Introduction to Quantum Mechanics

Problem 2.1

Prove the following three theorems:

- (a) For normalizable solutions, the separation constant E must be real. Hint: Write E (in Equation 2.7) as $E_0 + i\Gamma$ (with E_0 and Γ real), and show that if Equation 1.20 is to hold for all t, Γ must be zero.
- (b) The time-independent wave function $\psi(x)$ can always be taken to be real (unlike $\Psi(x,t)$, which is necessarily complex). Hint: If $\psi(x)$ satisfies Equation 2.5, for a given E, so too does its complex conjugate, and hence also the real linear combinations $(\psi + \psi^*)$ and $i(\psi \psi^*)$.
- (c) If V(x) is an even function (that is, V(-x) = V(x)) then $\psi(x)$ can always be taken to be either even or odd. Hint: If $\psi(x)$ satisfies Equation 2.5, for a given E, so too does $\psi(-x)$, and hence also the even and odd linear combinations $\psi(x) \pm \psi(-x)$.

Solution

(a) Suppose $E = E_0 + i\Gamma$ for some real E_0 and Γ . Then the time-dependent wave function $\Psi(x,t)$ can be written as

$$\begin{split} \Psi(x,t) &= \psi(x) e^{-i\frac{Et}{\hbar}} \\ &= \psi(x) e^{-i\frac{(E_0+i\Gamma)t}{\hbar}} \\ &= \psi(x) e^{\frac{\Gamma t}{\hbar}} e^{-i\frac{E_0t}{\hbar}}. \end{split}$$

Thus,

$$\begin{split} \int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, \mathrm{d}x &= \int_{-\infty}^{\infty} |\psi(x)|^2 e^{\frac{2\Gamma t}{\hbar}} \, \mathrm{d}x \\ &= e^{\frac{2\Gamma t}{\hbar}} \int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x, \end{split}$$

which varies with time, unless $\Gamma = 0$. Therefore, the separation constant E must be real.

(b) If $\psi(x)$ satisfies $\hat{H}\psi = E\psi$, then its complex conjugate $\psi^*(x)$ also satisfies $\hat{H}\psi^* = E\psi^*$.

If $\psi_1(x)$ and $\psi_2(x)$ are two solutions of $\hat{H}\psi = E\psi$, then any linear combination $\psi_3(x) = c_1\psi_1(x) + c_2\psi_2(x)$ is also a solution.

Thus for any complex solution $\psi(x)$, we can construct two real solutions $\psi_1(x) = \frac{1}{2}(\psi(x) + \psi^*(x))$ and $\psi_2(x) = \frac{1}{2i}(\psi(x) - \psi^*(x))$.

(c) If $\psi(x)$ satisfies $-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\mathrm{d}x^2}+V(x)\psi(x)=E\psi(x)$, then

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\mathrm{d}(-x)^2}+V(-x)\psi(-x)=-\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\mathrm{d}x^2}+V(x)\psi(-x)$$

$$= E\psi(-x),$$

which means $\psi(-x)$ is also a solution. Thus we can construct two solutions $\psi_1(x) = \frac{1}{2}(\psi(x) + \psi(-x))$, which is even, and $\psi_2(x) = \frac{1}{2}(\psi(x) - \psi(-x))$, which is odd.

Problem 2.2

Show that E must exceed the minimum value of V(x), for every normalizable solution to the time-independent Schrödinger equation. What is the classical analog to this statement? Hint: Rewrite Equation 2.5 in the form

$$\frac{\partial^2 \psi}{\mathrm{d}x^2} = \frac{2m}{\hbar^2} [V(x) - E] \psi.$$

if $E < V_{\min}$, then ψ and its second derivative always have the same sign—argue that such a function cannot be normalized.

Solution

Rewrite time-independent Schrödinger equation as

$$\frac{\partial^2 \psi}{\mathrm{d}x^2} = \frac{2m}{\hbar^2} [V(x) - E]\psi.$$

If $E < V_{\min}$, then V(x) - E > 0 for all x. Thus ψ and its second derivative always have the same sign, which means ψ cannot be normalized.

In classical mechanics, this statement is analogous that if the total energy of a particle is less than the minimum potential energy, the particle's kinetic energy is negative, then the particle cannot exist in the system.

Problem 2.3

Show that there is no acceptable solution to the (time-independent) Schrödinger equation for the infinite square well with E=0 or E<0. (This is a special case of the general theorem in Problem 2.2, but this time do it by explicitly solving the Schrödinger equation, and showing that you cannot satisfy the boundary conditions.)

Solution

When E = 0, the time-independent Schrödinger equation for the infinite square well becomes

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi = 0,$$

which leads to $\psi(x) = 0$, which is not normalizable.

When E < 0, the time-independent Schrödinger equation for the infinite square well becomes

$$\frac{\partial^2 \psi}{\mathrm{d}x^2} = \kappa^2 \psi,$$

where $\kappa = \frac{\sqrt{-2mE}}{\hbar}$. The general solution to this equation is

$$\psi(x) = Ae^{\kappa x} + Be^{-\kappa x},$$

then the boundary conditions $\psi(0) = \psi(a) = 0$ lead to A = B = 0, which means $\psi(x) = 0$, which is not normalizable.

Problem 2.4

Calculate $\langle x \rangle$, $\langle x^2 \rangle$, $\langle p \rangle$, $\langle p^2 \rangle$, σ_x , and σ_p , for the nth stationary state of the infinite square well. Check that the uncertainty principle is satisfied. Which state comes closest to the uncertainty limit?

Solution

The expectation value of x is

$$\begin{split} \langle x \rangle &= \int_0^a x \left| \psi_{n(x)} \right|^2 \mathrm{d}x \\ &= \int_0^a x \left(\sqrt{\frac{2}{a}} \sin \left(\frac{n\pi x}{a} \right) \right)^2 \mathrm{d}x \\ &= \frac{2}{a} \int_0^a x \sin^2 \left(\frac{n\pi x}{a} \right) \mathrm{d}x \\ &= \frac{1}{a} \left[\frac{1}{2} x^2 - \frac{a}{2n\pi} x \sin \left(\frac{2n\pi x}{a} \right) - \frac{a^2}{4n^2 \pi^2} \cos \left(\frac{2n\pi x}{a} \right) \right]_0^a \\ &= \frac{a}{2}. \end{split}$$

The expectation value of x^2 is

$$\begin{split} \langle x^2 \rangle &= \int_0^a x^2 \Big| \psi_{n(x)} \Big|^2 \, \mathrm{d}x \\ &= \int_0^a x^2 \left(\sqrt{\frac{2}{a}} \sin \left(\frac{n \pi x}{a} \right) \right)^2 \, \mathrm{d}x \\ &= \frac{2}{a} \int_0^a x^2 \sin^2 \left(\frac{n \pi x}{a} \right) \, \mathrm{d}x \\ &= \frac{1}{a} \left[\frac{1}{3} x^3 - \frac{a}{2n \pi} x^2 \sin \left(\frac{2n \pi x}{a} \right) - \frac{a^2}{2n^2 \pi^2} x \cos \left(\frac{2n \pi x}{a} \right) + \frac{a^3}{4n^3 \pi^3} \sin \left(\frac{2n \pi x}{a} \right) \Big]_0^a \\ &= \frac{1}{a} \left(\frac{a^3}{3} - \frac{a^3}{2n^2 \pi^2} \right) \\ &= a^2 \left(\frac{1}{3} - \frac{1}{2n^2 \pi^2} \right). \end{split}$$

The expectation value of p is

$$\langle p \rangle = m \frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t}$$
$$= 0$$

The expectation value of p^2 is

$$\begin{split} \langle p^2 \rangle &= \int_0^a \psi_n^*(x) \left(\frac{\hbar}{i} \frac{\mathrm{d}}{\mathrm{d}x} \right)^2 \psi_n \, \mathrm{d}x \\ &= -\hbar^2 \int_0^a \psi_n^*(x) \frac{\mathrm{d}^2 \psi_n}{\mathrm{d}x^2} \, \mathrm{d}x \\ &= -\hbar^2 \left(-\frac{2mE_n}{\hbar^2} \right) \int_0^a \left| \psi_{n(x)} \right|^2 \mathrm{d}x \\ &= 2mE_n \\ &= \frac{n^2 \pi^2 \hbar^2}{a^2}. \end{split}$$

The standard deviation of x is

$$\begin{split} \sigma_x &= \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \\ &= a \sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}. \end{split}$$

The standard deviation of p is

$$\begin{split} \sigma_p &= \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \\ &= \frac{n \pi \hbar}{a}. \end{split}$$

The uncertainty principle is

$$\begin{split} \sigma_x \sigma_p &= a \sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}} \cdot n\pi \frac{\hbar}{a} \\ &= \frac{\hbar}{2} \sqrt{n^2 \frac{\pi^2}{3} - 2} \\ &\geq \frac{\hbar}{2} \sqrt{\frac{\pi^2}{3} - 2} \\ &\geq \frac{\hbar}{2}. \end{split}$$

Problem 2.5

A particle in the infinite square well has as its initial wave function an even mixture of the first two stationary states:

$$\Psi(x,0) = A[\psi_1(x) + \psi_2(x)].$$

- (a) Normalize $\Psi(x,0)$. (That is, find A. This is very easy, if you exploit the orthonormality of ψ_1 and ψ_2 . Recall that, having normalized Ψ at t=0, you can rest assured that it stays normalized—if you doubt this, check it explicitly after doing part (b).)
- (b) Find $\Psi(x,t)$ and $|\Psi(x,t)|^2$. Express the latter as a sinusoidal function of time, as in Example 2.1. To simplify the result, let $\omega = \pi^2 \frac{\hbar}{2ma^2}$.
- (c) Compute $\langle x \rangle$. Notice that it oscillates in time. What is the angular frequency of the oscillation? What is the amplitude of the oscillation? (If your amplitude is greater than $\frac{a}{2}$, go directly to jail.)
- (d) Compute $\langle p \rangle$. (As Peter Lorre would say, "Do it ze kveek vay, Johnny!")
- (e) If you measured the energy of this particle, what values might you get, and what is the probability of getting each of them? Find the expectation value of H. How does it compare with E_1 and E_2 ?

$$\begin{split} &1=\int_0^a |\Psi(x,0)|^2\,\mathrm{d}x\\ &=A^2\int_0^a \left[\psi_1(x)+\psi_2(x)\right]^* [\psi_1(x)+\psi_2(x)]\,\mathrm{d}x\\ &=A^2\int_0^a \left[|\psi_1(x)|^2+|\psi_2(x)|^2+\psi_1^*(x)\psi_2(x)+\psi_2^*(x)\psi_1(x)\right]\mathrm{d}x\\ &=2A^2, \end{split}$$

so
$$A = \frac{1}{\sqrt{2}}$$
.

$$\Psi(x,t) = \frac{1}{\sqrt{2}} \left[\psi_1(x) e^{-i\frac{E_1 t}{h}} + \psi_2(x) e^{-i\frac{E_2 t}{h}} \right]$$

$$= \frac{1}{\sqrt{2}} \left[\psi_1(x) e^{-i\omega t} + \psi_2(x) e^{-4i\omega t} \right]$$

$$= \frac{1}{\sqrt{2}} \left[\sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) e^{-i\omega t} + \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) e^{-4i\omega t} \right]$$

$$= \frac{1}{\sqrt{a}} e^{-i\omega t} \left[\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right) e^{-3i\omega t} \right].$$

$$|\Psi(x,t)|^2 = \frac{1}{a} \left[\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right) e^{-3i\omega t} \right] \left[\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right) e^{3i\omega t} \right]$$

$$= \frac{1}{a} \left[\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2\sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right) \cos(3\omega t) \right].$$
(S)
$$\int_0^a dx \, dx \, dx$$

$$\begin{split} & \overset{\text{(c)}}{\langle x \rangle} = \int_0^a x |\Psi(x,t)|^2 \, \mathrm{d}x \\ & = \frac{1}{a} \int_0^a x \left[\sin^2 \left(\frac{\pi x}{a} \right) + \sin^2 \left(\frac{2\pi x}{a} \right) + 2 \sin \left(\frac{\pi x}{a} \right) \sin \left(\frac{2\pi x}{a} \right) \cos(3\omega t) \right] \mathrm{d}x \end{split}$$

$$\begin{split} &= \frac{1}{a} \int_0^a x \left[\sin^2 \left(\frac{\pi x}{a} \right) + \sin^2 \left(\frac{2\pi x}{a} \right) \right] \mathrm{d}x + \frac{2}{a} \cos(3\omega t) \int_0^a x \sin\left(\frac{\pi x}{a} \right) \sin\left(\frac{2\pi x}{a} \right) \mathrm{d}x \\ &= \frac{1}{a} \left[\frac{a^2}{4} + \frac{a^2}{4} \right] + \frac{1}{a} \cos(3\omega t) \int_0^a x \left[\cos\left(\frac{\pi x}{a} \right) - \cos\left(\frac{3\pi x}{a} \right) \right] \mathrm{d}x \\ &= \frac{a}{2} + \frac{1}{a} \cos(3\omega t) \left[\frac{a}{\pi} x \sin\left(\frac{\pi x}{a} \right) + \frac{a^2}{\pi^2} \cos\left(\frac{\pi x}{a} \right) - \frac{a}{3\pi} x \sin\left(\frac{3\pi x}{a} \right) - \frac{a^2}{9\pi^2} \cos\left(\frac{3\pi x}{a} \right) \right]_0^a \\ &= \frac{a}{2} + \frac{1}{a} \cos(3\omega t) \left[-\frac{a^2}{\pi^2} - \frac{a^2}{\pi^2} + \frac{a^2}{9\pi^2} + \frac{a^2}{9\pi^2} \right] \\ &= \frac{a}{2} - \frac{16}{9\pi^2} a \cos(3\omega t) \\ &= \frac{a}{2} \left[1 - \frac{32}{9\pi^2} \cos(3\omega t) \right], \end{split}$$

where the angular frequency of the oscillation is $3\omega = \frac{3\pi^2\hbar}{2ma^2}$ and the amplitude of the oscillation is $\frac{16a}{9\pi^2} \approx 0.18a$.

$$\begin{split} \langle p \rangle &= m \frac{\mathrm{d} \langle x \rangle}{\mathrm{d}t} \\ &= m \frac{\mathrm{d}}{\mathrm{d}t} \left[\frac{a}{2} \left(1 - \frac{32}{9\pi^2} \cos(3\omega t) \right) \right] \\ &= \frac{16ma}{9\pi^2} 3\omega \sin(3\omega t) \\ &= \frac{8\hbar}{3a} \sin(3\omega t). \end{split}$$

(e) The possible values of energy are $E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$ and $E_2 = \frac{2\pi^2 \hbar^2}{ma^2}$, with probability $\frac{1}{2}$ for each. The expectation value of H is

$$\begin{split} \langle H \rangle &= \frac{1}{2} E_1 + \frac{1}{2} E_2 \\ &= \frac{1}{2} \left(\frac{\pi^2 \hbar^2}{2ma^2} \right) + \frac{1}{2} \left(\frac{2\pi^2 \hbar^2}{ma^2} \right) \\ &= \frac{5\pi^2 \hbar^2}{4ma^2}. \end{split}$$

Problem 2.6

Although the overall phase constant of the wave function is of no physical significance (it cancels out whenever you calculate a measurable quantity), the relative phase of the coefficients in Equation 2.17 does matter. For example, suppose we change the relative phase of ψ_1 and ψ_2 in Problem 2.5:

$$\Psi(x,0) = A \big[\psi_1(x) + e^{i\phi} \psi_2(x) \big], \label{eq:psi_approx}$$

where ϕ is some constant. Find $\Psi(x,t)$, $|\Psi(x,t)|^2$, and $\langle x \rangle$, and compare your results with what you got before. Study the special cases $\phi = \frac{\pi}{2}$ and $\phi = \pi$. (For a graphi.alteal exploration of this problem see the applet in footnote 9 of this chapter.)

Solution

$$\begin{split} 1 &= \int_0^a |\Psi(x,0)|^2 \,\mathrm{d}x \\ &= A^2 \int_0^a \left[|\psi_1(x)|^2 + |\psi_2(x)|^2 + e^{i\phi} \psi_1^*(x) \psi_2(x) + e^{-i\phi} \psi_2^*(x) \psi_1(x) \right] \mathrm{d}x \\ &= 2A^2, \end{split}$$

so $A = \frac{1}{\sqrt{2}}$.

$$\begin{split} \Psi(x,t) &= \frac{1}{\sqrt{2}} \Big[\psi_1(x) e^{-i\frac{E_1 t}{\hbar}} + e^{i\phi} \psi_2(x) e^{-i\frac{E_2 t}{\hbar}} \Big] \\ &= \frac{1}{\sqrt{2}} \big[\psi_1(x) e^{-i\omega t} + e^{i\phi} \psi_2(x) e^{-4i\omega t} \big] \\ &= \frac{1}{\sqrt{2}} \left[\sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) e^{-i\omega t} + e^{i\phi} \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) e^{-4i\omega t} \right] \\ &= \frac{1}{\sqrt{a}} e^{-i\omega t} \left[\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right) e^{i\phi} e^{-3i\omega t} \right]. \end{split}$$

$$\begin{split} |\Psi(x,t)|^2 &= \frac{1}{a} \bigg[\sin \bigg(\pi \frac{x}{a} \bigg) + \sin \bigg(2 \pi \frac{x}{a} \bigg) e^{-3i\omega t} \bigg] \bigg[\sin \bigg(\pi \frac{x}{a} \bigg) + \sin \bigg(2 \pi \frac{x}{a} \bigg) e^{3i\omega t} \bigg] \\ &= \frac{1}{a} \bigg[\sin^2 \bigg(\pi \frac{x}{a} \bigg) + \sin^2 \bigg(2 \pi \frac{x}{a} \bigg) + \sin \bigg(\pi \frac{x}{a} \bigg) \sin \bigg(2 \pi \frac{x}{a} \bigg) (e^{i\phi} e^{-3i\omega t} + e^{-i\phi} e^{3i\omega t}) \bigg] \\ &= \frac{1}{a} \bigg[\sin^2 \bigg(\pi \frac{x}{a} \bigg) + \sin^2 \bigg(2 \pi \frac{x}{a} \bigg) + 2 \sin \bigg(\pi \frac{x}{a} \bigg) \sin \bigg(2 \pi \frac{x}{a} \bigg) \cos (3\omega t - \phi) \bigg]. \end{split}$$

Then
$$\langle x \rangle = \frac{a}{2} \left[1 - \frac{32}{9\pi^2} \cos(3\omega t - \phi) \right].$$

When $\phi = \frac{\pi}{2}$, $\langle x \rangle = \frac{a}{2} \left[1 + \frac{32}{9\pi^2} \sin(3\omega t) \right],$
When $\phi = \pi$, $\langle x \rangle = \frac{a}{2} \left[1 + \frac{32}{9\pi^2} \cos(3\omega t) \right].$

Problem 2.7

A particle in the infinite square well has the initial wave function

$$\Psi(x,0) = \begin{cases} Ax, & 0 \leq x \leq \frac{a}{2} \\ A(a-x), \frac{a}{2} \leq x \leq a. \end{cases}$$

- (a) Sketch $\Psi(x,0)$, and determine the constant A.
- (b) Find $\Psi(x,t)$.
- (c) What is the probability that a measurement of the energy would yield the value E_1 ?
- (d) Find the expectation value of the energy, using Equation 2.21.

Solution

(a)
$$1 = \int_0^a |\Psi(x,0)|^2 dx$$
$$= A^2 \left[\int_0^{\frac{a}{2}} x^2 dx + \int_{\frac{a}{2}}^a (a-x)^2 dx \right]$$
$$= A^2 \left[\frac{x^3}{3} \Big|_0^{\frac{a}{2}} - \frac{(a-x)^3}{3} \Big|_{\frac{a}{2}}^a \right]$$
$$= A^2 \left[\frac{a^3}{24} + \frac{a^3}{24} \right]$$
$$= \frac{A^2 a^3}{12},$$

so
$$A = \frac{2\sqrt{3}}{a\sqrt{a}}$$
.

$$\begin{split} c_n^{\left(\frac{\mathbf{b}}{\mathbf{b}}\right)} & \int_0^a \Psi(x,0) \psi_n^*(x) \, \mathrm{d}x \\ & = A \sqrt{\frac{2}{a}} \left[\int_0^{\frac{a}{2}} x \sin\left(\frac{n\pi x}{a}\right) \, \mathrm{d}x + \int_{\frac{a}{2}}^a (a-x) \sin\left(\frac{n\pi x}{a}\right) \, \mathrm{d}x \right] \\ & = A \sqrt{\frac{2}{a}} \frac{a}{n\pi} \left[-x \cos\left(\frac{n\pi x}{a}\right) \Big|_0^{\frac{a}{2}} + \int_0^{\frac{a}{2}} \cos\left(\frac{n\pi x}{a}\right) \, \mathrm{d}x - (a-x) \cos\left(\frac{n\pi x}{a}\right) \Big|_{\frac{a}{2}}^a - \int_{\frac{a}{2}}^a \cos\left(\frac{n\pi x}{a}\right) \, \mathrm{d}x \right] \\ & = A \sqrt{\frac{2}{a}} \frac{a}{n\pi} \left[\frac{a}{n\pi} \sin\left(\frac{n\pi x}{a}\right) \Big|_0^{\frac{a}{2}} - \frac{a}{n\pi} \sin\left(\frac{n\pi x}{a}\right) \Big|_{\frac{a}{2}}^a \right] \\ & = A \sqrt{\frac{2}{a}} \frac{a}{n\pi} \left[\frac{a}{n\pi} \sin\left(\frac{n\pi}{2}\right) + \frac{a}{n\pi} \sin\left(\frac{n\pi}{2}\right) \right] \\ & = \frac{4\sqrt{6}}{n^2\pi^2} \sin\left(n\frac{\pi}{2}\right) \\ & = \begin{cases} \frac{4\sqrt{6}}{n^2\pi^2} (-1)^{\frac{n-1}{2}} \text{ odd } n \\ 0 & \text{even } n \end{cases} \end{split}$$

So

$$\begin{split} \Psi(x,t) &= \sum_{n=1,3,5,\dots} c_n \psi_{n(x)} e^{-i\frac{E_n t}{\hbar}} \\ &= \sum_{n=1,3,5,\dots} \frac{4\sqrt{6}}{n^2 \pi^2} (-1)^{\frac{n-1}{2}} \sqrt{\frac{2}{a}} \sin \left(n\pi \frac{x}{a}\right) e^{-i\frac{E_n t}{\hbar}} \\ &= \frac{4\sqrt{6}}{\pi^2} \sqrt{\frac{2}{a}} \sum_{n=1,2,5} \frac{(-1)^{\frac{n-1}{2}}}{n^2} \sin \left(n\pi \frac{x}{a}\right) e^{-i\frac{E_n t}{\hbar}}, \end{split}$$

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

(c) The probability that a measurement of the energy would yield the value E_1 is

$$\begin{split} P(E_1) &= \left| c_1 \right|^2 \\ &= \left(\frac{4\sqrt{6}}{\pi^2} \right)^2 \\ &= \frac{96}{\pi^4} \approx 0.9855 \end{split}$$

(d) The expectation value of the energy is

$$\begin{split} \langle H \rangle &= \sum_{n=1,3,5,\dots} |c_n|^2 E_n \\ &= \sum_{n=1,3,5,\dots} \left(\frac{4\sqrt{6}}{n^2 \pi^2} \right)^2 \frac{n^2 \pi^2 \hbar^2}{2ma^2} \\ &= \sum_{n=1,3,5,\dots} \frac{48\hbar^2}{n^2 \pi^2 ma^2} \\ &= \frac{48\hbar^2}{\pi^2 ma^2} \sum_{n=1,3,5,\dots} \frac{1}{n^2} \\ &= \frac{48\hbar^2}{\pi^2 ma^2} \frac{\pi^2}{8} \\ &= \frac{6\hbar^2}{ma^2}. \end{split}$$

Problem 2.8

A particle of mass m in the infinite square well (of width a) starts out in the state

$$\Psi(x,0) = \begin{cases} A \ 0 \le x \le \frac{a}{2} \\ 0 \ \frac{a}{2} < x \le a \end{cases}$$

for some constant A, so it is (at t=0) equally likely to be found at any point in the left half of the well. What is the probability that a measurement of the energy (at some later time t) would yield the value $\frac{\pi^2 \hbar^2}{2ma^2}$?

$$1 = \int_0^a |\Psi(x,0)|^2 dx$$
$$= A^2 \left[\int_0^{\frac{a}{2}} dx \right]$$
$$= \frac{A^2 a}{2},$$

so
$$A = \sqrt{\frac{2}{a}}$$
.

$$c_1 = \int_0^a \Psi(x, 0) \psi_1^*(x) dx$$

$$= A \sqrt{\frac{2}{a}} \int_0^{\frac{a}{2}} \sin\left(\frac{\pi x}{a}\right) dx$$

$$= A \sqrt{\frac{2}{a}} \left(\frac{a}{\pi}\right) \left[-\cos\left(\frac{\pi x}{a}\right)\right]_0^{\frac{a}{2}}$$

$$= \frac{2}{\pi}.$$

The probability that a measurement of the energy would yield the value $\pi^2 \frac{\hbar^2}{2ma^2} = E_1$ is

$$\begin{split} P(E_1) &= \left| c_1 \right|^2 \\ &= \left(\frac{2}{\pi} \right)^2 \\ &= \frac{4}{\pi^2} \approx 0.4053. \end{split}$$

Problem 2.9

For the wave function in Example 2.2, find the expectation value of H, at time t = 0, the "old fashioned" way:

$$\langle H \rangle = \int \Psi(x,0)^* \hat{H} \Psi(x,0) \, \mathrm{d}x.$$

Compare the result we got in Example 2.3. Note: Because $\langle H \rangle$ is independent of time, there is no loss of generality in using t=0.

$$\begin{split} \hat{H}\Psi(x,0) &= \frac{-\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \Psi(x,0) \\ &= \frac{-\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} [Ax(a-x)] \\ &= \frac{-\hbar^2}{2m} (-2A) \\ &= \frac{\hbar^2 A}{m}. \\ \langle H \rangle &= \int \Psi(x,0)^* \hat{H} \Psi(x,0) \, \mathrm{d}x \\ &= \frac{\hbar^2 A^2}{m} \int_0^a x(a-x) \, \mathrm{d}x \end{split}$$

$$\begin{split} &= \frac{\hbar^2 A^2}{m} \left[a \frac{x^2}{2} - \frac{x^3}{3} \Big|_0^a \right] \\ &= \frac{\hbar^2 A^2 a^3}{6m} \\ &= \frac{5\hbar^2}{ma^2}. \end{split}$$

- (a) Construct $\psi_2(x)$.
- (b) Sketch ψ_0 , ψ_1 , and ψ_2 .
- (c) Check the orthogonality of ψ_0 , ψ_1 , and ψ_2 , by explicit integration. Hint: If you exploit the even-ness and odd-ness of the functions, there is really only one integral left to do.

Solution

$$\begin{split} \psi_0 &= \left(m\frac{\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}, \\ \hat{a}_+ \psi_0 &= \frac{1}{\sqrt{2\hbar m\omega}} (-i\hat{p} + m\omega\hat{x})\psi_0 \\ &= \frac{1}{\sqrt{2\hbar m\omega}} \left(m\frac{\omega}{\pi\hbar}\right)^{\frac{1}{4}} \left(-\hbar\frac{\mathrm{d}}{\mathrm{d}x} + m\omega x\right) e^{-\frac{m\omega}{2\hbar}x^2} \\ &= \frac{1}{\sqrt{2\hbar m\omega}} \left(m\frac{\omega}{\pi\hbar}\right)^{\frac{1}{4}} \left[-\hbar\left(-\frac{m\omega}{\hbar}x\right) + m\omega x\right] e^{-\frac{m\omega}{2\hbar}x^2} \\ &= \frac{1}{\sqrt{2\hbar m\omega}} \left(m\frac{\omega}{\pi\hbar}\right)^{\frac{1}{4}} 2m\omega x e^{-\frac{m\omega}{2\hbar}x^2}. \\ (\hat{a}_+)^2 \psi_0 &= \frac{1}{\sqrt{2\hbar m\omega}} (-i\hat{p} + m\omega\hat{x})(\hat{a}_+\psi_0) \\ &= \frac{1}{2\hbar m\omega} \left(m\frac{\omega}{\pi\hbar}\right)^{\frac{1}{4}} 2m\omega \left(-\hbar\frac{\mathrm{d}}{\mathrm{d}x} + m\omega x\right) x e^{-\frac{m\omega}{2\hbar}x^2} \\ &= \frac{1}{2\hbar m\omega} \left(m\frac{\omega}{\pi\hbar}\right)^{\frac{1}{4}} 2m\omega \left[-\hbar\left(1 - \frac{m\omega}{\hbar}x^2\right) + m\omega x^2\right] e^{-\frac{m\omega}{2\hbar}x^2} \\ &= \left(m\frac{\omega}{-\hbar}\right)^{\frac{1}{4}} \left[\frac{2m\omega}{\hbar}x^2 - 1\right] e^{-\frac{m\omega}{2\hbar}x^2}. \end{split}$$

Therefore,

$$\begin{split} \psi_2 &= \frac{1}{\sqrt{2}} \big(\hat{a}_+\big)^2 \psi_0 \\ &= \frac{1}{\sqrt{2}} \bigg(m \frac{\omega}{\pi \hbar} \bigg)^{\frac{1}{4}} \bigg[\frac{2m\omega}{\hbar} x^2 - 1 \bigg] e^{-\frac{m\omega}{2\hbar} x^2}. \end{split}$$

(b)

(c) As ψ_0 and ψ_2 are even and ψ_1 is odd, the only integral left to do is

$$\begin{split} \int_{-\infty}^{\infty} \psi_0^* \psi_2 \, \mathrm{d}x &= \int_{-\infty}^{\infty} \left(m \frac{\omega}{\pi \hbar} \right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar} x^2} \frac{1}{\sqrt{2}} \left(m \frac{\omega}{\pi \hbar} \right)^{\frac{1}{4}} \left[\frac{2m\omega}{\hbar} x^2 - 1 \right] e^{-\frac{m\omega}{2\hbar} x^2} \, \mathrm{d}x \\ &= \frac{1}{\sqrt{2}} \left(m \frac{\omega}{\pi \hbar} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \left[\frac{2m\omega}{\hbar} x^2 - 1 \right] e^{-\frac{m\omega}{\hbar} x^2} \, \mathrm{d}x \\ &= \frac{1}{\sqrt{2}} \left(m \frac{\omega}{\pi \hbar} \right)^{\frac{1}{2}} \left[\frac{2m\omega}{\hbar} \int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega}{\hbar} x^2} \, \mathrm{d}x - \int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar} x^2} \, \mathrm{d}x \right] \\ &= \frac{1}{\sqrt{2}} \left(m \frac{\omega}{\pi \hbar} \right)^{\frac{1}{2}} \left[\frac{2m\omega}{\hbar} \frac{\hbar}{2m\omega} \sqrt{\frac{\pi \hbar}{m\omega}} - \sqrt{\frac{\pi \hbar}{m\omega}} \right] \\ &= 0. \end{split}$$

Problem 2.11

- (a) Compute $\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$, and $\langle p^2 \rangle$, for the states ψ_0 (Equation 2.60) and ψ_1 (Equation 2.63), by explicit integration.
- (b) Check the uncertainty principle for these states.
- (c) Compute $\langle T \rangle$ and $\langle V \rangle$ for these states. (No new integration allowed!) Is their sum what you would expect?

Solution

(a) For $\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}$, which is even, we have

$$\begin{split} \langle x \rangle &= \int_{-\infty}^{\infty} x |\psi_0(x)|^2 \, \mathrm{d}x \\ &= 0, \\ \langle p \rangle &= m \frac{\mathrm{d}}{\mathrm{d}t} \langle x \rangle \\ &= 0, \\ \langle x^2 \rangle &= \int_{-\infty}^{\infty} x^2 |\psi_0(x)|^2 \, \mathrm{d}x \\ &= \int_{-\infty}^{\infty} x^2 \Big(\frac{m\omega}{\pi\hbar} \Big)^{\frac{1}{2}} e^{-\frac{m\omega}{\hbar}x^2} \, \mathrm{d}x \\ &= \Big(m \frac{\omega}{\pi\hbar} \Big)^{\frac{1}{2}} \int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega}{\hbar}x^2} \, \mathrm{d}x \\ &= \Big(m \frac{\omega}{\pi\hbar} \Big)^{\frac{1}{2}} \left[\frac{\hbar}{2m\omega} \sqrt{\frac{\pi\hbar}{m\omega}} \right] \end{split}$$

 $=\frac{\hbar}{2m\omega},$

$$\begin{split} \langle p^2 \rangle &= \int_{-\infty}^{\infty} \psi_0^* \left(\frac{\hbar}{i} \frac{\mathrm{d}}{\mathrm{d}x} \right)^2 \psi_0 \, \mathrm{d}x \\ &= -\hbar^2 \int_{-\infty}^{\infty} \psi_0^* \frac{\mathrm{d}^2 \psi_0}{\mathrm{d}x^2} \, \mathrm{d}x \\ &= -\hbar^2 \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} \frac{\mathrm{d}}{\mathrm{d}x} \left[-\frac{m\omega}{\hbar} x e^{-\frac{m\omega}{2\hbar}x^2} \right] \mathrm{d}x \\ &= \hbar m\omega \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} \left(1 - \frac{m\omega}{\hbar} x^2 \right) e^{-\frac{m\omega}{\hbar}x^2} \, \mathrm{d}x \\ &= \hbar m\omega \sqrt{\frac{m\omega}{\pi\hbar}} \left(\sqrt{\frac{\pi\hbar}{m\omega}} - \frac{m\omega}{\hbar} \frac{\hbar}{2m\omega} \sqrt{\frac{\pi\hbar}{m\omega}} \right) \\ &= \frac{\hbar m\omega}{2}. \end{split}$$
For $\psi_1 = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \sqrt{\frac{2m\omega}{\hbar}} x e^{-\frac{m\omega}{2\hbar}x^2}$, which is odd, we have
$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi_1(x)|^2 \, \mathrm{d}x \\ &= 0, \\ \langle p \rangle = m \frac{\mathrm{d}}{\mathrm{d}t} \langle x \rangle \\ &= 0, \\ \langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi_1(x)|^2 \, \mathrm{d}x \\ &= \sqrt{\frac{m\omega}{\pi\hbar}} \frac{2m\omega}{\hbar} \int_{-\infty}^{\infty} x^4 e^{-\frac{m\omega}{\hbar}x^2} \, \mathrm{d}x \\ &= \sqrt{\frac{m\omega}{\pi\hbar}} \frac{2m\omega}{\hbar} \left[\frac{3\hbar^2}{4m^2\omega^2} \sqrt{\frac{\pi\hbar}{m\omega}} \right] \\ &= \frac{3\hbar}{2m\omega}, \end{split}$$

Find $\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$, $\langle p^2 \rangle$, and $\langle T \rangle$, for the *n*th stationary state of the harmonic oscillator, using the method of Example 2.5. Check that the uncertainty principle is satisfied.

Solution

The expectation value of x is

$$\langle x \rangle = \sqrt{\frac{\hbar}{2m\omega}} \int_{-\infty}^{\infty} \psi_n^* (\hat{a}_+ + \hat{a}_-) \psi_n \, \mathrm{d}x$$

$$\begin{split} &=\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n+1}\int_{-\infty}^{\infty}\psi_n^*\psi_{n+1}+\sqrt{n}\int_{-\infty}^{\infty}\psi_n^*\psi_{n-1}\,\mathrm{d}x\right]\\ &=0. \end{split}$$

Thus the expectation value of p is

$$\langle p \rangle = \frac{\mathrm{d}}{\mathrm{d}t} \langle x \rangle$$

= 0.

The expectation value of x^2 is

$$\begin{split} \langle x^2 \rangle &= \frac{\hbar}{2m\omega} \int_{-\infty}^{\infty} \psi_n^* (\hat{a}_+ + \hat{a}_-)^2 \psi_n \, \mathrm{d}x \\ &= \frac{\hbar}{2m\omega} \int_{-\infty}^{\infty} \psi_n^* (\hat{a}_+^2 + \hat{a}_-^2 + \hat{a}_+ \hat{a}_- + \hat{a}_- \hat{a}_+) \psi_n \, \mathrm{d}x \\ &= \frac{\hbar}{2m\omega} \left[\sqrt{n+1} \int_{-\infty}^{\infty} \psi_n^* \hat{a}_+ \psi_{n+1} + \sqrt{n} \int_{-\infty}^{\infty} \psi_n^* \hat{a}_- \psi_{n-1} \, \mathrm{d}x + (n+n+1) \int_{-\infty}^{\infty} \psi_n^* \psi_n \, \mathrm{d}x \right] \\ &= \frac{\hbar}{2m\omega} \left[\sqrt{n+1} \sqrt{n+2} \int_{-\infty}^{\infty} \psi_n^* \psi_{n+2} + n \sqrt{n-1} \int_{-\infty}^{\infty} \psi_n^* \psi_{n-2} \, \mathrm{d}x + 2n + 1 \right] \\ &= \left(n + \frac{1}{2} \right) \frac{\hbar}{m\omega}. \end{split}$$

The expectation value of p^2 is

$$\begin{split} \langle p^2 \rangle &= -\hbar m \frac{\omega}{2} \int_{-\infty}^{\infty} \psi_n^* (\hat{a}_+ - \hat{a}_-)^2 \psi_n \, \mathrm{d}x \\ &= -\hbar m \frac{\omega}{2} \int_{-\infty}^{\infty} \psi_n^* (\hat{a}_+^2 + \hat{a}_-^2 - \hat{a}_+ \hat{a}_- - \hat{a}_- \hat{a}_+) \psi_n \, \mathrm{d}x \\ &= -\hbar m \frac{\omega}{2} \left[\sqrt{n+1} \int_{-\infty}^{\infty} \psi_n^* \hat{a}_+ \psi_{n+1} + \sqrt{n} \int_{-\infty}^{\infty} \psi_n^* \hat{a}_- \psi_{n-1} \, \mathrm{d}x - (n+n+1) \int_{-\infty}^{\infty} \psi_n^* \psi_n \, \mathrm{d}x \right] \\ &= -\hbar m \frac{\omega}{2} \left[\sqrt{n+1} \sqrt{n+2} \int_{-\infty}^{\infty} \psi_n^* \psi_{n+2} + n \sqrt{n-1} \int_{-\infty}^{\infty} \psi_n^* \psi_{n-2} \, \mathrm{d}x - (2n+1) \right] \\ &= \left(n + \frac{1}{2} \right) \hbar m \omega. \end{split}$$

The expectation value of T is

$$\langle T \rangle = \frac{1}{2m} \langle p^2 \rangle$$

= $\frac{1}{2} \left(n + \frac{1}{2} \right) \hbar \omega$.

The standard deviation of x is

$$\begin{split} \sigma_x &= \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \\ &= \sqrt{\left(n + \frac{1}{2}\right) \frac{\hbar}{m \omega}}. \end{split}$$

The standard deviation of p is

$$\begin{split} \sigma_p &= \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \\ &= \sqrt{\left(n + \frac{1}{2}\right) \hbar m \omega}. \end{split}$$

The uncertainty principle is

$$\begin{split} \sigma_x \sigma_p &= \sqrt{\left(n + \frac{1}{2}\right) \frac{\hbar}{m \omega}} \sqrt{\left(n + \frac{1}{2}\right) \hbar m \omega} \\ &= \left(n + \frac{1}{2}\right) \hbar \geq \frac{\hbar}{2}. \end{split}$$

Problem 2.13

A particle in the harmonic oscillator potential starts out in the state

$$\Psi(x,0) = A[3\psi_0(x) + 4\psi_1(x)].$$

- (a) Find A.
- (b) Construct $\Psi(x,t)$ and $|\Psi(x,t)|^2$. Don't get too excited if $|\Psi(x,t)|^2$ oscillates at exactly the classical frequency; what would it have been had I specified $\psi_2(x)$, instead of $\psi_1(x)$?
- (c) Find $\langle x \rangle$ and $\langle p \rangle$. Check that Ehrenfest's theorem (Equation 1.38) holds, for this wave function.
- (d) If you measured the energy of this particle, what values might you get, and with what probabilities?

(a)
$$1 = \int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx$$

$$= |A|^2 (9+16),$$

so
$$A = \frac{1}{5}$$
.

$$\begin{split} \Psi(x,t) &= \frac{1}{5} \Big[3\psi_0(x) e^{-i\frac{E_0t}{\hbar}} + 4\psi_1(x) e^{-i\frac{E_1t}{\hbar}} \Big] \\ &= \frac{1}{5} \Big[3\psi_0(x) e^{-\frac{1}{2}i\omega t} + 4\psi_1(x) e^{-\frac{3}{2}i\omega t} \Big]. \\ &|\Psi(x,t)|^2 = \frac{1}{25} \Big[9|\psi_0(x)|^2 + 16|\psi_1(x)|^2 + 12\psi_0(x)\psi_1(x) \big(e^{i\omega t} + e^{-i\omega t} \big) \Big] \end{split}$$

$$\begin{aligned} &=\frac{1}{25}\left[9|\psi_0(x)|^2+16|\psi_1(x)|^2+24\psi_0(x)\psi_1(x)\cos(\omega t)\right]. \end{aligned}$$
 (c)
$$\langle x\rangle = \int_{-\infty}^{\infty}\Psi(x,0)^*x\Psi(x,0)\,\mathrm{d}x \\ &=\frac{1}{25}\left[9\int_{-\infty}^{\infty}\psi_0x\psi_0\,\mathrm{d}x+16\int_{-\infty}^{\infty}\psi_1x\psi_1\,\mathrm{d}x+24\cos(\omega t)\int_{-\infty}^{\infty}\psi_0x\psi_1\,\mathrm{d}x\right] \\ &=\frac{24}{25}\cos(\omega t)\int_{-\infty}^{\infty}\psi_0x\psi_1\,\mathrm{d}x \\ &=\frac{24}{25}\cos(\omega t)\sqrt{\frac{m\omega}{\pi\hbar}}\sqrt{\frac{2m\omega}{\hbar}}\int_{-\infty}^{\infty}xe^{-\frac{m\omega}{2\hbar}x^2}xe^{-\frac{m\omega}{2\hbar}x^2}\,\mathrm{d}x \\ &=\frac{24}{25}\cos(\omega t)\sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty}e^{-\frac{m\omega}{\hbar}x^2}\,\mathrm{d}x \\ &=\frac{24}{25}\sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t). \end{aligned}$$

Then,

$$\langle p \rangle = m \frac{\mathrm{d}}{\mathrm{d}t} \langle x \rangle$$
$$= -\frac{24}{25} \sqrt{\frac{\hbar m \omega}{2}} \sin(\omega t).$$

We have

$$\frac{\mathrm{d}\langle p\rangle}{\mathrm{d}t} = -\frac{24}{25}\sqrt{\frac{\hbar m\omega}{2}}\omega\cos(\omega t),$$

and

$$\frac{\mathrm{d}V}{\mathrm{d}x} = m\omega^2 x.$$

Therefore,

$$\begin{split} -\langle \frac{\mathrm{d}V}{\mathrm{d}x} \rangle &= -m\omega^2 \langle x \rangle \\ &= -\frac{24}{25} \sqrt{\frac{\hbar m\omega}{2}} \omega \cos(\omega t) \\ &= \frac{\mathrm{d}\langle p \rangle}{\mathrm{d}t}, \end{split}$$

so Ehrenfest's theorem holds.

(d) We can get the energy $E_0 = \frac{\hbar\omega}{2}$ with probability $\frac{9}{25}$ and the energy $E_1 = \frac{3\hbar\omega}{2}$ with probability $\frac{16}{25}$.

In the ground state of the harmonic oscillator, what is the probability (correct to three significant digits) of finding the particle outside the classically allowed region? Hint: Classically, the energy of an oscillator is $E = (\frac{1}{2})ka^2 = (\frac{1}{2})m\omega^2a^2$, where a is the amplitude. So the "classically allowed region" for an oscillator of energy E extends from $-\sqrt{\frac{2E}{m\omega^2}}$ to $+\sqrt{\frac{2E}{m\omega^2}}$. Look in a math table under "Normal Distribution" or "Error Function" for the numerical value of the integral, or evaluate it by computer.

Solution

For the ground state of the harmonic oscillator,

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2},$$

the probability of finding the particle outside the classically allowed region $(-x_0, x_0)$ is

$$\begin{split} P &= 2 \int_{x_0}^{\infty} \left| \psi_0(x) \right|^2 \mathrm{d}x \\ &= 2 \sqrt{\frac{m\omega}{\pi\hbar}} \int_{x_0}^{\infty} e^{-\frac{m\omega}{\hbar}x^2} \, \mathrm{d}x \\ &= 2 \sqrt{\frac{m\omega}{\pi\hbar}} \sqrt{\frac{\pi\hbar}{m\omega}} \Big(1 - 2F\Big(\sqrt{2}\Big)\Big) \\ &\approx 0.157, \end{split}$$

Problem 2.15

Use the recursion formula

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)}a_j$$

to work out $H_5(\xi)$ and $H_6(\xi)$. Invoke the convention that the coefficient of the highest power of ξ is 2^n to fix the overall constant.

Solution

n = 5:

$$a_3 = \frac{-2 \times 4}{2 \times 3} a_1 = -\frac{4}{3} a_1$$

$$a_5 = \frac{-2 \times 2}{4 \times 5} a_3 = -\frac{1}{5} a_3 = \frac{4}{15} a_1,$$

then,

$$\begin{split} H_5(\xi) &= a_1 \xi + a_3 \xi^3 + a_5 \xi^5 \\ &= a_1 \bigg(\xi - \frac{4}{3} \xi^3 + \frac{4}{15} \xi^5 \bigg), \end{split}$$

setting $a_1 = 15 \cdot \frac{2^5}{4} = 120$, we have

$$\begin{split} H_5(\xi) &= 120 \bigg(\xi - \frac{4}{3} \xi^3 + \frac{4}{15} \xi^5 \bigg) \\ &= 32 \xi^5 - 160 \xi^3 + 120 \xi. \end{split}$$

n = 6:

$$\begin{split} a_2 &= \frac{-2 \times 6}{1 \times 2} a_0 = -6 a_0, \\ a_4 &= \frac{-2 \times 4}{3 \times 4} a_2 = -\frac{2}{3} a_2 = 4 a_0, \\ a_6 &= \frac{-2 \times 2}{5 \times 6} a_4 = -\frac{2}{15} a_4 = -\frac{8}{15} a_0, \end{split}$$

then,

$$\begin{split} H_6(\xi) &= a_0 + a_2 \xi^2 + a_4 \xi^4 + a_6 \xi^6 \\ &= a_0 \bigg(1 - 6 \xi^2 + 4 \xi^4 - \frac{8}{15} \xi^6 \bigg). \end{split}$$

Setting $a_0 = -15 \cdot \frac{2^6}{8} = -120$, we have

$$\begin{split} H_6(\xi) &= -120 \bigg(1 - 6 \xi^2 + 4 \xi^4 - \frac{8}{15} \xi^6 \bigg) \\ &= 64 \xi^6 - 480 \xi^4 + 720 \xi^2 - 120. \end{split}$$

Problem 2.16

In this problem we explore some of the more useful theorems (stated without proof) involving Hermite polynomials.

(a) The Rodrigues formula says that

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{\mathrm{d}^n}{\mathrm{d}\xi^n} e^{-\xi^2}.$$

Use it to derive H_3 and H_4 .

(b) The following recursion relation gives you $H_{n+1}(\xi)$ in terms of the two preceding Hermite polynomials:

$$H_{n+1}(\xi) = 2\xi H_{n(\xi)} - 2nH_{n-1}(\xi).$$

Use it, together with your answer in (a), to obtain H_5 and H_6 .

(c) If you differentiate an nth-order polynomial, you get a polynomial of order (n-1). For the Hermite polynomials, in fact,

$$\frac{\mathrm{d}H_n}{\mathrm{d}\xi} = 2nH_{n-1}(\xi).$$

Check this, by differentiating H_5 and H_6 .

(d) $H_n(\xi)$ is the nth z-derivative, at z=0, of the generating function

$$e^{-z^2+2z\xi}=\sum_{n=0}^\infty\frac{z^n}{n!}H_n(\xi).$$

Use this to obtain H_1 , H_2 , and H_3 .

Solution

(a)
$$\frac{\mathrm{d}}{\mathrm{d}\xi}e^{-\xi^2} = -2\xi e^{-\xi^2},$$

$$\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}e^{-\xi^2} = \frac{\mathrm{d}}{\mathrm{d}\xi}\left(-2\xi e^{-\xi^2}\right)$$

$$= (4\xi^2 - 2)e^{-\xi^2},$$

$$\frac{\mathrm{d}^3}{\mathrm{d}\xi^3}e^{-\xi^2} = \frac{\mathrm{d}}{\mathrm{d}\xi}(4\xi^2 - 2)e^{-\xi^2}$$

$$= (-8\xi^3 + 12\xi)e^{-\xi^2},$$

$$\frac{\mathrm{d}^4}{\mathrm{d}\xi^4}e^{-\xi^2} = \frac{\mathrm{d}}{\mathrm{d}\xi}(-8\xi^3 + 12\xi)e^{-\xi^2}$$

$$= (16\xi^4 - 48\xi^2 + 12)e^{-\xi^2}.$$

Therefore, we have

$$\begin{split} H_3(\xi) &= (-1)^3 e^{\xi^2} \frac{\mathrm{d}^3}{\mathrm{d}\xi^3} e^{-\xi^2} \\ &= -e^{\xi^2} \big(-8\xi^3 + 12\xi \big) e^{-\xi^2} \\ &= 8\xi^3 - 12\xi, \\ H_4(\xi) &= (-1)^4 e^{\xi^2} \frac{\mathrm{d}^4}{\mathrm{d}\xi^4} e^{-\xi^2} \\ &= e^{\xi^2} \big(16\xi^4 - 48\xi^2 + 12 \big) e^{-\xi^2} \\ &= 16\xi^4 - 48\xi^2 + 12. \end{split}$$

(b)
$$H_5(\xi) = 2\xi H_4(\xi) - 2 \times 4H_3(\xi)$$

$$= 2\xi (16\xi^4 - 48\xi^2 + 12) - 8(8\xi^3 - 12\xi)$$

$$= 32\xi^5 - 96\xi^3 + 24\xi - 64\xi^3 + 96\xi$$

$$= 32\xi^5 - 160\xi^3 + 120\xi,$$

$$H_6(\xi) = 2\xi H_5(\xi) - 2 \times 5H_4(\xi)$$

$$= 2\xi (32\xi^5 - 160\xi^3 + 120\xi) - 10(16\xi^4 - 48\xi^2 + 12)$$

$$= 64\xi^6 - 320\xi^4 + 240\xi^2 - 160\xi^4 + 480\xi^2 - 120$$

$$= 64\xi^6 - 480\xi^4 + 720\xi^2 - 120.$$

(c)
$$\frac{\mathrm{d}H_5}{\mathrm{d}\xi} = \frac{\mathrm{d}}{\mathrm{d}\xi} (32\xi^5 - 160\xi^3 + 120\xi)$$

$$= 160\xi^4 - 480\xi^2 + 120$$

$$= 10(16\xi^4 - 48\xi^2 + 12)$$

$$= 10H_4(\xi)$$

$$= 2 \times 5H_4(\xi),$$

$$\frac{\mathrm{d}H_6}{\mathrm{d}\xi} = \frac{\mathrm{d}}{\mathrm{d}\xi} (64\xi^6 - 480\xi^4 + 720\xi^2 - 120)$$

$$= 384\xi^5 - 1920\xi^3 + 1440\xi$$

$$= 12(32\xi^5 - 160\xi^3 + 120\xi)$$

$$= 12H_5(\xi)$$

$$= 2 \times 6H_5(\xi).$$
(d)
$$\frac{\mathrm{d}}{\mathrm{d}z} e^{-z^2 + 2z\xi} = (-2z + 2\xi)e^{-z^2 + 2z\xi},$$

setting z = 0 gives us $H_1(\xi) = 2\xi$.

$$\begin{split} \frac{\mathrm{d}^2}{\mathrm{d}z^2} e^{-z^2 + 2z\xi} &= \frac{\mathrm{d}}{\mathrm{d}z} \Big((-2z + 2\xi) e^{-z^2 + 2z\xi} \Big) \\ &= -2e^{-z^2 + 2z\xi} + (-2z + 2\xi) (-2z + 2\xi) e^{-z^2 + 2z\xi} \\ &= [-2 + (-2z + 2\xi)^2] e^{(-z^2 + 2z\xi)}, \end{split}$$

setting z = 0 gives us $H_2(\xi) = 4\xi^2 - 2$.

$$\begin{split} \frac{\mathrm{d}^3}{\mathrm{d}z^3} e^{-z^2 + 2z\xi} &= \frac{\mathrm{d}}{\mathrm{d}z} \Big(\big[-2 + (-2z + 2\xi)^2 \big] e^{(-z^2 + 2z\xi)} \Big) \\ &= -2 \times 2 (-2z + 2\xi) e^{(-z^2 + 2z\xi)} + \big[-2 + (-2z + 2\xi)^2 \big] (-2z + 2\xi) e^{(-z^2 + 2z\xi)} \\ &= \big[(-2z + 2\xi)^3 - 6(-2z + 2\xi) \big] e^{(-z^2 + 2z\xi)}, \end{split}$$

setting z = 0 gives us $H_3(\xi) = 8\xi^3 - 12\xi$.

Problem 2.17

Show that $[Ae^{ikx} + Be^{-ikx}]$ and $[C\cos kx + D\sin kx]$ are equivalent ways of writing the same function of x, and determine the constants C and D in terms of A and B, and vice versa. Comment: In quantum mechanics, when V = 0, the exponentials represent traveling waves, and are most convenient in discussing the free particle, whereas sines and cosines correspond to standing waves, which arise naturally in the case of the infinite square well.

$$C\cos kx + D\sin kx = Ae^{ikx} + Be^{-ikx}$$
$$= A[\cos kx + i\sin kx] + B[\cos kx - i\sin kx]$$

$$= (A+B)\cos kx + i(A-B)\sin kx,$$

so we have

$$\begin{split} C &= A + B, \\ D &= i(A - B). \end{split}$$

$$Ae^{ikx} + Be^{-ikx} = C\cos kx + D\sin kx \\ &= \frac{C}{2} \left(e^{ikx} + e^{-ikx}\right) + \frac{D}{2}i\left(e^{ikx} - e^{-ikx}\right) \\ &= \left(\frac{C}{2} + \frac{D}{2}i\right)e^{ikx} + \left(\frac{C}{2} - \frac{D}{2}i\right)e^{-ikx}, \end{split}$$

so we have

$$A = \frac{C}{2} + \frac{D}{2}i,$$

$$B = \frac{C}{2} - \frac{D}{2}i.$$

Problem 2.18

Find the probability current

$$J(x,t) = \frac{i\hbar}{2m} \bigg(\Psi \frac{\partial \Psi^*}{\mathrm{d}x} - \Psi^* \frac{\partial \Psi}{\mathrm{d}x} \bigg)$$

for the free particle wave function Equation

$$\Psi_{k(x,t)} = Ae^{i\left(kx - \frac{\hbar k^2}{2m}t\right)},$$

Which direction does the probability flow?

Solution

$$\begin{split} J(x,t) &= \frac{i\hbar}{2m} \bigg(\Psi \frac{\partial \Psi^*}{\mathrm{d}x} - \Psi^* \frac{\partial \Psi}{\mathrm{d}x} \bigg) \\ &= \frac{i\hbar}{2m} |A|^2 \bigg[e^{i \left(kx - \frac{\hbar k^2}{2m}t\right)} (-ik) e^{-i \left(kx - \frac{\hbar k^2}{2m}t\right)} - e^{-i \left(kx - \frac{\hbar k^2}{2m}t\right)} (ik) e^{i \left(kx - \frac{\hbar k^2}{2m}t\right)} \bigg] \\ &= \frac{i\hbar}{2m} |A|^2 (-2ik) \\ &= \frac{\hbar k}{m} |A|^2. \end{split}$$

It flows in the positive x direction.

This problem is designed to guide you through a "proof" of Plancherel's theorem, by starting with the theory of ordinary Fourier series on a *finite* interval, and allowing that interval to expand to infinity.

(a) Dirichlet's theorem says that "any" function f(x) on the interval [-a, +a] can be expanded as a Fourier series:

$$f(x) = \sum_{n=0}^{\infty} \left[a_n \sin\left(\frac{n\pi x}{a}\right) + b_n \cos\left(\frac{n\pi x}{a}\right) \right].$$

Show that this can be written equivalently as

$$f(x) = \sum_{n = -\infty}^{\infty} c_n e^{i\frac{n\pi x}{a}}.$$

What is c_n , in terms of a_n and b_n ?

(b) Show (by appropriate modification of Fourier's trick) that

$$c_n = \frac{1}{2a} \int_{-a}^{+a} f(x) e^{-i\frac{n\pi x}{a}} \, \mathrm{d}x.$$

(c) Eliminate n and c_n in favor of the new variables $k = \left(\frac{n\pi}{a}\right)$ and $F(k) = \sqrt{\frac{2}{\pi}}ac_n$. Show that (a) and (b) now become

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n = -\infty}^{\infty} F(k)e^{ikx} \Delta k; F(k) = \frac{1}{\sqrt{2\pi}} \int_{-a}^{+a} f(x)e^{-ikx} dx,$$

where Δk is the increment in k from one n to the next.

(d) Take the limit $a \to \infty$ to obtain Plancherel's theorem. Comment: In view of their quite different origins, it is surprising (and delightful) that the two formulas—one for F(k) in terms of f(x), the other for f(x) in terms of F(k)—have such a similar structure in the limit $a \to \infty$.

Solution

$$\begin{split} f(x) &= \sum_{n=0}^{\infty} \left[a_n \sin \left(\frac{n \pi x}{a} \right) + b_n \cos \left(\frac{n \pi x}{a} \right) \right] \\ &= b_0 + \sum_{n=1}^{\infty} a_n \sin \left(\frac{n \pi x}{a} \right) + \sum_{n=1}^{\infty} b_n \cos \left(\frac{n \pi x}{a} \right) \\ &= b_0 + \sum_{n=1}^{\infty} \frac{a_n}{2i} \left[e^{i \frac{n \pi x}{a}} - e^{-i \frac{n \pi x}{a}} \right] + \sum_{n=1}^{\infty} \frac{b_n}{2} \left[e^{i \frac{n \pi x}{a}} + e^{-i \frac{n \pi x}{a}} \right] \\ &= b_0 + \sum_{n=1}^{\infty} \left(\frac{a_n}{2i} + \frac{b_n}{2} \right) e^{i \frac{n \pi x}{a}} + \sum_{n=1}^{\infty} \left(-\frac{a_n}{2i} + \frac{b_n}{2} \right) e^{-i \frac{n \pi x}{a}}. \end{split}$$

Let

$$\begin{split} c_0 &= b_0, \\ c_n &= \frac{a_n}{2i} + \frac{b_n}{2} \quad n > 0, \\ c_n &= -\frac{a_{-n}}{2i} + \frac{b_{-n}}{2} \quad n < 0, \end{split}$$

then we have

$$\begin{split} f(x) &= \sum_{n=-\infty}^{\infty} c_n e^{i\frac{n\pi x}{a}}. \\ \text{(b)} &\quad \frac{1}{2a} \int_{-a}^{+a} f(x) e^{-i\frac{n\pi x}{a}} &= \frac{1}{2a} \int_{-a}^{+a} \left[\sum_{m=-\infty}^{\infty} c_m e^{i\frac{m\pi x}{a}} \right] e^{-i\frac{n\pi x}{a}} \, \mathrm{d}x \\ &= \frac{1}{2a} \sum_{m=-\infty}^{\infty} c_m \int_{-a}^{+a} e^{i\frac{(m-n)\pi x}{a}} \, \mathrm{d}x, \end{split}$$

where when m = n,

$$\int_{-a}^{+a} e^{i\frac{(m-n)\pi x}{a}} dx = \int_{-a}^{+a} e^0 dx$$
$$= 2a,$$

and when $m \neq n$,

$$\begin{split} \int_{-a}^{+a} e^{i\frac{(m-n)\pi x}{a}} \, \mathrm{d}x &= \frac{e^{i\frac{(m-n)\pi x}{a}} \Big|_{-a}^{a}}{i(m-n)\frac{\pi}{a}} \\ &= \frac{e^{i(m-n)\pi} - e^{-i(m-n)\pi}}{i(m-n)\frac{\pi}{a}} \\ &= \frac{(-1)^{m-n} - (-1)^{n-m}}{i(m-n)\frac{\pi}{a}} \\ &= 0, \end{split}$$

then we have

$$\frac{1}{2a} \int_{-a}^{+a} f(x)e^{-i\frac{n\pi x}{a}} = \frac{1}{2a} \sum_{m=-\infty}^{\infty} c_m [2a\delta_{mn}]$$

$$= \sum_{m=-\infty}^{\infty} c_m \delta_{mn}$$

$$= c_n.$$
(c)
$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{i\frac{n\pi x}{a}}$$

$$= \sum_{n=-\infty}^{\infty} \sqrt{\frac{\pi}{2}} \frac{1}{a} F(k) e^{ikx}$$

$$\begin{split} &= \sum_{n=-\infty}^{\infty} \sqrt{\frac{1}{2\pi}} \frac{\pi}{a} F(k) e^{ikx} \\ &= \sqrt{\frac{1}{2\pi}} \sum_{n=-\infty}^{\infty} F(k) e^{ikx} \Delta k, \end{split}$$

and

$$F(k) = \sqrt{\frac{2}{\pi}} a c_n$$

$$= \sqrt{\frac{1}{2\pi}} \int_{-a}^{+a} f(x) e^{-i\frac{n\pi x}{a}} dx$$

$$= \sqrt{\frac{1}{2\pi}} \int_{-a}^{+a} f(x) e^{-ikx} dx.$$
(d)
$$f(x) = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk.$$

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

(a)
$$1 = \int_{-\infty}^{+\infty} |\Psi(x,0)|^2 dx$$
$$= |A|^2 \int_{-\infty}^{+\infty} e^{-2a|x|} dx$$
$$= 2|A|^2 \int_0^{+\infty} e^{-2ax} dx$$
$$= 2|A|^2 \frac{e^{-2ax}}{-2a} \Big|_0^{+\infty}$$
$$= \frac{|A|^2}{a},$$

so $A = \sqrt{a}$. (b)

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx} dx$$

$$= 2 \frac{A}{\sqrt{2\pi}} \int_{0}^{+\infty} e^{-ax} \cos(kx) dx$$

$$= \frac{A}{\sqrt{2\pi}} \int_{0}^{+\infty} e^{-ax} [e^{ikx} + e^{-ikx}] dx$$

$$= \frac{A}{\sqrt{2\pi}} \left[\int_{0}^{+\infty} e^{(ik-a)x} dx + \int_{0}^{+\infty} e^{(-ik-a)x} dx \right]$$

$$= \frac{A}{\sqrt{2\pi}} \left[\frac{e^{(ik-a)x}}{ik-a} + \frac{e^{(-ik-a)x}}{-ik-a} \right] \Big|_{0}^{+\infty}$$

$$= \frac{A}{\sqrt{2\pi}} \left[\frac{-1}{ik-a} + \frac{1}{ik+a} \right]$$

$$= \frac{A}{\sqrt{2\pi}} \frac{-ik-a+ik-a}{(ik-a)(ik+a)}$$

$$= \sqrt{\frac{a}{\sqrt{2\pi}}} \frac{2a}{a^2+k^2}.$$
(c)
$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i\left(kx-\frac{hk^2}{2m}t\right)} dk$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \sqrt{\frac{a}{2\pi}} \frac{2a}{a^2+k^2} e^{i\left(kx-\frac{hk^2}{2m}t\right)} dk$$

$$= \frac{a^{\frac{3}{2}}}{\pi} \int_{-\infty}^{+\infty} \frac{e^{i\left(kx-\frac{hk^2}{2m}t\right)}}{a^2+k^2} dk.$$

(d) For very large $a, \Psi(x,0)$ is a sharp spike and

$$\phi(k) \approx \sqrt{\frac{a}{2\pi}} \frac{2a}{a^2} = \sqrt{\frac{2}{\pi a}}$$

is broad and flat, position is well-defined but momentum is ill-defined. For very small a, $\Psi(x,0)$ is broad and flat and

$$\phi(k) \approx \sqrt{\frac{a}{2\pi}} \frac{2a}{k^2} = \sqrt{\frac{2a^3}{\pi}} \frac{1}{k^2}$$

is a sharp spike, position is ill-defined but momentum is well-defined.

Problem 2.21

A free particle has the initial wave function

$$\Psi(x,0) = Ae^{-ax^2},$$

where A and a are (real and positive) constants.

- (a) Normalize $\Psi(x,0)$.
- (b) Find $\Psi(x,t)$. Hint: Integrals of the form

$$\int_{-\infty}^{+\infty} e^{-(ax^2 + bx)} \, \mathrm{d}x$$

can be handled by "completing the square": Let $y \equiv \sqrt{a}(x + \frac{b}{2a})$, and note that $(ax^2 + bx) = y^2 - \frac{b^2}{4a}$. Answer:

$$\Psi(x,t) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \frac{1}{\gamma} e^{-a\frac{x^2}{\gamma^2}}, \text{ where } \gamma \equiv \sqrt{1 + \frac{2i\hbar t}{m}}.$$

(c) Find $|\Psi(x,t)|^2$. Express your answer in terms of the quantity

$$w \equiv \sqrt{\frac{a}{1 + \left(\frac{2\hbar t}{m}\right)^2}}.$$

Sketch $|\Psi|^2$ (as a function of x) at t=0, and again for some very large t. Qualitatively, what happens to $|\Psi|^2$, as time goes on?

- (d) Find $\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$, $\langle p^2 \rangle$, σ_x , and σ_p . Partial answer: $\langle p^2 \rangle = a\hbar^2$, but it may take some algebra to reduce it to this simple form.
- (e) Does the uncertainty principle hold? At what time t does the system come closest to the uncertainty limit?

(a)
$$1 = \int_{-\infty}^{+\infty} |\Psi(x,0)|^2 dx$$
$$= |A|^2 \int_{-\infty}^{+\infty} e^{-2ax^2} dx$$
$$= |A|^2 \sqrt{\frac{2\pi}{4a}}$$

$$=|A|^2\sqrt{\frac{\pi}{2a}},$$

so
$$A = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}}$$
.
(b)
$$\int_{-\infty}^{+\infty} e^{-(ax^2 + bx)} dx = \int_{-\infty}^{+\infty} e^{-y^2 + \frac{b^2}{4a}} \frac{1}{\sqrt{a}} dy$$

$$= \frac{1}{\sqrt{a}} e^{\frac{b^2}{4a}} \int_{-\infty}^{+\infty} e^{-y^2} dy$$

$$= \frac{1}{\sqrt{a}} e^{\frac{b^2}{4a}} \sqrt{\pi}$$

$$= \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}.$$

(c)

$$\begin{split} \phi(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx} \, \mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} A e^{-ax^2} e^{-ikx} \, \mathrm{d}x \\ &= \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-(ax^2 + ikx)} \, \mathrm{d}x \\ &= \frac{A}{\sqrt{2\pi}} \sqrt{\frac{\pi}{a}} e^{-\frac{k^2}{4a}} \\ &= \frac{\frac{2a}{\pi}}{\sqrt{2\pi}} \sqrt{\frac{\pi}{a}} e^{-\frac{k^2}{4a}} \\ &= \frac{\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}}{\sqrt{2\pi}} \sqrt{\frac{\pi}{a}} e^{-\frac{k^2}{4a}} \\ &= \frac{e^{-\frac{k^2}{4a}}}{(2\pi a)^{\frac{1}{4}}}. \end{split}$$

$$\Psi(x,t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} \, \mathrm{d}k \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{e^{-\frac{k^2}{4a}}}{(2\pi a)^{\frac{1}{4}}} e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} \, \mathrm{d}k \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{(2\pi a)^{\frac{1}{4}}} \int_{-\infty}^{+\infty} e^{-\frac{k^2}{4a}} e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} \, \mathrm{d}k \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{(2\pi a)^{\frac{1}{4}}} \int_{-\infty}^{+\infty} e^{-\left[\left(\frac{1}{4a} + \frac{\hbar k_1}{2m}\right)k^2 - ixk\right]} \, \mathrm{d}k \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{(2\pi a)^{\frac{1}{4}}} \sqrt{\frac{\pi}{\frac{1}{4a} + \frac{i\hbar t}{2m}}} e^{-\frac{x^2}{4\left(\frac{1}{4a} + \frac{i\hbar t}{2m}\right)}} \\ &= \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \frac{e^{-\frac{\alpha x^2}{1-2\frac{i\hbar t}{2m}}}}{\sqrt{1 + \frac{2i\hbar t}{m}}} e^{-\frac{x^2}{1-\frac{2i\hbar t}}}} \\ &= \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \frac{1}{\gamma} e^{-\frac{\alpha x^2}{\gamma^2}}, \end{split}$$
 where $\gamma = \sqrt{1 + \frac{2i\hbar t}{m}}$.
$$|\Psi(x,t)|^2 = \sqrt{\frac{2a}{\pi}} \frac{e^{-\frac{i\pi^2}{1+\frac{2i\hbar t}{m}}} e^{-\frac{i\pi^2}{1-\frac{2i\hbar t}}}}{\sqrt{\left(1 + \frac{2i\hbar t}{m}\right)\left(1 - \frac{2i\hbar t}{m}\right)}} = \sqrt{\frac{2a}{\pi}} \frac{e^{-\frac{2ax^2}{1-2\frac{i\hbar t}{m}}}}{\sqrt{1 + \left(\frac{2i\hbar t}{m}\right)^2}}$$

$$=\sqrt{\frac{2}{\pi}}\omega e^{-2\omega^2x^2},$$

where $\omega = \sqrt{\frac{a}{1 + \left(\frac{2\hbar t}{m}\right)^2}}$.

As t increases, the wave function spreads out.

(d)
$$\langle x \rangle = \int_{-\infty}^{+\infty} x |\Psi(x,t)|^2 \, \mathrm{d}x$$

$$= 0;$$

$$\langle p \rangle = m \frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t}$$
$$= 0:$$

$$\begin{split} \langle x^2 \rangle &= \int_{-\infty}^{+\infty} x^2 |\Psi(x,t)|^2 \, \mathrm{d}x \\ &= \sqrt{\frac{2}{\pi}} \omega \int_{-\infty}^{+\infty} x^2 e^{-2\omega^2 x^2} \, \mathrm{d}x \\ &= \sqrt{\frac{2}{\pi}} \omega \left(\frac{1}{4\omega^2}\right) \left[x e^{-2\omega^2 x^2} \Big|_{-\infty}^{+\infty} + \int_{-\infty}^{+\infty} e^{-2\omega^2 x^2} \, \mathrm{d}x \right] \\ &= \sqrt{\frac{2}{\pi}} \omega \left(\frac{1}{4\omega^2}\right) \sqrt{2\pi} \left(\frac{1}{2\omega}\right) \\ &= \frac{1}{4\omega^2}; \end{split}$$

$$\begin{split} \langle p^2 \rangle &= \int_{-\infty}^{+\infty} \Psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x} \right)^2 \Psi(x,t) \, \mathrm{d}x \\ &= -\hbar^2 \int_{-\infty}^{+\infty} \Psi^*(x,t) \frac{\partial^2 \Psi}{\partial x^2} \, \mathrm{d}x \\ &= -\hbar^2 \sqrt{\frac{2a}{\pi}} \frac{1}{\sqrt{\left(1 + \frac{2i\hbar t}{m}\right)\left(1 - \frac{2i\hbar t}{m}\right)}} \int_{-\infty}^{+\infty} e^{-\frac{ax^2}{1 - \frac{2i\hbar t}{m}}} \frac{\partial^2}{\partial x^2} e^{-\frac{ax^2}{1 + \frac{2i\hbar t}{m}}} \, \mathrm{d}x \\ &= -\hbar^2 \sqrt{\frac{2a}{\pi}} \frac{1}{\sqrt{1 + \left(\frac{2\hbar t}{m}\right)^2}} \left(\frac{-2a}{1 + \frac{2i\hbar t}{m}} \right) \int_{-\infty}^{+\infty} e^{-\frac{ax^2}{1 - \frac{2i\hbar t}{m}}} \frac{\partial}{\partial x} x e^{-\frac{ax^2}{1 + \frac{2i\hbar t}{m}}} \, \mathrm{d}x \\ &= \hbar^2 \sqrt{\frac{2a}{\pi}} \frac{1}{\sqrt{1 + \left(\frac{2\hbar t}{m}\right)^2}} \left(\frac{2a}{1 + \frac{2i\hbar t}{m}} \right) \int_{-\infty}^{+\infty} e^{-\frac{ax^2}{1 - \frac{2i\hbar t}{m}}} \left(1 - \frac{2ax^2}{1 + \frac{2i\hbar t}{m}} \right) e^{-\frac{ax^2}{1 + \frac{2i\hbar t}{m}}} \, \mathrm{d}x \\ &= \frac{2\hbar^2 \sqrt{\frac{2a}{\pi}} a}{\left(1 + \frac{2i\hbar t}{m}\right)^2 \sqrt{1 + \left(\frac{2\hbar t}{m}\right)^2}} \int_{-\infty}^{+\infty} e^{-\frac{2ax^2}{1 + \left(\frac{2\hbar t}{m}\right)^2}} \left(1 + \frac{2i\hbar t}{m} - 2ax^2 \right) \, \mathrm{d}x \end{split}$$

$$\begin{split} &= \frac{2\hbar^2 \sqrt{\frac{2a}{\pi}}a}{\left(1 + \frac{2i\hbar t}{m}\right)^2 \sqrt{1 + \left(\frac{2\hbar t}{m}\right)^2}} \left[\sqrt{\frac{\pi \left(1 + \left(\frac{2\hbar t}{m}\right)^2\right)}{2a}} \left(1 + \frac{2i\hbar t}{m}\right) - 2a\frac{1}{4\omega^3} \sqrt{\frac{\pi}{2}} \right] \\ &= \frac{2\hbar^2 \sqrt{\frac{2a}{\pi}}a}{\left(1 + \frac{2i\hbar t}{m}\right)^2 \sqrt{1 + \left(\frac{2\hbar t}{m}\right)^2}} \left[\sqrt{\frac{\pi \left(1 + \left(\frac{2\hbar t}{m}\right)^2\right)}{2a}} \left(1 + \frac{2i\hbar t}{m}\right) - 2a\frac{\left(1 + \left(\frac{2\hbar t}{m}\right)^2\right) \sqrt{1 + \left(\frac{2\hbar t}{m}\right)^2}}{4a\sqrt{a}} \sqrt{\frac{\pi}{2}} \right] \\ &= \frac{2\hbar^2 \sqrt{\frac{2a}{\pi}}a}{\left(1 + \frac{2i\hbar t}{m}\right)^2 \sqrt{1 + \left(\frac{2\hbar t}{m}\right)^2}} \left[\sqrt{\frac{\pi}{2}}\frac{1}{\omega} \left(1 + \frac{2i\hbar t}{m}\right) - \frac{1 + \left(\frac{2\hbar t}{m}\right)^2}{2\omega} \sqrt{\frac{\pi}{2}} \right] \\ &= \frac{2\hbar^2 a\frac{\sqrt{a}}{\omega}}{1 + \frac{2i\hbar t}{m}} \sqrt{1 + \left(\frac{2\hbar t}{m}\right)^2} - \frac{\hbar^2 a\frac{\sqrt{a}}{\omega} \left(1 + \left(\frac{2\hbar t}{m}\right)^2\right)}{\left(1 + \frac{2i\hbar t}{m}\right)^2} \\ &= \frac{2\hbar^2 a}{1 + \frac{2i\hbar t}{m}} - \frac{\hbar^2 a \left(1 + \left(\frac{2\hbar t}{m}\right)^2\right)}{\left(1 + \frac{2i\hbar t}{m}\right)^2} \\ &= \hbar^2 a \left[\frac{2\left(1 + \left(\frac{2i\hbar t}{m}\right)\right) - \left(1 + \left(\frac{2\hbar t}{m}\right)^2\right)}{\left(1 + \frac{2i\hbar t}{m}\right)} \right] \\ &= \hbar^2 a \left[\frac{1 - \left(\frac{2\hbar t}{m}\right)^2 + \frac{4i\hbar t}{m}}{1 - \left(\frac{2\hbar t}{m}\right)^2 + \frac{4i\hbar t}{m}} \right] \\ &= \hbar^2 a. \end{split}$$

$$\begin{split} \sigma_x &= \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \\ &= \sqrt{\frac{1}{4\omega^2} - 0} \\ &= \frac{1}{2\omega}, \end{split}$$

and

$$\sigma_{p} = \sqrt{\langle p^{2} \rangle - \langle p \rangle^{2}}$$

$$= \sqrt{\hbar^{2} a - 0}$$

$$= \hbar \sqrt{a}.$$
(e)
$$\sigma_{x} \sigma_{p} = \frac{1}{2\omega} \hbar \sqrt{a}$$

$$= \frac{\hbar}{2} \sqrt{1 + \left(\frac{2\hbar t}{m}\right)^{2}} \ge \frac{\hbar}{2}.$$

The uncertainty principle holds, and the system comes closest to the uncertainty limit at t = 0.

Evaluate the following integrals:

(a)
$$\int_{-1}^{+1} (x^3 - 3x^2 + 2x - 1)\delta(x + 2) dx$$
.
(b) $\int_{0}^{\infty} [\cos(3x) + 2]\delta(x - \pi) dx$.
(c) $\int_{-1}^{+1} \exp(|x| + 3)\delta(x - 2) dx$.

(b)
$$\int_{0}^{\infty} [\cos(3x) + 2] \delta(x - \pi) dx$$
.

(c)
$$\int_{-1}^{9+1} \exp(|x|+3)\delta(x-2) dx$$

Solution

(a)
$$\int_{-1}^{+1} (x^3 - 3x^2 + 2x - 1) \delta(x + 2) dx = (x^3 - 3x^2 + 2x - 1) \Big|_{x = -2}$$
$$= (-2)^3 - 3(-2)^2 + 2(-2) - 1$$
$$= -8 - 12 - 4 - 1$$
$$= -25.$$

(b)
$$\int_0^\infty [\cos(3x) + 2] \delta(x - \pi) \, \mathrm{d}x = [\cos(3x) + 2]|_{x = \pi}$$

$$= \cos(3\pi) + 2$$

$$= -1 + 2$$

$$= 1.$$

(c)
$$\int_{-1}^{+1} \exp(|x| + 3)\delta(x - 2) \, \mathrm{d}x = 0$$

Problem 2.23

Delta functions live under integral signs, and two expressions $(D_1(x))$ and $D_2(x)$ involving delta functions are said to be equal if

$$\int_{-\infty}^{+\infty} f(x) D_1(x) \,\mathrm{d}x = \int_{-\infty}^{+\infty} f(x) D_2(x) \,\mathrm{d}x,$$

for every (ordinary) function f(x).

(a) Show that

$$\delta(cx) = \frac{1}{|c|} \delta(x),$$

where c is a real constant. (Be sure to check the case where c is negative.)

(b) Let $\theta(x)$ be the step function:

$$\theta(x) \equiv \begin{cases} 1, & x > 0 \\ 0, & x < 0. \end{cases}$$

(In the rare case where it actually matters, we define $\theta(0)$ to be $\frac{1}{2}$.) Show that $\frac{\mathrm{d}\theta}{\mathrm{d}x} = \delta(x).$

Solution

(a) Let y = cx, then dy = c dx, then

$$\int_{-\infty}^{+\infty} f(x)\delta(cx) \, \mathrm{d}x = \begin{cases} \frac{1}{c} \int_{-\infty}^{+\infty} f\left(\frac{y}{c}\right)\delta(y) \, \mathrm{d}y = \frac{1}{c}f(0) & c > 0\\ \frac{1}{c} \int_{+\infty}^{-\infty} f\left(\frac{y}{c}\right)\delta(y) \, \mathrm{d}y = -\frac{1}{c} \int_{-\infty}^{+\infty} f\left(\frac{y}{c}\right)\delta(y) \, \mathrm{d}y = -\frac{1}{c}f(0) & c < 0 \end{cases}$$
$$= \frac{1}{|c|} f(0)$$
$$= \int_{-\infty}^{+\infty} f(x) \frac{1}{|c|} \delta(x) \, \mathrm{d}x,$$

so
$$\delta(cx) = \frac{1}{|c|}\delta(x)$$
.

$$\int_{-\infty}^{+\infty} f(x) \frac{d\theta}{dx} dx = f\theta \mid_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \theta(x) \frac{df}{dx} dx$$

$$= f(+\infty) - \int_{0}^{+\infty} \frac{df}{dx} dx$$

$$= f(+\infty) - (f(\infty) - f(0))$$

$$= f(0)$$

$$= \int_{-\infty}^{+\infty} f(x)\delta(x) dx,$$

so
$$\frac{\mathrm{d}\theta}{\mathrm{d}x} = \delta(x)$$
.

Check the uncertainty principle for the wave function in

$$\begin{split} \psi(x) &= \frac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha|x|}{\hbar^2}} \\ &= \begin{cases} \frac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha x}{\hbar^2}} & x \geq 0 \\ \frac{\sqrt{m\alpha}}{\hbar} e^{\frac{m\alpha x}{\hbar^2}} & x \leq 0. \end{cases} \end{split}$$

Hint: Calculating $\langle p^2 \rangle$ can be tricky, because the derivative of ψ has a step discontinuity at x = 0. You may want to use the result in Problem 2.23(b). Partial answer: $\langle p^2 \rangle = \left(\frac{m\alpha}{\hbar}\right)^2$.

$$\begin{split} \langle x \rangle &= 0; \\ \langle p^2 \rangle &= m \frac{\mathrm{d} \langle x \rangle}{\mathrm{d}t} \\ &= 0; \\ \langle x^2 \rangle &= \int_{-\infty}^{+\infty} x^2 |\psi(x)|^2 \, \mathrm{d}x \\ &= 2 \frac{m\alpha}{\hbar^2} \int_0^{+\infty} x^2 e^{-\frac{2m\alpha x}{\hbar^2}} \, \mathrm{d}x \end{split}$$

$$\begin{split} &=\frac{2m\alpha}{\hbar^2}\frac{h^2}{2m\alpha}\int_0^{+\infty}2xe^{-\frac{2m\alpha x}{\hbar^2}}\,\mathrm{d}x\\ &=2\frac{h^2}{2m\alpha}\int_0^{+\infty}e^{-\frac{2m\alpha x}{\hbar^2}}\,\mathrm{d}x\\ &=\frac{h^2}{2m\alpha}\frac{h^2}{2m\alpha}\\ &=\frac{h^4}{2m^2\alpha^2}\\ &\frac{\mathrm{d}\psi}{\mathrm{d}x}=\begin{cases} \frac{\sqrt{m\alpha}}{\hbar}\left(-\frac{m\alpha}{\hbar^2}\right)e^{-\frac{m\alpha x}{\hbar^2}}&x\geq0\\ \frac{\sqrt{m\alpha}}{\hbar}\left(\frac{m\alpha}{\hbar^2}\right)e^{-\frac{m\alpha x}{\hbar^2}}&x\leq0.\\ &=\left(\frac{\sqrt{m\alpha}}{\hbar}\right)^3\left[-\theta(x)e^{-\frac{m\alpha x}{\hbar^2}}+\theta(-x)e^{\frac{m\alpha x}{\hbar^2}}\right]\\ &=\left(\frac{\sqrt{m\alpha}}{\hbar}\right)^3\left[-\delta(x)e^{-\frac{m\alpha x}{\hbar^2}}+\theta(x)\frac{m\alpha}{\hbar^2}e^{-\frac{m\alpha x}{\hbar^2}}-\delta(-x)e^{\frac{m\alpha x}{\hbar^2}}+\theta(-x)\frac{m\alpha}{\hbar^2}e^{\frac{m\alpha x}{\hbar^2}}\right]\\ &=\left(\frac{\sqrt{m\alpha}}{\hbar}\right)^3\left[-\delta(x)\left(e^{-\frac{m\alpha x}{\hbar^2}}+e^{\frac{m\alpha x}{\hbar^2}}\right)+\frac{m\alpha}{\hbar^2}(\theta(x)+\theta(-x))e^{-\frac{m\alpha x}{\hbar^2}}\right]\\ &=\left(\frac{\sqrt{m\alpha}}{\hbar}\right)^3\left[-2\delta(x)+\frac{m\alpha}{\hbar^2}e^{-\frac{m\alpha x}{\hbar^2}}\right]\\ &=\left(\frac{\sqrt{m\alpha}}{\hbar}\right)^3\left[-2\delta(x)+\frac{m\alpha}{\hbar^2}e^{-\frac{m\alpha x}{\hbar^2}}\right]\\ &=\left(\frac{\sqrt{m\alpha}}{\hbar}\right)^4\int_{-\infty}^{+\infty}e^{-\frac{m\alpha x}{\hbar^2}}\left[-2\delta(x)+\frac{m\alpha}{\hbar^2}e^{-\frac{m\alpha x}{\hbar^2}}\right]\mathrm{d}x\\ &=-\hbar^2\left(\frac{\sqrt{m\alpha}}{\hbar}\right)^4\int_{-\infty}^{+\infty}e^{-\frac{m\alpha x}{\hbar^2}}\left[-2\delta(x)+\frac{m\alpha}{\hbar^2}e^{-\frac{m\alpha x}{\hbar^2}}\right]\mathrm{d}x\\ &=-\left(\frac{m\alpha}{\hbar}\right)^2\left[-2\int_{-\infty}^{+\infty}\delta(x)e^{-\frac{m\alpha x}{\hbar^2}}\mathrm{d}x+2\frac{m\alpha}{\hbar^2}\int_0^{+\infty}e^{-\frac{2m\alpha xx}{\hbar^2}}\mathrm{d}x\right]\\ &=-\left(\frac{m\alpha}{\hbar}\right)^2\left[-2+\frac{2m\alpha}{\hbar^2}\frac{\hbar^2}{2m\alpha}\right]\\ &=\left(\frac{m\alpha}{\hbar}\right)^2. \end{cases}$$

$$\begin{split} &=\frac{\hbar^2}{\sqrt{2}m\alpha};\\ \sigma_p &= \sqrt{\langle p^2\rangle - \langle p\rangle^2}\\ &= \sqrt{\left(\frac{m\alpha}{\hbar}\right)^2 - 0}\\ &= \frac{m\alpha}{\hbar}.\\ \sigma_x \sigma_p &= \frac{\hbar^2}{\sqrt{2}m\alpha} \frac{m\alpha}{\hbar}\\ &= \frac{\hbar}{\sqrt{2}} \geq \frac{\hbar}{2}. \end{split}$$

Check that the bound state of the delta-function Well

$$\psi_{\mathrm{bound}}(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha|x|}{\hbar^2}}$$

is orthogonal to the scattering states

$$\psi_{\text{scattering}}(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Fe^{ikx} + Ge^{-ikx} & x > 0 \end{cases}$$

Solution

$$\begin{split} \langle \psi_{\text{bound}}(x), \psi_{\text{scattering}}(x) \rangle &= \int_{-\infty}^{+\infty} \psi_{\text{bound}}^*(x) \psi_{\text{scattering}}(x) \, \mathrm{d}x \\ &= \frac{\sqrt{m\alpha}}{\hbar} \left[\int_{-\infty}^{0} e^{\frac{m\alpha x}{\hbar^2}} \left(A e^{ikx} + B e^{-ikx} \right) \, \mathrm{d}x + \int_{0}^{+\infty} e^{-\frac{m\alpha x}{\hbar^2}} \left(F e^{ikx} + G e^{-ikx} \right) \, \mathrm{d}x \right] \\ &= \frac{\sqrt{m\alpha}}{\hbar} \left[A \int_{-\infty}^{0} e^{\left(\frac{m\alpha}{\hbar^2} + ik\right)x} \, \mathrm{d}x + B \int_{-\infty}^{0} e^{\left(\frac{m\alpha}{\hbar^2} - ik\right)x} \, \mathrm{d}x \right. \\ &+ F \int_{0}^{+\infty} e^{\left(-\frac{m\alpha}{\hbar^2} + ik\right)x} \, \mathrm{d}x + G \int_{0}^{+\infty} e^{\left(-\frac{m\alpha}{\hbar^2} - ik\right)x} \, \mathrm{d}x \right] \\ &= \frac{\sqrt{m\alpha}}{\hbar} \left[A \frac{e^{\left(\frac{m\alpha}{\hbar^2} + ik\right)x}}{\frac{m\alpha}{\hbar^2} + ik} \bigg|_{-\infty}^{0} + B \frac{e^{\left(\frac{m\alpha}{\hbar^2} - ik\right)x}}{\frac{m\alpha}{\hbar^2} - ik} \bigg|_{-\infty}^{0} + F \frac{e^{\left(-\frac{m\alpha}{\hbar^2} + ik\right)x}}{-\frac{m\alpha}{\hbar^2} + ik} \bigg|_{0}^{+\infty} + G \frac{e^{\left(-\frac{m\alpha}{\hbar^2} - ik\right)x}}{-\frac{m\alpha}{\hbar^2} - ik} \bigg|_{0}^{+\infty} \right] \\ &= \frac{\sqrt{m\alpha}}{\hbar} \left[\frac{A}{\frac{m\alpha}{\hbar^2} + ik} + \frac{B}{\frac{m\alpha}{\hbar^2} - ik} - \frac{F}{-\frac{m\alpha}{\hbar^2} + ik} - \frac{G}{-\frac{m\alpha}{\hbar^2} - ik}} \right] \end{split}$$

$$\begin{split} &=\frac{\sqrt{m\alpha}}{\hbar}\left[\frac{A+G}{\frac{m\alpha}{\hbar^2}+ik}+\frac{B+F}{\frac{m\alpha}{\hbar^2}-ik}\right]\\ &=\frac{\sqrt{m\alpha}}{\hbar}\left[\frac{(A+G)\left(\frac{m\alpha}{\hbar^2}-ik\right)+(B+F)\left(\frac{m\alpha}{\hbar^2}+ik\right)}{\left(\frac{m\alpha}{\hbar^2}\right)^2+k^2}\right]\\ &=\frac{\sqrt{m\alpha}}{\hbar}\left[\frac{(A+B+F+G)\left(\frac{m\alpha}{\hbar^2}\right)+ik(B+F-A-G)}{\left(\frac{m\alpha}{\hbar^2}\right)^2+k^2}\right]\\ &=\frac{\sqrt{m\alpha}}{\hbar}\left[\frac{(A+B+A+B)\left(\frac{m\alpha}{\hbar^2}\right)+ik(B-A+A(1+2i\beta)-B(1-2i\beta)\right)}{\left(\frac{m\alpha}{\hbar^2}\right)^2+k^2}\right]\\ &=\frac{\sqrt{m\alpha}}{\hbar}\left[\frac{2(A+B)\frac{m\alpha}{\hbar^2}-2k\beta(A+B)}{\left(\frac{m\alpha}{\hbar^2}\right)^2+k^2}\right]\\ &=\frac{\sqrt{m\alpha}}{\hbar}\left[\frac{2(A+B)\frac{m\alpha}{\hbar^2}-2k\beta(A+B)}{\left(\frac{m\alpha}{\hbar^2}\right)^2+k^2}\right]\\ &=\frac{\sqrt{m\alpha}}{\hbar}\left[\frac{2(A+B)\frac{m\alpha}{\hbar^2}-2\frac{m\alpha}{\hbar^2}(A+B)}{\left(\frac{m\alpha}{\hbar^2}\right)^2+k^2}\right]\\ &=0 \end{split}$$

What is the Fourier transform of $\delta(x)$? Using Plancherel's theorem, show that

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} \, \mathrm{d}k.$$

Comment: This formula gives any respectable mathematician apoplexy. Although the integral is clearly infinite when x=0, it doesn't converge (to zero or anything else) when $x\neq 0$, since the integrand oscillates forever. There are ways to patch it up (for instance, you can integrate from -L to +L, and interpret Equation 2.147 to mean the average value of the finite integral, as $L\to\infty$). The source of the problem is that the delta function doesn't meet the requirement (square-integrability) for Plancherel's theorem (see footnote 42). In spite of this, Equation 2.147 can be extremely useful, if handled with care.

$$\Delta(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \delta(x) e^{-ikx} \, \mathrm{d}x$$

$$= \frac{1}{\sqrt{2\pi}}$$

$$\delta(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Delta(k) e^{ikx} \, \mathrm{d}k$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ikx} \, \mathrm{d}k$$

Consider the double delta-function potential

$$V(x) = -\alpha [\delta(x+a) + \delta(x-a)],$$

where α and a are positive constants.

- (a) Sketch this potential.
- (b) How many bound states does it possess? Find the allowed energies, for $\alpha = \frac{\hbar^2}{ma}$ and for $\alpha = \frac{\hbar^2}{4ma}$, and sketch the wave functions.
- (c) What are the bound state energies in the limiting cases (i) $a \to 0$ and (ii) $a \to \infty$ (holding α fixed)? Explain why your answers are reasonable, by comparison with the single delta-function well.

Solution

- (a)
- (b) As V is even, the solutions can be even or odd. For even solutions,

$$\psi(x) = \begin{cases} Ae^{\kappa x} & x < -a \\ B(e^{\kappa x} + e^{-\kappa x}) & -a < x < a \\ Ae^{-\kappa x} & x > a \end{cases}$$

Continuity of ψ at $x = \pm a$ gives

$$Ae^{-\kappa a} = B(e^{\kappa a} + e^{-\kappa a}),$$

or

$$A = B(1 + e^{2\kappa a}).$$

Continuity of $\frac{d\psi}{dx}$ at $x = \pm a$ gives

$$\lim_{\varepsilon \to 0} \left(\frac{\mathrm{d}\psi}{\mathrm{d}x} \Big|_{a-\varepsilon}^{a+\varepsilon} \right) = -\frac{2m\alpha}{\hbar^2} \psi(a)$$

$$-\kappa A e^{-\kappa a} - B(\kappa e^{\kappa a} - \kappa e^{-\kappa a}) = -\frac{2m\alpha}{\hbar^2} A e^{-\kappa a}$$

$$\left(\frac{2m\alpha}{\hbar^2} - \kappa \right) A e^{-\kappa a} = B(\kappa e^{\kappa a} - \kappa e^{-\kappa a})$$

$$\left(\frac{2m\alpha}{\hbar^2} - \kappa \right) B(e^{\kappa a} + e^{-\kappa a}) = B(\kappa e^{\kappa a} - \kappa e^{-\kappa a})$$

$$\frac{2m\alpha}{\hbar^2} (e^{\kappa a} + e^{-\kappa a}) = 2\kappa e^{\kappa a}$$

$$e^{-2\kappa a} = \frac{\hbar^2 \kappa}{m\alpha} - 1,$$

which has only one solution; For odd solutions,

$$\psi(x) = \begin{cases} -Ae^{\kappa x} & x < -a \\ B(e^{\kappa x} - e^{-\kappa x}) & -a < x < a \\ Ae^{-\kappa x} & x > a \end{cases}$$

Continuity of ψ at $x = \pm a$ gives

$$Ae^{-\kappa a} = B(e^{\kappa a} - e^{-\kappa a}),$$

or

$$A = B(e^{2\kappa a} - 1).$$

Continuity of $\frac{d\psi}{dx}$ at $x = \pm a$ gives

$$\lim_{\varepsilon \to 0} \left(\frac{\mathrm{d}\psi}{\mathrm{d}x} \right|_{a-\varepsilon}^{a+\varepsilon} \right) = -\frac{2m\alpha}{\hbar^2} \psi(a)$$

$$-\kappa A e^{-\kappa a} - B(\kappa e^{\kappa a} + \kappa e^{-\kappa a}) = -\frac{2m\alpha}{\hbar^2} A e^{-\kappa a}$$

$$\left(\frac{2m\alpha}{\hbar^2} - \kappa \right) A e^{-\kappa a} = B\kappa (e^{\kappa a} + e^{-\kappa a})$$

$$\left(\frac{2m\alpha}{\hbar^2} - \kappa \right) B(e^{\kappa a} - e^{-\kappa a}) = B\kappa (e^{\kappa a} + e^{-\kappa a})$$

$$\frac{2m\alpha}{\hbar^2} (e^{\kappa a} - e^{-\kappa a}) = 2\kappa e^{\kappa a}$$

$$e^{-2\kappa a} = 1 - \frac{\hbar^2 \kappa}{m\alpha},$$

which has one solution if $\alpha > \frac{\hbar^2}{2ma}$, and no solutions if $\alpha \leq \frac{\hbar^2}{2ma}$. In conclusion, there are two bound states if $\alpha > \frac{\hbar^2}{2ma}$, and one bound state if $\alpha \leq \frac{\hbar^2}{2ma}$.

(c) (i) When $a \to 0$, there is only one (even) bound state, the equation says

$$\frac{\hbar^2 \kappa}{m\alpha} - 1 = e^{-2\kappa a} \approx 1$$
$$\kappa = \frac{2m\alpha}{\hbar^2}.$$

Then the energy is

$$E = -\frac{\kappa^2 \hbar^2}{2m}$$
$$= -\frac{2m\alpha^2}{\hbar^2}$$
$$= -\frac{m(2\alpha)^2}{2\hbar^2},$$

which is just the energy of a single delta-function well with strength 2α .

(ii) When $a \to \infty$, there are two bound states, the even one says

$$\frac{\hbar^2\kappa}{m\alpha}-1=e^{-2\kappa a}\approx 0$$

$$\kappa=\frac{m\alpha}{\hbar^2}.$$

Then the energy is

$$\begin{split} E &= -\frac{\kappa^2 \hbar^2}{2m} \\ &= -\frac{m\alpha^2}{2\hbar^2}; \end{split}$$

and the odd one says

$$1 - \frac{\hbar^2 \kappa}{m\alpha} = e^{-2\kappa a} \approx 0$$

$$\kappa = \frac{m\alpha}{\hbar^2}.$$

Then the energy is

$$E = -\frac{\kappa^2 \hbar^2}{2m}$$
$$= -\frac{m\alpha^2}{2\hbar^2};$$

Problem 2.28

Find the transmission coefficient, for the potential in Problem 2.27.