PHY V2500: QUANTUM MECHANICS I

Problem Set 4

Due October 23, 2025

Problem 1

The wave function for a particular state for a one dimensional system is given by

$$\psi(x) = A\,e^{-i\omega t}\,x\,e^{-ax}$$

where x is the in the range $0 \le x \le \infty$.

a) Determine the normalization factor A.

b) Calculate the expectation values $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$ and $\langle p^2\rangle$.

c) Verify the uncertainty relation for x and p using your results.

Solution

We will need integrals of the form $\int x^n e^{-2ax}$. We evaluate this as

$$\int_0^\infty dx\,x^n e^{-2ax} = \frac{1}{(2a)^{n+1}}\int du\,u^n e^{-u} = \frac{n!}{(2a)^{n+1}}$$

where $u = 2ax$. Notice also that

$$I(n) = \int du\,u^n e^{-u} = \frac{u^n e^{-u}}{(-1)}\Big]_0^\infty + \int du\,n\,u^{n-1}e^{-u} = n\,I(n-1)$$

This shows that $I(n) = n!$.

a) For normalization, we find

$$1 = |A|^2 \int dx\,x^2\,e^{-2ax} = \frac{|A|^2}{4a^3}$$

This gives $A = 2a^{\frac{3}{2}}$.

b) We also have

$$\begin{aligned}
\langle x\rangle &= 4a^3 \int dx\,x^3 e^{-2ax} = \frac{3}{2a} \\
\langle p\rangle &= 4a^3 \int xe^{-ax}\left(-i\hbar\frac{\partial}{\partial x}\right)xe^{-ax} = 4a^3(-i\hbar)\int dx\,[x - ax^2]e^{-2ax} \\
&= 4a^3(-i\hbar)\left[\frac{1}{(2a)^2} - \frac{a2!}{(2a)^3}\right] = 0 \\
\langle x^2\rangle &= 4a^3 \int dx\,x^4 e^{-2ax} = \frac{3}{a^2} \\
\langle p^2\rangle &= 4a^3(-\hbar^2)\int dx\,xe^{-ax}\frac{\partial^2}{\partial x^2}(xe^{-ax}) = 4a^3(-\hbar^2)\int dx\,xe^{-ax}(a^2x - 2ax)e^{-ax} \\
&= 4a^3(-\hbar^2)\left[a^2\frac{2}{(2a)^3} + (-2a)\frac{1}{4a^2}\right] = \hbar^2 a^2
\end{aligned}$$

c) From the results given above,

$$\Delta x^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{3}{4a^2}, \qquad \Delta p^2 = \langle p^2 \rangle - \langle p \rangle^2 = \hbar^2 a^2$$

We find

$$\Delta x \, \Delta p = \frac{\sqrt{3}}{2a} \, \hbar a = \sqrt{3} \, \frac{\hbar}{2}$$

This is consistent with the uncertainty principle $\Delta x \, \Delta p \geq (\hbar/2)$.

Problem 2

Consider the harmonic oscillator problem discussed in class. The oscillator is initially (at time $t = 0$) given to be in the state described by the wave function

$$\psi(x) = \frac{1}{\sqrt{2}} \, (u_1 + u_2)$$

where $u_0 = \langle x|1\rangle$ and $u_1 = \langle x|2\rangle$ are the wave functions for the first and second excited states, respectively. Obtain ψ at time $t > 0$ and calculate the probability to find the particle in the range $-\infty < x < 0$. (*Caution*: You cannot use orthogonality since the required range is only the half-line.)

Solution

The states have the energies $E_1 = (1 + \frac{1}{2})\hbar\omega$, $E_2 = (2 + \frac{1}{2})\hbar\omega$. Thus the state at time t is given by

$$\psi(x,t) = \frac{1}{\sqrt{2}} e^{-i3\omega t/2} \left(u_1 + e^{-i\omega t} u_2 \right)$$

The required probability is given by

$$\int_0^\infty dx \, |\psi|^2 = \int_0^\infty dx \, \frac{1}{2} \left[u_1^2 + u_2^2 + u_1 u_2 (e^{i\omega t} + e^{-i\omega t}) \right] = \int_0^\infty dx \, \frac{1}{2} \left[u_1^2 + u_2^2 + 2 u_1 u_2 \cos \omega t \right]$$

The integrals we need are

$$\begin{aligned}
\int_0^\infty d\xi \, \xi e^{-\xi^2} &= \frac{1}{2} \int_0^\infty du e^{-u} = \frac{1}{2} \\
\int_0^\infty d\xi \, \xi^3 e^{-\xi^2} &= \frac{1}{2} \int_0^\infty du u \, e^{-u} = \frac{1}{2} \\
\int_0^\infty d\xi \, e^{-\xi^2} &= \frac{\sqrt{\pi}}{2} \\
\int_0^\infty d\xi \, \xi^2 e^{-\xi^2} &= \frac{\sqrt{\pi}}{4} \\
\int_0^\infty d\xi \, \xi^4 e^{-\xi^2} &= \frac{3\sqrt{\pi}}{8}
\end{aligned}$$

The last two follow from the integral

$$\int_0^\infty d\xi \, e^{\lambda \xi^2} e^{-\xi^2} = \frac{1}{2} \frac{\sqrt{\pi}}{(1-\lambda)^{\frac{1}{2}}}$$

by expanding both sides in powers of λ. The wave functions in terms of the Hermite polynomials give

$$\begin{aligned} u_1 &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \sqrt{2}\xi\, e^{-\frac{1}{2}\xi^2} \\ u_2 &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{(4\xi^2-2)}{\sqrt{8}}\, e^{-\frac{1}{2}\xi^2}, \qquad \xi = \sqrt{\frac{m\omega}{\hbar}}\, x \end{aligned}$$

These give

$$\begin{aligned} \int_0^\infty dx\, u_1^2 &= \frac{1}{\sqrt{\pi}} \int_0^\infty d\xi\, 2\xi^2\, e^{-\xi^2} = \frac{1}{2} \\ \int_0^\infty dx\, u_2^2 &= \frac{1}{\sqrt{\pi}} \int_0^\infty d\xi\, \frac{(16\xi^4 - 16\xi^2 + 4)}{8}\, e^{-\xi^2} = \frac{(6-4+2)}{8} = \frac{1}{2} \\ \int_0^\infty dx\, u_1 u_2 &= \frac{1}{\sqrt{\pi}} \int_0^\infty d\xi\, \frac{(4\xi^2-2)}{\sqrt{8}} \frac{2\xi}{\sqrt{2}} e^{-\xi^2} = \frac{1}{\sqrt{\pi}} \int_0^\infty d\xi\, (2\xi^3 - \xi) e^{-\xi^2} \\ &= \frac{1}{2\sqrt{\pi}} \end{aligned}$$

This gives

$$\int_0^\infty dx\, |\psi|^2 = \frac{1}{2} + \frac{1}{2\sqrt{\pi}} \cos\omega t$$

Problem 3

Consider the harmonic oscillator with the Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2\, \hat{x}^2$$

A particle is created in the state given by the wave function

$$\psi = \begin{cases} C(1 - |x|/a) & |x| \le a \\ 0 & |x| > a \end{cases}$$

This wave function is thus a bump around the origin vanishing beyond a on both sides. Calculate the expectation value of the Hamiltonian for this wave function.Your answer will be a function of a; let us call this as $\mathcal{E}(a)$. Minimize $\mathcal{E}(a)$ with respect to a and then use it back in $\mathcal{E}(a)$ to obtain the minimum value for $\mathcal{E}$ for this type of wave function.

Solution

We start with the normalization of ψ. Notice that ψ is an even function, so we can write

$$\begin{aligned} \int dx |\psi|^2 &= 2|C|^2 \int_0^a dx (1 - x/a)^2 = 2|C|^2 \int_0^a dx \left(1 - 2\frac{x}{a} + \frac{x^2}{a^2}\right) \\ &= 2|C|^2 \left(a - \frac{1}{a} a^2 + \frac{1}{a^2} \frac{a^3}{3}\right) = |C|^2 \frac{2a}{3} \end{aligned}$$

This gives $C = \sqrt{3/2a}$. The expectation value of the Hamiltonian is of the form

$$\langle H \rangle = \int dx\, \psi^* H \psi$$

Notice that

$$\frac{\partial}{\partial x}\psi = \begin{cases} -\frac{1}{a} & x > 0 \\ \frac{1}{a} & x < 0 \end{cases}$$

The derivative is discontinuous at $x = 0$ and the second derivative is undefined there. We avoid this by writing the expectation value of H as

$$\langle H \rangle = \frac{\hbar^2}{2m} \int \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} + \frac{m\omega^2}{2} \int \psi^* x^2 \psi$$

The required integrals are

$$\begin{aligned} \int \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} &= \frac{3}{2a} 2 \int_0^a (1/a)^2 = \frac{3}{a^2} \\ \int \psi^* x^2 \psi &= \frac{3}{2a} 2 \int_0^a dx\, x^2 \big(1 - (x/a)\big)^2 = \frac{3}{2a} 2 \int_0^a dx \left(x^2 - 2\frac{x^3}{a} + \frac{x^4}{a^2}\right) \\ &= \frac{a^2}{10} \end{aligned}$$

Thus

$$\mathcal{E}(a) = \langle H \rangle = \frac{3\hbar^2}{2ma^2} + \frac{m\omega^2 a^2}{20}$$

We minimize with respect to a; this gives the condition

$$\frac{m\omega^2 a}{10} = 3\frac{\hbar^2}{ma^3} \implies a^2 = a_*^2 = \sqrt{30}(\hbar/m\omega)$$

Using this back in $\mathcal{E}(a)$,

$$\mathcal{E}(a_*) = \frac{\sqrt{30}}{10}\hbar\omega \approx 0.547\,\hbar\omega$$

Notice that this is fairly close to the actual ground state energy $E_0 = \frac{1}{2}\hbar\omega$.

Problem 4

A wave function of the form $\psi \sim e^{ikx}$ is not localized as $\psi^*\psi$ is the same for all x. The probability to find the particle is the same everywhere. An approximately localized state can be obtained as a combination of the plane wave states. A simple example of that, in one dimension, is

$$\psi = \frac{1}{(\pi\sigma^2)^{1/4}} \exp\left[iq(x - x_0) - i\frac{\hbar q^2 t}{m}\right] \exp\left[-\frac{(x - x_0 - vt)^2}{2\sigma^2}\right]$$

where $v = \hbar q/m$. Here q and x_0 are free (and constant) parameters, and σ is another parameter giving the extent of localization. For this expression, calculate $\psi^*\psi$ and the probability current J. Calculate the time-derivative of $\psi^*\psi$ and express it in terms of J.

Solution

By direct calculation

$$\rho = \psi^* \psi = \frac{1}{\sqrt{\pi\sigma^2}} \exp\left(-\frac{(x-z)^2}{\sigma^2}\right), \qquad z = x_0 + vt$$

Thus

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -\frac{1}{\sigma^2} 2(x-z)\dot{z}\,\rho = 2\frac{(x-z)}{\sigma^2}\,v\,\rho \\ \frac{\partial \rho}{\partial x} &= -2\frac{(x-z)}{\sigma^2}\,\rho \end{aligned}$$

Similarly

$$\begin{aligned} J &= -\frac{i\hbar}{2m}\left[\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\,\psi\right] \\ &= -\frac{i\hbar}{2m}\left[\psi^* \left(iq - \frac{(x-z)}{\sigma^2}\right)\psi - \text{complex conjugate}\right] = \frac{\hbar q}{m}\,\rho = v\rho \\ \frac{\partial J}{\partial x} &= v\frac{\partial \rho}{\partial x} = -2\frac{(x-z)}{\sigma^2} v\rho \end{aligned}$$

We see from these equations that

$$\frac{\partial \rho}{\partial t} = -\frac{\partial J}{\partial x}$$