Problem 3.49

(a) Write down the time-dependent "Schrödinger equation" in momentum space, for a free particle, and solve it. *Answer:* $\exp\left(-ip^2t/2m\hbar\right)\Phi(p,0)$.

(b) Find $\Phi(p,0)$ for the traveling gaussian wave packet (Problem 2.42), and construct $\Phi(p,t)$ for this case. Also construct $|\Phi(p,t)|^2$, and note that it is independent of time.

(c) Calculate $\langle p\rangle$ and $\langle p^2\rangle$ by evaluating the appropriate integrals involving Φ, and compare your answers to Problem 2.42.

(d) Show that $\langle H\rangle = \langle p\rangle^2/2m + \langle H\rangle_0$ (where the subscript 0 denotes the *stationary* gaussian), and comment on this result.

Solution

Part (a)

The governing equation for the position-space wave function of a particle with mass m is Schrödinger's equation.

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi(x,t), \quad -\infty < x < \infty,\ t > 0$$

For a free particle in particular, the potential energy function $V(x,t)$ is zero.

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} \tag{1}$$

Because this is a linear PDE over the whole line ($-\infty < x < \infty$), the Fourier transform can be applied to solve it. The Fourier transform of $\Psi(x,t)$ is defined here by

$$\Phi(p,t) = \mathscr{F}\{\Psi(x,t)\} = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\Psi(x,t)\,dx$$

in order to obtain the momentum-space wave function $\Phi(p,t)$. The temporal derivative transforms as follows.

$$\begin{aligned}
\mathscr{F}\left\{\frac{\partial\Psi}{\partial t}\right\} &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\frac{\partial\Psi}{\partial t}\,dx \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\frac{\partial}{\partial t}\left[e^{-ipx/\hbar}\Psi(x,t)\right]dx \\
&= \frac{1}{\sqrt{2\pi\hbar}}\frac{d}{dt}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\Psi(x,t)\,dx \\
&= \frac{d}{dt}\left[\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\Psi(x,t)\,dx\right] \\
&= \frac{d\Phi}{dt}
\end{aligned}$$

The spatial derivative transforms as follows.

$$\begin{aligned}
\mathscr{F}\left\{\frac{\partial^2\Psi}{\partial x^2}\right\} &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\frac{\partial^2\Psi}{\partial x^2}\,dx \\
&= \frac{1}{\sqrt{2\pi\hbar}}\left[\underbrace{e^{-ipx/\hbar}\frac{\partial\Psi}{\partial x}\bigg|_{-\infty}^{\infty}}_{=\,0} - \int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left(e^{-ipx/\hbar}\right)\frac{\partial\Psi}{\partial x}\,dx\right] \\
&= \frac{1}{\sqrt{2\pi\hbar}}\left[-\int_{-\infty}^{\infty}\left(-\frac{ip}{\hbar}e^{-ipx/\hbar}\right)\frac{\partial\Psi}{\partial x}\,dx\right] \\
&= \frac{ip}{\hbar}\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\frac{\partial\Psi}{\partial x}\,dx \\
&= \frac{ip}{\hbar}\frac{1}{\sqrt{2\pi\hbar}}\left[\underbrace{e^{-ipx/\hbar}\Psi(x,t)\bigg|_{-\infty}^{\infty}}_{=\,0} - \int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left(e^{-ipx/\hbar}\right)\Psi(x,t)\,dx\right] \\
&= \frac{ip}{\hbar}\frac{1}{\sqrt{2\pi\hbar}}\left[-\int_{-\infty}^{\infty}\left(-\frac{ip}{\hbar}e^{-ipx/\hbar}\right)\Psi(x,t)\,dx\right] \\
&= \frac{i^2p^2}{\hbar^2}\left[\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\Psi(x,t)\,dx\right] \\
&= -\frac{p^2}{\hbar^2}\Phi(p,t)
\end{aligned}$$

Take the Fourier transform of both sides of equation (1).

$$\mathscr{F}\left\{i\hbar\frac{\partial\Psi}{\partial t}\right\} = \mathscr{F}\left\{-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}\right\}$$

Use the fact that the Fourier transform is linear.

$$i\hbar\mathscr{F}\left\{\frac{\partial\Psi}{\partial t}\right\} = -\frac{\hbar^2}{2m}\mathscr{F}\left\{\frac{\partial^2\Psi}{\partial x^2}\right\}$$

Transform the derivatives.

$$i\hbar\left(\frac{d\Phi}{dt}\right) = -\frac{\hbar^2}{2m}\left[-\frac{p^2}{\hbar^2}\Phi(p,t)\right]$$

$$i\hbar\frac{d\Phi}{dt} = \frac{p^2}{2m}\Phi(p,t)$$

$$\frac{d\Phi}{dt} = -\frac{ip^2}{2m\hbar}\Phi(p,t)$$

Solve this ODE by separating variables.

$$\frac{d\Phi}{\Phi} = -\frac{ip^2}{2m\hbar}\,dt$$

Integrate both sides.

$$\ln\Phi = -\frac{ip^2}{2m\hbar}t + C(p)$$

Exponentiate both sides.

$$e^{\ln \Phi} = \exp\left[-\frac{ip^2}{2m\hbar}t + C(p)\right]$$

$$\Phi(p,t) = e^{C(p)} \exp\left(-\frac{ip^2}{2m\hbar}t\right)$$

Set $t = 0$ to determine $e^{C(p)}$.

$$\Phi(p,0) = e^{C(p)}$$

Therefore, the momentum-space wave function for a free particle is

$$\boxed{\Phi(p,t) = \Phi(p,0) \exp\left(-\frac{ip^2}{2m\hbar}t\right).}$$

Part (b)

For a travelling gaussian wave packet, the initial position-space wave function is $\Psi(x,0) = Ae^{-ax^2}e^{-ilx}$. Normalize it to determine A.

$$\begin{aligned}
1 &= \int_{-\infty}^{\infty} |\Psi(x,0)|^2 \, dx \\
&= \int_{-\infty}^{\infty} (Ae^{-ax^2}e^{ilx})(Ae^{-ax^2}e^{-ilx}) \, dx \\
&= \int_{-\infty}^{\infty} A^2 e^{-2ax^2} \, dx \\
&= 2A^2 \int_0^{\infty} \exp\left[-\frac{x^2}{\left(\frac{1}{\sqrt{2a}}\right)^2}\right] dx \\
&= 2A^2 \cdot \sqrt{\pi}\left(\frac{\frac{1}{\sqrt{2a}}}{2}\right) \\
&= A^2\sqrt{\frac{\pi}{2a}}
\end{aligned}$$

Solve for A.

$$A = \left(\frac{2a}{\pi}\right)^{1/4}$$

As a result,

$$\Psi(x,0) = \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2}e^{ilx},$$

and the momentum-space wave function becomes

$$\begin{aligned}
\Phi(p,t) &= \exp\left(-\frac{ip^2}{2m\hbar}t\right)\Phi(p,0) \\
&= \exp\left(-\frac{ip^2}{2m\hbar}t\right)\mathscr{F}\{\Psi(x,0)\} \\
&= \exp\left(-\frac{ip^2}{2m\hbar}t\right)\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\Psi(x,0)\,dx \\
&= \exp\left(-\frac{ip^2}{2m\hbar}t\right)\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2}e^{ilx}\,dx \\
&= \left(\frac{a}{2\pi^3\hbar^2}\right)^{1/4}\exp\left(-\frac{ip^2}{2m\hbar}t\right)\int_{-\infty}^{\infty}\exp\left[-ax^2+i\left(-\frac{p}{\hbar}+l\right)x\right]dx \\
&= \left(\frac{a}{2\pi^3\hbar^2}\right)^{1/4}\exp\left(-\frac{ip^2}{2m\hbar}t\right)\int_{-\infty}^{\infty}\exp\left[-a\left(x^2+i\frac{\hbar l-p}{\hbar a}x\right)\right]dx \\
&= \left(\frac{a}{2\pi^3\hbar^2}\right)^{1/4}\exp\left(-\frac{ip^2}{2m\hbar}t\right)\int_{-\infty}^{\infty}\exp\left\{-a\left[x^2+i\frac{\hbar l-p}{\hbar a}x+i^2\frac{(\hbar l-p)^2}{4\hbar^2a^2}\right]\right\}\exp\left[ai^2\frac{(\hbar l-p)^2}{4\hbar^2a^2}\right]dx \\
&= \left(\frac{a}{2\pi^3\hbar^2}\right)^{1/4}\exp\left(-\frac{ip^2}{2m\hbar}t\right)\exp\left[-\frac{(\hbar l-p)^2}{4\hbar^2a}\right]\int_{-\infty}^{\infty}\exp\left[-a\left(x+i\frac{\hbar l-p}{2\hbar a}\right)^2\right]dx.
\end{aligned}$$

Make the following substitution.

$$u = x + i\frac{\hbar l-p}{2\hbar a}$$

$$du = dx$$

Consequently,

$$\begin{aligned}
\Phi(p,t) &= \left(\frac{a}{2\pi^3\hbar^2}\right)^{1/4}\exp\left(-\frac{ip^2}{2m\hbar}t\right)\exp\left[-\frac{(\hbar l-p)^2}{4\hbar^2a}\right]\int_{-\infty}^{\infty} e^{-au^2}\,du \\
&= \left(\frac{a}{2\pi^3\hbar^2}\right)^{1/4}\exp\left(-\frac{ip^2}{2m\hbar}t\right)\exp\left[-\frac{(\hbar l-p)^2}{4\hbar^2a}\right]\sqrt{\frac{\pi}{a}} \\
&= \left(\frac{1}{2\pi\hbar^2a}\right)^{1/4}\exp\left(-\frac{ip^2}{2m\hbar}t\right)\exp\left[-\frac{(p-\hbar l)^2}{4\hbar^2a}\right],
\end{aligned}$$

and the probability distribution for the particle's momentum is

$$\begin{aligned}
|\Phi(p,t)|^2 &= \Phi^*(p,t)\Phi(p,t) \\
&= \left\{\left(\frac{1}{2\pi\hbar^2a}\right)^{1/4}\exp\left(\frac{ip^2}{2m\hbar}t\right)\exp\left[-\frac{(p-\hbar l)^2}{4\hbar^2a}\right]\right\}\left\{\left(\frac{1}{2\pi\hbar^2a}\right)^{1/4}\exp\left(-\frac{ip^2}{2m\hbar}t\right)\exp\left[-\frac{(p-\hbar l)^2}{4\hbar^2a}\right]\right\} \\
&= \sqrt{\frac{1}{2\pi\hbar^2a}}\exp\left[-\frac{(p-\hbar l)^2}{2\hbar^2a}\right].
\end{aligned}$$

Part (c)

Now calculate the expectation value of p at time t.

$$\langle p\rangle = \langle \Phi \,|\, \hat{p} \,|\, \Phi\rangle = \int_{-\infty}^{\infty} \Phi^*(p,t)p\Phi(p,t)\,dp = \int_{-\infty}^{\infty} p|\Phi(p,t)|^2\,dp$$

$$= \sqrt{\frac{1}{2\pi\hbar^2 a}}\int_{-\infty}^{\infty} p\exp\left[-\frac{(p-\hbar l)^2}{2\hbar^2 a}\right]dp$$

Make the substitution,

$$v = p - \hbar l \quad \rightarrow \quad p = v + \hbar l$$

$$dv = dp.$$

Then

$$\begin{aligned}
\langle p\rangle &= \sqrt{\frac{1}{2\pi\hbar^2 a}}\int_{-\infty}^{\infty}(v+\hbar l)\exp\left(-\frac{v^2}{2\hbar^2 a}\right)dv \\
&= \frac{1}{\sqrt{2\pi\hbar^2 a}}\left[\underbrace{\int_{-\infty}^{\infty} v\exp\left(-\frac{v^2}{2\hbar^2 a}\right)dv}_{=\,0} + \hbar l\int_{-\infty}^{\infty}\exp\left(-\frac{v^2}{2\hbar^2 a}\right)dv\right] \\
&= \frac{1}{\sqrt{2\pi\hbar^2 a}}\left[\hbar l\left(\sqrt{\pi}\cdot\sqrt{2\hbar^2 a}\right)\right] \\
&= \hbar l,
\end{aligned}$$

which is the same result obtained in Problem 2.42. Now calculate the expectation value of p^2 at time t.

$$\begin{aligned}
\langle p^2\rangle = \langle \Phi \,|\, \hat{p}^2 \,|\, \Phi\rangle &= \int_{-\infty}^{\infty}\Phi^*(p,t)p^2\Phi(p,t)\,dp \\
&= \int_{-\infty}^{\infty} p^2|\Phi(p,t)|^2\,dp \\
&= \sqrt{\frac{1}{2\pi\hbar^2 a}}\int_{-\infty}^{\infty} p^2\exp\left[-\frac{(p-\hbar l)^2}{2\hbar^2 a}\right]dp \\
&= \frac{1}{\sqrt{2\pi\hbar^2 a}}\int_{-\infty}^{\infty}(v+\hbar l)^2\exp\left(-\frac{v^2}{2\hbar^2 a}\right)dv \\
&= \frac{1}{\sqrt{2\pi\hbar^2 a}}\int_{-\infty}^{\infty}(v^2+2\hbar l v+\hbar^2 l^2)\exp\left(-\frac{v^2}{2\hbar^2 a}\right)dv \\
&= \frac{1}{\sqrt{2\pi\hbar^2 a}}\left[\int_{-\infty}^{\infty} v^2\exp\left(-\frac{v^2}{2\hbar^2 a}\right)dv + 2\hbar l\underbrace{\int_{-\infty}^{\infty} v\exp\left(-\frac{v^2}{2\hbar^2 a}\right)dv}_{=\,0}\right. \\
&\qquad\left. + \hbar^2 l^2\int_{-\infty}^{\infty}\exp\left(-\frac{v^2}{2\hbar^2 a}\right)dv\right]
\end{aligned}$$

Evaluate the integrals and simplify the answer.

$$\begin{aligned}\langle p^2\rangle &= \frac{1}{\sqrt{2\pi\hbar^2 a}}\left[\sqrt{\pi}\cdot\frac{(2\hbar^2 a)^{3/2}}{2} + \hbar^2 l^2\left(\sqrt{\pi}\cdot\sqrt{2\hbar^2 a}\right)\right] \\ &= \frac{2\hbar^2 a}{2} + \hbar^2 l^2 \\ &= \hbar^2 a + \hbar^2 l^2 \\ &= \hbar^2(a + l^2)\end{aligned}$$

This is the same result obtained in Problem 2.42.

Part (d)

Finally, calculate the expectation value of energy.

$$\begin{aligned}\langle H\rangle &= \left\langle \frac{p^2}{2m} + V\right\rangle \\ &= \left\langle \frac{p^2}{2m} + 0\right\rangle \\ &= \frac{1}{2m}\langle p^2\rangle \\ &= \frac{1}{2m}(\hbar^2 a + \hbar^2 l^2) \\ &= \frac{(\hbar l)^2}{2m} + \frac{a\hbar^2}{2m} \\ &= \frac{\langle p\rangle^2}{2m} + \frac{\langle p^2\rangle_0}{2m} \\ &= \underbrace{\frac{\langle p\rangle^2}{2m}}_{\substack{\text{energy due}\\ \text{to motion}}} + \underbrace{\langle H\rangle_0}_{\substack{\text{energy of}\\ \text{stationary}\\ \text{wave packet}}}\end{aligned}$$

The stationary gaussian wave packet (with $l = 0$) was analyzed in Problem 2.21, and there it was found that $\langle p^2\rangle_0 = a\hbar^2$.