frac{1}{L} \left(\frac{2L^2}{25\pi^2} - \frac{2L^2}{9\pi^2} \right)$$

$$\langle x(t) \rangle = -\frac{32L}{225\pi^2} \cos((\omega_4 - \omega_1)t)$$

(d) The expectation value of momentum is

$$\langle p_x(t) \rangle = -i\hbar \int \psi^*(x, t) \frac{\partial}{\partial x} \psi(x, t) dx = \frac{-i\hbar}{2} \int_{-L/2}^{L/2} \left((\psi_1^* + \psi_4^*) \frac{\partial}{\partial x} (\psi_1 + \psi_4) \right) dx$$

The terms $\int_{-L/2}^{L/2} \psi_4^* \frac{\partial \psi_4}{\partial x} dx = 0$ and $\int_{-L/2}^{L/2} \psi_1^* \frac{\partial \psi_1}{\partial x} dx = 0$ by symmetry, leaving

$$\begin{aligned} \langle p_x(t) \rangle &= \frac{-i\hbar}{2} \frac{2}{L} \frac{4\pi}{L} e^{-i(\omega_4 - \omega_1)t} \int_{-L/2}^{L/2} \cos\left(\frac{\pi x}{L}\right) \cos\left(\frac{4\pi x}{L}\right) dx + \\ &\quad \frac{i\hbar}{2} \frac{2\pi}{L} e^{i(\omega_4 - \omega_1)t} \int_{-L/2}^{L/2} \sin\left(\frac{4\pi x}{L}\right) \sin\left(\frac{\pi x}{L}\right) dx \\ \langle p_x(t) \rangle &= \frac{-i\hbar}{2} \frac{8\pi}{L^2} e^{-i(\omega_4 - \omega_1)t} \frac{2L}{15\pi} + \frac{i\hbar}{2} \frac{2\pi}{L^2} e^{i(\omega_4 - \omega_1)t} \frac{8L}{15\pi} \end{aligned}$$

$$\langle p_x(t) \rangle = \frac{-i\hbar}{15L} (e^{-i(\omega_4 - \omega_1)t} \cancel{+} e^{i(\omega_4 - \omega_1)t})$$

and

$$\langle p_x(t) \rangle = \frac{16\hbar}{15L} \sin((\omega_4 - \omega_1)t)$$

(e) The current density is

$$J_x(x, t) = \frac{-ie\hbar}{2m} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right)$$

$$J_x(x, t) = \frac{-ie\hbar}{4m} \left((\psi_1^* + \psi_4^*) \frac{\partial}{\partial x} (\psi_1 + \psi_4) - (\psi_1 + \psi_4) \frac{\partial}{\partial x} (\psi_1^* + \psi_4^*) \right)$$

$$\begin{aligned} J_x(x, t) &= \frac{-ie\hbar}{2Lm} \left(\cos\left(\frac{\pi x}{L}\right) \frac{\partial}{\partial x} \sin\left(\frac{4\pi x}{L}\right) (e^{i(\omega_1 - \omega_4)t} - e^{-i(\omega_1 - \omega_4)t}) + \right. \\ &\quad \left. \sin\left(\frac{4\pi x}{L}\right) \frac{\partial}{\partial x} \cos\left(\frac{\pi x}{L}\right) (e^{-i(\omega_1 - \omega_4)t} - e^{i(\omega_1 - \omega_4)t}) \right) \end{aligned}$$

$$J_x(x, t) = \frac{-e\hbar}{Lm} \left(\cos\left(\frac{\pi x}{L}\right) \frac{\partial}{\partial x} \sin\left(\frac{4\pi x}{L}\right) - \sin\left(\frac{4\pi x}{L}\right) \frac{\partial}{\partial x} \cos\left(\frac{\pi x}{L}\right) \right) \sin((\omega_4 - \omega_1)t)$$

$$J_x(x, t) = \frac{-\pi e\hbar}{mL^2} \left(4 \cos\left(\frac{\pi x}{L}\right) \cos\left(4\pi \frac{x}{L}\right) + \sin\left(4\pi \frac{x}{L}\right) \sin\left(\frac{\pi x}{L}\right) \right) \sin((\omega_4 - \omega_1)t)$$

Problem 5.6

The Hamiltonian \hat{H} in the Schrödinger equation is Hermitian and so it is its own Hermitian adjoint, i.e., $\hat{H} = \hat{H}^\dagger$. The time dependence of the expectation value of the observable A associated with operator \hat{A} is found from

$$\frac{d}{dt}\langle A \rangle = \langle \frac{\partial \psi}{\partial t} | \hat{A} | \psi \rangle + \langle \psi | \frac{\partial}{\partial t} \hat{A} | \psi \rangle + \langle \psi | \hat{A} | \frac{\partial \psi}{\partial t} \rangle$$

which may be rewritten as

$$\frac{d}{dt}\langle A \rangle = \frac{i}{\hbar} \langle \psi | \hat{H} \hat{A} | \psi \rangle - \frac{i}{\hbar} \langle \psi | \hat{A} \hat{H} | \psi \rangle + \langle \psi | \frac{\partial}{\partial t} \hat{A} | \psi \rangle$$

$$\frac{d}{dt}\langle A \rangle = \frac{i}{\hbar} \langle \psi | \hat{H} \hat{A} - \hat{A} \hat{H} | \psi \rangle + \langle \psi | \frac{\partial}{\partial t} \hat{A} | \psi \rangle$$

where we used the Hermitian property of \hat{H} and the fact that the Schrödinger equation is

$$\frac{-i}{\hbar} \hat{H} | \psi \rangle = | \frac{\partial \psi}{\partial t} \rangle$$

Hence,

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

If the Hamiltonian commutes with the operator \hat{A} , then $[\hat{H}, \hat{A}] = 0$, and we may conclude that

$$\frac{d}{dt}\langle A \rangle = \langle \frac{\partial}{\partial t} \hat{A} \rangle$$

Problem 5.7

- (a) The position operator \hat{x} is Hermitian if it is its own Hermitian adjoint, i.e., $\hat{x}^\dagger = \hat{x}$ or $\langle \psi | x | \phi \rangle = \langle \phi | x | \psi \rangle^*$. For the operator \hat{x} this is easy to show

$$\langle \psi | x | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x) (x \psi(x)) dx = \int_{-\infty}^{\infty} (x \psi^*(x)) \psi(x) dx = \int_{-\infty}^{\infty} (x \psi(x))^* \psi(x) dx = \langle x \psi | \psi \rangle$$

(b) To show that the operator $\frac{d}{dx}$ is anti-Hermitian we integrate by parts and make use of the fact that the wavefunction $\psi(x) \rightarrow 0$ as $x \rightarrow \pm\infty$

$$\begin{aligned}\langle \psi | \frac{d}{dx} \psi \rangle &= \int_{-\infty}^{\infty} \psi^*(x) \left(i\hbar \frac{d}{dx} \psi(x) \right) dx = \psi^*(x) \psi(x) \Big|_{x=-\infty}^{x=\infty} - \int_{-\infty}^{\infty} \left(\frac{d}{dx} \psi^*(x) \right) \psi(x) dx \\ \langle \psi | \frac{d}{dx} \psi \rangle &= - \int_{-\infty}^{\infty} \left(\frac{d}{dx} \psi(x) \right)^* \psi(x) dx = - \langle \frac{d}{dx} \psi | \psi \rangle\end{aligned}$$

and $\left(\frac{d}{dx} \right)^\dagger = - \frac{d}{dx}$.

(c) Because the operator $\frac{d}{dx}$ is anti-Hermitian, it follows that the momentum operator

$$-i\hbar \frac{d}{dx}$$
 is Hermitian since $\left(-i\hbar \frac{d}{dx} \right)^\dagger = i\hbar \left(- \frac{d}{dx} \right) = -i\hbar \frac{d}{dx}$.

Problem 5.8

(a) The Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

and the momentum operator is

$$\hat{p} = -i\hbar \frac{d}{dx}$$

To find the commutator $[\hat{H}, \hat{p}]$ we have it act on the arbitrary wave function $\psi(x)$ so that

$$\begin{aligned}[\hat{H}, \hat{p}]\psi &= \hat{H}\hat{p}\psi - \hat{p}\hat{H}\psi \\ &= \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right) \left(-i\hbar \frac{d\psi}{dx} \right) - \left(-i\hbar \frac{d}{dx} \right) \left(-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi \right) \\ &= i\frac{\hbar^3}{2m} \frac{d^3\psi}{dx^3} - i\hbar V \frac{d\psi}{dx} - i\frac{\hbar^3}{2m} \frac{d^3\psi}{dx^3} + i\hbar \psi \frac{dV}{dx} + i\hbar V \frac{d\psi}{dx} \\ &= i\hbar \frac{dV}{dx} \psi\end{aligned}$$

and

$$[\hat{H}, \hat{p}] = i\hbar \frac{dV}{dx}$$

(b) Solutions of the time-independent Schrödinger equation are eigenfunctions of the Hamiltonian. If the solutions are also eigenstates of the momentum operator then the operators \hat{H} and \hat{p} must commute, i.e. $[\hat{H}, \hat{p}] = 0$. Hence, from part (a), we require

$$[\hat{H}, \hat{p}] = i\hbar \frac{dV}{dx} = 0. \text{ This can only be satisfied if the potential is a constant (which}$$

can be set to zero) over all space. We may conclude that only free particles can be in such eigenstates of momentum.