Problem 2.20

A free particle has the initial wave function

$$\Psi(x,0) = Ae^{-a|x|},$$

where A and a are positive real constants.

(a) Normalize $\Psi(x,0)$.

(b) Find $\phi(k)$.

(c) Construct $\Psi(x,t)$, in the form of an integral.

(d) Discuss the limiting cases (a very large, and a very small).

Solution

The governing equation for the wave function is the Schrödinger 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, $V = 0$, and the equation simplifies to

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

Let there be a prescribed initial condition, $\Psi(x,0) = \Psi_0(x)$. Since the PDE is linear and $-\infty < x < \infty$, the Fourier transform can be applied to solve it. The Fourier transform of $\Psi(x,t)$ is defined here as

$$\mathcal{F}\{\Psi(x,t)\} = \tilde{\Psi}(k,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx}\Psi(x,t)\,dx.$$

As a result, the partial derivatives of Ψ transform as follows.

$$\mathcal{F}\left\{\frac{\partial^n \Psi}{\partial x^n}\right\} = (ik)^n\tilde{\Psi}(k,t)$$
$$\mathcal{F}\left\{\frac{\partial^n \Psi}{\partial t^n}\right\} = \frac{d^n\tilde{\Psi}}{dt^n}$$

Take the Fourier transform of both sides of the Schrödinger equation.

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

Since the transform is a linear operator, the constants can be brought in front.

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

Transform the derivatives.

$$i\hbar\frac{d\tilde{\Psi}}{dt} = -\frac{\hbar^2}{2m}(ik)^2\tilde{\Psi}(k,t)$$

By using the Fourier transform, Schrödinger's equation has become a first-order ODE. Solve it now.

$$\frac{\frac{d\tilde{\Psi}}{dt}}{\tilde{\Psi}} = -\frac{i\hbar}{2m}k^2$$

$$\frac{d}{dt}\ln\tilde{\Psi} = -\frac{i\hbar}{2m}k^2$$

$$\ln\tilde{\Psi} = -\frac{i\hbar}{2m}k^2 t + C(k)$$

$$\tilde{\Psi}(k,t) = B(k)\exp\left(-\frac{i\hbar}{2m}k^2 t\right)$$

To determine $B(k)$, transform the given initial condition,

$$\Psi(x,0) = \Psi_0(x) \quad \rightarrow \quad \mathcal{F}\{\Psi(x,0)\} = \mathcal{F}\{\Psi_0(x)\} \quad \rightarrow \quad \tilde{\Psi}(k,0) = \tilde{\Psi}_0(k),$$

and then apply it.

$$\tilde{\Psi}(k,0) = B(k) = \tilde{\Psi}_0(k)$$

Consequently, the transformed solution to Schrödinger's equation is

$$\tilde{\Psi}(k,t) = \tilde{\Psi}_0(k)\exp\left(-\frac{i\hbar}{2m}k^2 t\right).$$

Now take the inverse Fourier transform to get $\Psi(x,t)$.

$$\begin{aligned}\Psi(x,t) &= \mathcal{F}^{-1}\left\{\tilde{\Psi}(k,t)\right\} \\ &= \mathcal{F}^{-1}\left\{\tilde{\Psi}_0(k)\exp\left(-\frac{i\hbar}{2m}k^2 t\right)\right\} \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\tilde{\Psi}_0(k)\exp\left(-\frac{i\hbar}{2m}k^2 t\right)dk\end{aligned}$$

Therefore, the solution to the Schrödinger equation for a free particle is

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\left(ikx - \frac{i\hbar}{2m}k^2 t\right)\tilde{\Psi}_0(k)\,dk.}$$

Part (a)

Normalize the initial wave function by requiring the integral of $|\Psi(x,0)|^2$ over the whole line to be 1.

$$\begin{aligned}1 = \int_{-\infty}^{\infty}|\Psi(x,0)|^2\,dx = \int_{-\infty}^{\infty}A^2 e^{-2a|x|}\,dx = 2A^2\int_0^{\infty}e^{-2a|x|}\,dx &= 2A^2\int_0^{\infty}e^{-2ax}\,dx \\ &= 2A^2\left(\frac{1}{-2a}e^{-2ax}\Big|_0^{\infty}\right) \\ &= 2A^2\left(\frac{1}{2a}\right) \\ &= \frac{A^2}{a}\end{aligned}$$

Solve for A.

$$A = \sqrt{a}$$

As a result, the initial wave function is

$$\Psi_0(x) = \sqrt{a}e^{-a|x|}.$$

Part (b)

$\phi(k)$ is the Fourier transform of the initial wave function.

$$\begin{aligned}
\phi(k) &= \tilde{\Psi}_0(k) \\
&= \mathcal{F}\left\{\Psi_0(x)\right\} \\
&= \mathcal{F}\left\{\sqrt{a}e^{-a|x|}\right\} \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx}\sqrt{a}e^{-a|x|}\,dx \\
&= \sqrt{\frac{a}{2\pi}}\int_{-\infty}^{\infty} e^{-ikx-a|x|}\,dx \\
&= \sqrt{\frac{a}{2\pi}}\left(\int_{-\infty}^{0} e^{-ikx+ax}\,dx + \int_{0}^{\infty} e^{-ikx-ax}\,dx\right) \\
&= \sqrt{\frac{a}{2\pi}}\left[\int_{-\infty}^{0} e^{(-ik+a)x}\,dx + \int_{0}^{\infty} e^{(-ik-a)x}\,dx\right] \\
&= \sqrt{\frac{a}{2\pi}}\left[\frac{1}{-ik+a}e^{(-ik+a)x}\bigg|_{-\infty}^{0} + \frac{1}{-ik-a}e^{(-ik-a)x}\bigg|_{0}^{\infty}\right] \\
&= \sqrt{\frac{a}{2\pi}}\left(\frac{1}{-ik+a} + \frac{1}{ik+a}\right) \\
&= \sqrt{\frac{a}{2\pi}}\left[\frac{(ik+a)+(-ik+a)}{(-ik+a)(ik+a)}\right] \\
&= \sqrt{\frac{a}{2\pi}}\left(\frac{2a}{k^2+a^2}\right)
\end{aligned}$$

Part (c)

Substitute the initial wave function into the boxed formula for $\Psi(x,t)$.

$$\begin{aligned}
\Psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \exp\left(ikx - \frac{i\hbar}{2m}k^2t\right)\tilde{\Psi}_0(k)\,dk \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \exp\left(ikx - \frac{i\hbar}{2m}k^2t\right)\sqrt{\frac{a}{2\pi}}\left(\frac{2a}{k^2+a^2}\right)dk \\
&= \frac{a^{3/2}}{\pi}\int_{-\infty}^{\infty} \exp\left(ikx - \frac{i\hbar}{2m}k^2t\right)\frac{dk}{k^2+a^2}
\end{aligned}$$

Part (d)

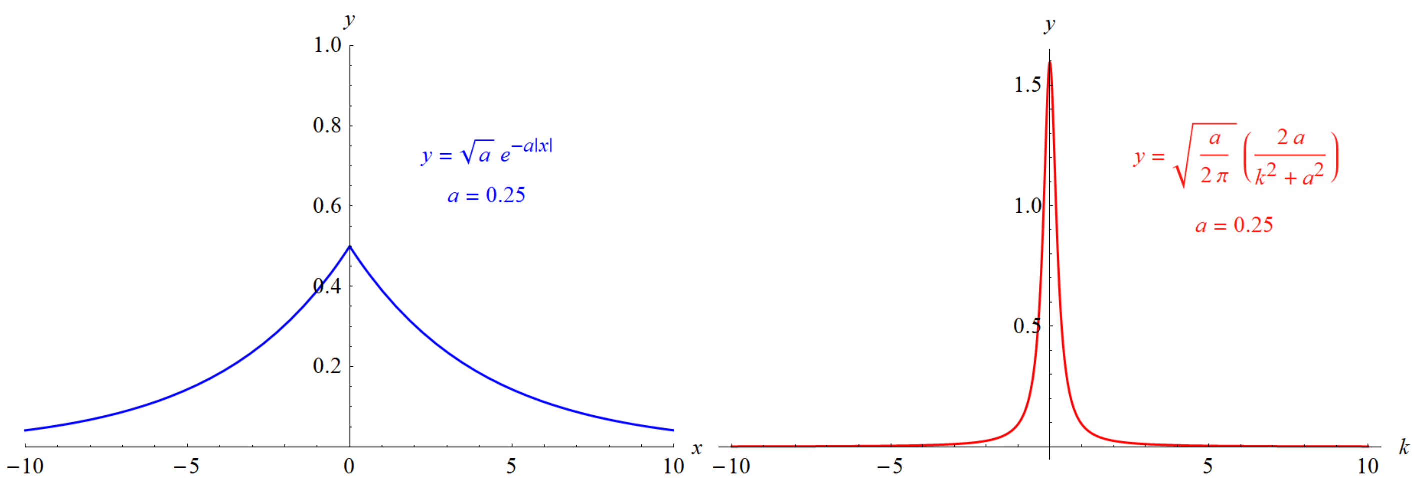
Take the limit of $\Psi(x,t)$ as $a \to 0$.

$$\begin{aligned}\lim_{a\to 0}\Psi(x,t) &= \lim_{a\to 0}\frac{a^{3/2}}{\pi}\int_{-\infty}^{\infty}\exp\left(ikx-\frac{i\hbar}{2m}k^2t\right)\frac{dk}{k^2+a^2}\\ &= \frac{1}{\pi}\int_{-\infty}^{\infty}\exp\left(ikx-\frac{i\hbar}{2m}k^2t\right)\lim_{a\to 0}\left(\frac{a^{3/2}}{k^2+a^2}\right)dk\\ &= \frac{1}{\pi}\int_{-\infty}^{\infty}\exp\left(ikx-\frac{i\hbar}{2m}k^2t\right)(0)\,dk\\ &= 0\end{aligned}$$

Take the limit of $\Psi(x,t)$ as $a \to \infty$, using l'Hôpital's rule whenever it's needed.

$$\begin{aligned}\lim_{a\to \infty}\Psi(x,t) &= \lim_{a\to \infty}\frac{a^{3/2}}{\pi}\int_{-\infty}^{\infty}\exp\left(ikx-\frac{i\hbar}{2m}k^2t\right)\frac{dk}{k^2+a^2}\\ &= \frac{1}{\pi}\int_{-\infty}^{\infty}\exp\left(ikx-\frac{i\hbar}{2m}k^2t\right)\lim_{a\to \infty}\left(\frac{a^{3/2}}{k^2+a^2}\right)dk\\ &\overset{\frac{\infty}{\infty}}{\underset{\text{H}}{=}} \frac{1}{\pi}\int_{-\infty}^{\infty}\exp\left(ikx-\frac{i\hbar}{2m}k^2t\right)\lim_{a\to \infty}\left(\frac{\frac{3}{2}a^{1/2}}{2a}\right)dk\\ &= \frac{1}{\pi}\int_{-\infty}^{\infty}\exp\left(ikx-\frac{i\hbar}{2m}k^2t\right)\lim_{a\to \infty}\left(\frac{3}{4}\frac{1}{a^{1/2}}\right)dk\\ &= \frac{1}{\pi}\int_{-\infty}^{\infty}\exp\left(ikx-\frac{i\hbar}{2m}k^2t\right)(0)\,dk\\ &= 0\end{aligned}$$

Note that k is related to momentum by $p = \hbar k$, so the Fourier transform of $\Psi(x,0)$ is basically the wave function for the particle's momentum at $t = 0$. For low a, the following graphs indicate a low certainty in the particle's position and a high certainty in the particle's momentum initially.



For high a, the following graphs indicate a high certainty in the particle's position and a low certainty in the particle's momentum initially.