S2014

PROBLEM 2: Particle in a Box

A particle of mass m is in the ground state of a one dimension box of length L. At $t = 0$, the box suddenly expands *symmetrically* to *three* times its size, leaving the wavefunction of the particle undisturbed. Assume the particle was in the ground state before the expansion.

a) Solve the Schrodinger equation and calculate the eigenenergies and eigenfunctions in the box before and *after* the expansion (show all your work). (3 Points)

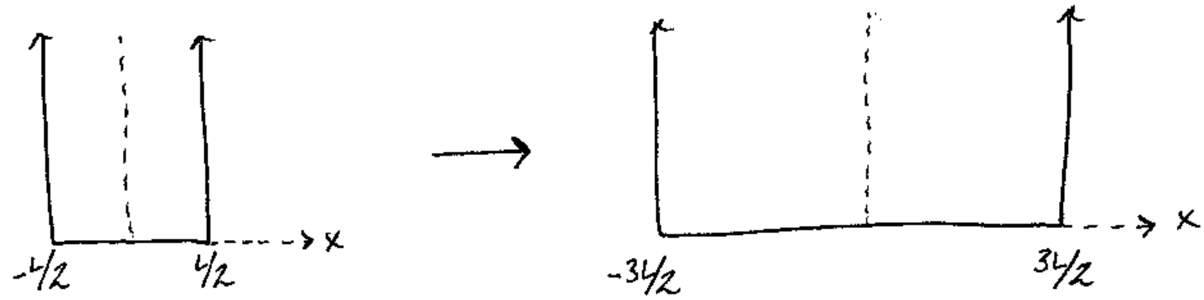
b) What is the probability of finding the particle in the ground state immediately after the expansion? (4 Points)

c) Compute the wave function of the particle $\psi(x, t)$ for $t \geq 0$. Hint: express your answer as a superposition of eigenstates. (3 Points)

Hint: $\int_{-\pi/2}^{\pi/2} \mathrm{d}\theta \, \cos\theta \cos(q\theta) = \frac{2}{1-q^2} \cos\left(q\frac{\pi}{2}\right)$,

$\int_{-\pi/2}^{\pi/2} \mathrm{d}\theta \, \cos\theta \sin(q\theta) = 0.$

(a)



Assuming this is an infinite square well, the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi,$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}.$$

The general solution of this equation is

$$\psi(x) = A\sin(kx) + B\cos(kx),$$

where A and B are constants. Applying boundary conditions will allow us to more specifically determine the wavefunction. At each boundary, the wavefunction must be zero since the potential is infinite outside of our box.

(a), cont'd...

In the initial case, our boundary conditions give us

$$\psi(-L/2) = A\sin\left(-\frac{kL}{2}\right) + B\cos\left(-\frac{kL}{2}\right) = 0$$
$$= B\cos\left(\frac{kL}{2}\right) - A\sin\left(\frac{kL}{2}\right) = 0$$

and

$$\psi(L/2) = A\sin\left(\frac{kL}{2}\right) + B\cos\left(\frac{kL}{2}\right) = 0.$$

We can set

$$\frac{kL}{2} = n\frac{\pi}{2} \quad .$$

For $n = 1, 3, 5, \ldots$ we must have $\cos\left(\frac{kL}{2}\right) = 0$, so it must be the case that $A = 0$. Thus, for odd values of n, our wavefunction is

$$\psi_{odd} = B\cos(kx)$$
$$\psi_{odd} = B\cos\left(\frac{n\pi x}{L}\right).$$

For $n = 2, 4, 6, \ldots$ we must have $\sin\left(\frac{kL}{2}\right) = 0$, so it must be the case that $B = 0$. So for even values of n, our wavefunction is

$$\psi_{even} = A\sin\left(\frac{n\pi x}{L}\right).$$

Now we must normalize these functions. In general,

$$\int_{\text{all space}} |\psi(x)|^2\, dx = 1.$$

(a), cont'd...

For ψ_{odd} ...

$$B^2 \int_{-L/2}^{L/2} \cos^2\left(\frac{n\pi x}{L}\right) dx = 1$$

$$B^2 \left[\frac{1}{2}\left(L + \frac{L\sin(n\pi)}{n\pi}\right)\right] = 1$$

But $\sin(n\pi) = 0$ for <u>all</u> values of n, so we are left with

$$B^2\left(\frac{1}{2}L\right) = 1$$

$$B = \sqrt{\frac{2}{L}}$$

and

$$\psi_{odd} = \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right) \quad , \quad n = 1, 3, 5, \ldots$$

Similarly, for ψ_{even} ...

$$A^2 \int_{-L/2}^{L/2} \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

$$A^2 \left[\frac{1}{2}\left(L - \frac{L\sin(n\pi)}{n\pi}\right)\right] = 1$$

$$A = \sqrt{\frac{2}{L}}$$

and

$$\psi_{even} = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad n = 2, 4, 6, \ldots$$

(a), cont'd...

The ground state corresponds to $n=1$, so our ground state wavefunction initially is

$$\boxed{\psi^{i}_{\text{ground}} = \sqrt{\frac{2}{L}}\cos\left(\frac{\pi x}{L}\right)}$$

We originally set

$$k = \frac{\sqrt{2mE}}{\hbar},$$

but we also know

$$k = \frac{n\pi}{L}.$$

So

$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{L}$$

$$2mE = \frac{n^2\pi^2\hbar^2}{L^2}$$

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

are our initial general eigenenergies. For $n=1$, the ground state energy is initially

$$\boxed{E^{i}_{\text{ground}} = \frac{\pi^2\hbar^2}{2mL^2}}$$

Now we want to do the same analysis <u>after</u> expansion.

(a), cont'd...

Since the well expanded symmetrically, our general wavefunction is still

$$\psi(x) = A\sin(kx) + B\cos(kx).$$

What has changed are our boundaries. We must have

$$\psi(-3L/2) = B\cos\left(\frac{3kL}{2}\right) - A\sin\left(\frac{3kL}{2}\right) = 0$$

and

$$\psi(3L/2) = A\sin\left(\frac{3kL}{2}\right) + B\cos\left(\frac{3kL}{2}\right) = 0.$$

Again, we set

$$\frac{3kL}{2} = n\frac{\pi}{2}.$$

For $n \in$ odds, we must have

$$\psi_{odd} = B\cos(kx)$$

$$\psi_{odd} = B\cos\left(\frac{n\pi x}{3L}\right)$$

For $n \in$ evens, we must have

$$\psi_{even} = A\sin\left(\frac{n\pi x}{3L}\right)$$

As before, we must normalize.

(a), cont'd...

For ψ_{odd} ...

$$B^2 \int_{-3L/2}^{3L/2} \cos^2\left(\frac{n\pi x}{3L}\right) dx = 1$$

$$B^2 \left[\frac{3L}{2n\pi}\left(n\pi + \sin(n\pi)\right)\right] = 1.$$

Again, $\sin(n\pi) = 0 \;\; \forall n$, so

$$B^2\left(\frac{3L}{2}\right) = 1$$

$$B = \sqrt{\frac{2}{3L}}$$

and

$$\psi_{odd} = \sqrt{\frac{2}{3L}} \cos\left(\frac{n\pi x}{3L}\right), \quad n = 1, 3, 5, \ldots$$

Similarly, for ψ_{even} ...

$$A^2 \int_{-3L/2}^{3L/2} \sin^2\left(\frac{n\pi x}{3L}\right) dx = 1$$

$$A^2 \left[\frac{3L}{2n\pi}\left(n\pi - \sin(n\pi)\right)\right] = 1$$

$$A = \sqrt{\frac{2}{3L}}$$

and

$$\psi_{even} = \sqrt{\frac{2}{3L}} \sin\left(\frac{n\pi x}{3L}\right), \quad n = 2, 4, 6, \ldots$$

(a), cont'd...

The ground state corresponds to $n=1$, so our ground state wavefunction at $t=0$ is

$$\boxed{\psi^f_{ground} = \sqrt{\frac{2}{3L}} \cos\left(\frac{\pi x}{3L}\right)}$$

We know

$$k = \frac{\sqrt{2mE}}{\hbar},$$

but now

$$k = \frac{n\pi}{3L}.$$

So

$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{3L}$$

$$2mE = \frac{n^2\pi^2\hbar^2}{9L^2}$$

$$E = \frac{n^2\pi^2\hbar^2}{18mL^2}$$

are the eigenenergies at $t=0$. For the ground state,

$$\boxed{E^f_{ground} = \frac{\pi^2\hbar^2}{18mL^2}}.$$

(b)

The amplitude of the transition is given by

$$C = \int_{\text{all space}} \psi^{*f}_{\text{ground}} \cdot \psi^{i}_{\text{ground}} \, dx$$

$$= \int \left(\sqrt{\frac{2}{3L}} \cos\left(\frac{\pi x}{3L}\right)\right)\left(\sqrt{\frac{2}{L}} \cos\left(\frac{\pi x}{L}\right)\right) dx$$

$$= \frac{2}{L\sqrt{3}} \int \cos\left(\frac{\pi x}{3L}\right) \cos\left(\frac{\pi x}{L}\right) dx$$

$$= \frac{2}{L\sqrt{3}} \int \frac{1}{2}\left[\cos\left(\frac{\pi x}{3L} - \frac{\pi x}{L}\right) + \cos\left(\frac{\pi x}{3L} + \frac{\pi x}{L}\right)\right] dx$$

$$= \frac{1}{L\sqrt{3}} \int \left[\cos\left(-\frac{2\pi x}{3L}\right) + \cos\left(\frac{4\pi x}{3L}\right)\right] dx$$

$$= \frac{1}{L\sqrt{3}} \left[\int \cos\left(\frac{2\pi x}{3L}\right) dx + \int \cos\left(\frac{4\pi x}{3L}\right) dx\right]$$

$$= \frac{1}{L\sqrt{3}} \left[\frac{3L}{2\pi} \sin\left(\frac{2\pi x}{3L}\right) + \frac{3L}{4\pi} \sin\left(\frac{4\pi x}{3L}\right)\right]\Bigg|_{-L/2}^{L/2}$$

$$= \frac{\sqrt{3}}{2\pi}\left(\sin\left(\frac{\pi}{3}\right) + \sin\left(\frac{\pi}{3}\right)\right) + \frac{\sqrt{3}}{4\pi}\left(\sin\left(\frac{2\pi}{3}\right) + \sin\left(\frac{2\pi}{3}\right)\right)$$

$$= \frac{\sqrt{3}}{\pi}\left(\frac{\sqrt{3}}{2}\right) + \frac{\sqrt{3}}{2\pi}\left(\frac{\sqrt{3}}{2}\right)$$

$$= \frac{3}{2\pi} + \frac{3}{4\pi}$$

$$= \frac{9}{4\pi}$$

(b), cont'd...

The probability of finding the particle in the ground state immediately after the expansion is then

$$P = |C|^2$$

$$= \left(\frac{9}{4\pi}\right)^2$$

$$\boxed{P = \frac{81}{16\pi^2}} \approx 0.51$$

(c)

In general, we should have

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n e^{\frac{-iE_n^f t}{\hbar}} \psi_n^f(x),$$

where "f" signifies after the expansion. The coefficients are simply

$$c_n = \int_{-L/2}^{L/2} \psi_n^{*f} \cdot \psi_{ground}^{i} \, dx$$

$$= \int_{-L/2}^{L/2} \psi_n^{*f} \cdot \sqrt{\frac{2}{L}} \cos\left(\frac{\pi x}{L}\right) dx$$

where

$$\psi_n^f = \begin{cases} \sqrt{2/3L} \cos\left(\frac{n\pi x}{3L}\right), & n = 1,3,5,\ldots \\ \sqrt{2/3L} \sin\left(\frac{n\pi x}{3L}\right), & n = 2,4,6,\ldots \end{cases}$$

So

$$\boxed{\psi(x,t) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} \int_{-L/2}^{L/2} \psi_n^{*f} \cos\left(\frac{\pi x}{L}\right) e^{-iE_n^f t/\hbar} dx},$$

where

$$E_n^f = \frac{n^2 \pi^2 \hbar^2}{18 m L^2}.$$