Solutions:
Homework Set 4

Due September 4

1. In this problem we consider the spreading of wave packets of a free particle in one dimension. The Hamiltonian is

$$H = \frac{p^2}{2m} \tag{1}$$

   (a) Let the wave function at time $t = 0$ be

$$\psi_0(x) = \psi(x, t = 0) = Ce^{-x^2/(4L^2)}, \tag{2}$$

   where C and L are constants (with L real).

   Normalize the wave function and find C, choosing C real and positive, $C > 0$.

   Then determine $\langle x \rangle$, $\langle p \rangle$ and $\Delta x \equiv \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ at $t = 0$.

$$1 = \int dx |\psi_0(x)|^2 = |C|^2 \int dx e^{-x^2/2L^2} = |C|^2 \sqrt{2\pi L^2} \tag{3}$$

   Choosing positive, real C:

$$C = \frac{1}{(2\pi L^2)^{1/4}} \tag{4}$$

$$\psi_0(x) = \frac{1}{\sqrt{2\pi L^2}} e^{-x^2/(4L^2)} \tag{5}$$

$$\langle x\rangle = \int dx x|\psi_0|^2 = \frac{1}{\sqrt{2\pi L^2}}\int dx\ xe^{-x^2/(2L^2)} \tag{6}$$

$$= 0 \tag{7}$$

$$\langle p\rangle = \frac{1}{\sqrt{2\pi L^2}}\int dx\ e^{-x^2/(4L^2)}\left(-i\frac{d}{dx}\right)e^{-x^2/(4L^2)} \tag{8}$$

$$= 0 \tag{9}$$

$$\Delta x^2 = \langle x^2\rangle = \frac{1}{\sqrt{2\pi L^2}}\int x^2 e^{-x^2/2L^2} = \frac{1}{\sqrt{2\pi L^2}}(L^2)\sqrt{2\pi L^2} \tag{10}$$

$$= L^2 \tag{11}$$

$$\Delta x = L \tag{12}$$

(b) Compute the initial momentum space wave function $\psi_0(p)$, and from that compute $\Delta p \equiv \sqrt{\langle p^2\rangle - \langle p\rangle^2}$.

Compare $\Delta x \Delta p$ to the minimum value allowed by the uncertainty principle

$$\Psi_0(p) = \frac{1}{\sqrt{2\pi L^2}}\int dx e^{-ipx/\hbar}\psi_0(x) \tag{13}$$

$$= \frac{1}{\sqrt{2\pi L^2}}\frac{1}{\sqrt{2\pi L^2}}\int dx e^{-x^2/4L^2 - ipx/\hbar} \tag{14}$$

$$= \left(\frac{2L^2}{\pi\hbar^2}\right)^{1/4} e^{-p^2L^2/\hbar^2} \tag{15}$$

$$\Delta p^2 = \langle p^2\rangle = \sqrt{\frac{2L^2}{\pi\hbar^2}}\int dp p^2 e^{-2p^2L^2/\hbar^2} \tag{16}$$

$$= \sqrt{\frac{2L^2}{\pi\hbar^2}}\left(\frac{\hbar^2}{4L^2}\right)\sqrt{\frac{\pi\hbar^2}{2L^2}} \tag{17}$$

$$= \frac{\hbar^2}{4L^2} \tag{18}$$

$$\Delta p = \frac{\hbar}{2L} \tag{19}$$

$$\Delta x \Delta p = \frac{\hbar}{2} \tag{20}$$

This is the minimum value allowed by the uncertainty principle

(c) Now compute $\psi(p,t)$ for any time t. Use it to find $\langle p\rangle$ and Δp for any time t.

$$\psi(p,t) = \langle p|e^{-itH/\hbar}|\psi\rangle = e^{-itp^2/2m\hbar}\psi_0(p) \tag{21}$$

$$= \left(\frac{2L^2}{\pi\hbar^2}\right)^{1/4} e^{-p^2L^2/\hbar^2 - itp^2/2m\hbar} \tag{22}$$

$$\langle p\rangle(t) = \int dp\; p|\psi(p,t)|^2 = \int dp\sqrt{\frac{2L^2}{\pi\hbar^2}}pe^{-p^2L^2/\hbar^2} \tag{23}$$

$$= 0 \tag{24}$$

$$\Delta p^2 = \int dp p^2|\psi(p,t)|^2 = \int dp\sqrt{\frac{2L^2}{\pi\hbar^2}}p^2e^{-p^2L^2/\hbar^2} \tag{25}$$

$$= \frac{\hbar^2}{4L^2} \tag{26}$$

The mean and dispersion is independent of time (and the same as at $t = 0$.)

(d) Now compute $\psi(x,t)$ for any time t. Express your answer in terms of the quantity,

$$D = L + \frac{it\hbar}{2mL}, \tag{27}$$

(a useful abbreviation). Then find $\langle x\rangle$ and Δx for any time t. Notice what happens to the product $\Delta x\Delta p$ for times $t > 0$.

$$\psi(x,t) = \langle x|e^{-itH\hbar}|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\left(\frac{2L^2}{\pi\hbar^2}\right)^{1/4}\int dp\exp(\frac{-p^2L^2}{\hbar^2} - \frac{itp2}{2m\hbar} + \frac{ipx}{\hbar}) \tag{28}$$

$$= \frac{1}{(2\pi)^{1/4}}\frac{1}{\sqrt{D}}e^{-x^2/4LD} \tag{29}$$

For expressing $\langle x\rangle$ the following quantities are useful:

$$\psi(x,t)^* = \frac{1}{(2\pi)^{1/4}}\frac{1}{\sqrt{D^*}}e^{-x^2/4LD^*} \tag{30}$$

$$DD^* = |D|^2 = L^2 + \frac{t^2\hbar^2}{4m^2L^2} \tag{31}$$

$$\frac{1}{D}\frac{1}{D^*} = \frac{D + D^*}{DD^*} = \frac{2L}{|D|^2} \tag{32}$$

$$\implies |\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{|D|^2}}e^{-x^2/2|D|^2} \tag{33}$$

Finally, we can write

$$\langle x\rangle(t) = \int dx x|\psi(x,t)|^2 \tag{34}$$

$$= \frac{1}{\sqrt{2\pi|D|^2}} \int dx x e^{-x^2/2|D|^2} \tag{35}$$

$$= 0 \tag{36}$$

$$\Delta x^2 = \frac{1}{\sqrt{2\pi|D|^2}} \int dx x^2 e^{-x^2/2|D|^2} \tag{37}$$

$$= |D|^2 \tag{38}$$

$$\Delta x = \sqrt{L^2 + \frac{t^2\hbar^2}{4m^2L^2}} \tag{39}$$

(e) If you had not done a detailed calculation you could estimate Δx as a function of t by using the uncertainty principle. Do this and compare to the results of the detailed calculation

If $\Delta x =$ L, then $\Delta p = \frac{\hbar^2}{2\Delta x} = \frac{\hbar}{2L}$.

So $\Delta v = \frac{\Delta p}{m} = \frac{\hbar}{2mL}$. So in time it should spread by $\Delta v t = \frac{\hbar t}{2mL}$.

This is the same as the explicit formula when t is large:

$$\Delta x \to \sqrt{\frac{t^2\hbar^2}{4m^2L^2}} = \frac{t\hbar}{2mL} \tag{40}$$

2. Consider a single, spinless particle moving in one dimension, confined by rigid walls at $x = 0$ and $x = a$.

   That is, a particle in an infinite square well

$$H = \frac{p^2}{2m} + V(x), \tag{41}$$

$$V(x) = \begin{cases} \infty & x > a \\ 0 & 0 \le x \le a\ , \\ \infty & x < 0 \end{cases} \tag{42}$$

   so that the wavefunction satisfies the free particle Schrödinger equation for $0 \le x \le a$, but the probability of measuring the particle with position $x < 0$ or $x > a$ is zero.

   (a) Find an expression for the energy eigenstates $\psi_n(x)$ and eigenvalues E_n. Is there any degeneracy?

In the interval $0 \leq x \leq a$, the wavefunction satisfies the equation

$$H|\psi_n\rangle = E_n|\psi_n\rangle \tag{43}$$

$$\implies \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) = E_n\psi_n(x) \tag{44}$$

with boundary condition $\psi(0) = \psi(a) = 0$.

The normalized solutions are

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \tag{45}$$

with $n \in \{1, 2, \ldots\}$.

The energies are

$$E_n = \frac{n^2\hbar^2\pi^2}{2ma^2}. \tag{46}$$

Eigenstates with energy E_n are unique (up to an overall phase), and so there is no degeneracy.

(b) For each energy eigenstate, evaluate

$$\Delta x^2 \Delta p^2 \equiv \left(\langle x^2\rangle - \langle x\rangle^2\right)\left(\langle p^2\rangle - \langle p\rangle^2\right) \tag{47}$$

We need to compute $\langle x\rangle$, $\langle x^2\rangle$, $\langle p\rangle$, and $\langle p^2\rangle$ for ψ_n:

$$\langle x^2\rangle = \frac{2}{a}\int_0^a dx\ x^2\sin^2\left(\frac{n\pi x}{a}\right) \tag{48}$$

$$= \frac{a^2}{3} - \frac{a^2}{2\pi^2 n^2} \tag{49}$$

$$\langle x\rangle = \frac{2}{a}\int_0^a dx\ x\sin^2\left(\frac{n\pi x}{a}\right) \tag{50}$$

$$= \frac{a}{2} \tag{51}$$

$$\langle p\rangle = \frac{2}{a}\int_0^a dx \sin\left(\frac{n\pi x}{a}\right)\left(-i\hbar\frac{d}{dx}\right)\sin\left(\frac{n\pi x}{a}\right) \tag{52}$$

$$= -i\hbar\frac{2n\pi}{a^2}\int_0^a dx \sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{n\pi x}{a}\right) \tag{53}$$

$$= 0 \tag{54}$$

$$\langle p^2\rangle = \frac{2}{a}\int_0^a dx \sin\left(\frac{n\pi x}{a}\right)\left(-\hbar^2\frac{d^2}{dx^2}\right)\sin\left(\frac{n\pi x}{a}\right) \tag{55}$$

$$= \hbar^2\frac{2}{a}\left(\frac{n\pi}{a}\right)^2\int_0^a dx \sin^2\left(\frac{n\pi x}{a}\right) \tag{56}$$

$$= \frac{\hbar^2 n^2\pi^2}{a^2} \tag{57}$$

$$\Delta x^2 = \langle x^2\rangle - \langle x\rangle^2 \tag{58}$$

$$= \frac{a^2}{3} - \frac{a^2}{2\pi^2 n^2} - \frac{a^2}{4} \tag{59}$$

$$= a^2\left[\frac{1}{12} - \frac{1}{2\pi^2 n^2}\right] \tag{60}$$

$$\Delta p^2 = \langle p^2\rangle = \frac{\hbar^2 n^2\pi^2}{a^2} \tag{61}$$

$$\Delta x^2\Delta p^2 = \hbar^2 n^2\pi^2\left[\frac{1}{12} - \frac{1}{2\pi^2 n^2}\right] \tag{62}$$

(c) For which energy eigenstate is this the smallest? How does it compare to the minimum allowed by the uncertainty principle?

This is smallest for the ground state, $n = 1$

$$\Delta x^2\Delta p^2 = \hbar^2\pi^2\left[\frac{1}{12} - \frac{1}{2\pi^2}\right] \tag{63}$$

$$= \frac{\hbar^2}{4}\left[\frac{\pi^2}{3} - 2\right] \simeq 1.3\frac{\hbar^2}{4} \tag{64}$$

$$\geq \frac{\hbar^2}{4} \tag{65}$$