

Homework 7 - Infinite Square Well

Question 1:

Consider a particle of mass m confined in a symmetric one-dimensional potential well. The initial state of the particle is given by the wave function

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

1. Find b .
2. What are the probabilities of measuring any of the five lowest energies of the system?
3. Calculate the mean value of the particles energy $\langle E \rangle$.
4. Find the state of the system at time t .

Solution:

1. Using the normalization condition $\langle \Psi | \Psi \rangle = 1$, we have

$$\begin{aligned} \langle \Psi(x, 0) | \Psi(x, 0) \rangle &= |b|^2 \left[\int_{-a/2}^0 \left(1 + \frac{2}{a}x\right)^2 dx + \int_0^{a/2} \left(1 - \frac{2}{a}x\right)^2 dx \right] \\ &= |b|^2 \left[\left(x + \frac{2}{a}x^2 + \frac{4}{3a^2}x^3\right) \Big|_{-a/2}^0 + \left(x - \frac{2}{a}x^2 + \frac{4}{3a^2}x^3\right) \Big|_0^{a/2} \right] \\ &= |b|^2 \left[-\left(-\frac{a}{2} + \frac{a}{2} - \frac{a}{6}\right) + \left(\frac{a}{2} - \frac{a}{2} + \frac{a}{6}\right) \right] \\ &= \frac{a}{3} |b|^2, \end{aligned}$$

hence

$$\boxed{|b| = \sqrt{\frac{3}{a}}}.$$

2. The eigenstates for an infinite well potential at $0 \leq x \leq a$ are

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi n x}{a}\right), \quad \text{with the associated energies } E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2},$$

and the general solution is of the form

$$\psi(x) = \sum_n c_n \psi_n(x),$$

and the probability to measure the E_n is $|c_n|^2$. Therefore, let us use this coordinate and write

$$\Psi(x, 0) = \sqrt{\frac{3}{a}} \begin{cases} \frac{2}{a}x, & 0 \leq x \leq \frac{a}{2}, \\ 2\left(1 - \frac{x}{a}\right), & \frac{a}{2} \leq x \leq a, \end{cases}$$

so that

$$c_n = \langle \psi_n | \Psi(x, 0) \rangle = \sqrt{\frac{2}{a}} \sqrt{\frac{3}{a}} \left[\int_0^{a/2} \frac{2}{a} x \sin\left(\frac{\pi n x}{a}\right) dx + \int_{a/2}^a 2\left(1 - \frac{x}{a}\right) \sin\left(\frac{\pi n x}{a}\right) dx \right].$$

The integrals are

$$\begin{aligned}
\int_0^{a/2} \frac{2}{a} x \sin\left(\frac{\pi n x}{a}\right) dx &= -\frac{2}{\pi n} \int_0^{a/2} x \frac{d}{dx} \left[\cos\left(\frac{\pi n x}{a}\right) \right] dx \\
&= -\frac{2}{\pi n} \left[x \cos\left(\frac{\pi n x}{a}\right) \right]_0^{a/2} + \frac{2}{\pi n} \int_0^{a/2} \cos\left(\frac{\pi n x}{a}\right) dx \\
&= -\frac{a}{\pi n} \cos\left(\frac{\pi n}{2}\right) + 2 \frac{a}{\pi^2 n^2} \sin\left(\frac{\pi n}{2}\right), \\
\int_{a/2}^a 2 \left(1 - \frac{x}{a}\right) \sin\left(\frac{\pi n x}{a}\right) dx &= 2 \int_{a/2}^a \sin\left(\frac{\pi n x}{a}\right) dx - \int_{a/2}^a \frac{2}{a} x \sin\left(\frac{\pi n x}{a}\right) dx \\
&= -2 \frac{a}{n\pi} \left(\cos(\pi n) - \cos\left(\frac{\pi n}{2}\right) \right) - \left(\frac{2}{\pi n} \left[-x \cos\left(\frac{\pi n x}{a}\right) \right]_{a/2}^a + \frac{2}{\pi n} \int_{a/2}^a \cos\left(\frac{\pi n x}{a}\right) dx \right) \\
&= -2 \frac{a}{n\pi} \left(\cos(\pi n) - \cos\left(\frac{\pi n}{2}\right) \right) - \left(\frac{2}{\pi n} \left[-a \cos(\pi n) + \frac{a}{2} \cos\left(\frac{\pi n}{2}\right) \right] - \frac{2a}{\pi^2 n^2} \sin\left(\frac{\pi n}{2}\right) \right) \\
&= \frac{a}{n\pi} \cos\left(\frac{\pi n}{2}\right) + \frac{2a}{\pi^2 n^2} \sin\left(\frac{\pi n}{2}\right),
\end{aligned}$$

therefore

$$c_n = \frac{4\sqrt{6}}{\pi^2 n^2} \sin\left(\frac{\pi n}{2}\right) \rightarrow \boxed{P(\langle E \rangle = E_n) = \frac{96}{(n^2 \pi^2)^2} \sin^2\left(\frac{n\pi}{2}\right)}.$$

In particular

$$\boxed{P_{2n} = 0 \quad \text{and} \quad P_{2n+1} = \frac{96}{(2n+1)^4 \pi^4}},$$

$$\begin{aligned}
P_0 &= P_2 = P_4 = 0, \\
P_1 &= \frac{96}{\pi^4} \approx 0.9855, \\
P_3 &= \frac{96}{81\pi^4} \approx 0.0122, \\
P_5 &= \frac{96}{625\pi^4} \approx 0.0016.
\end{aligned}$$

3. The mean value is simply

$$\begin{aligned}
\langle E \rangle &= \sum_n P_n E_n \\
&= \sum_n |\langle \psi_n | \Psi \rangle|^2 E_n \\
&= \sum_k \frac{96}{(2k+1)^4 \pi^4} \frac{\hbar^2 \pi^2 (2k+1)^2}{2ma^2} \\
&= \frac{48\hbar^2}{m\pi^2 a^2} \sum_k \frac{1}{(2k+1)^2},
\end{aligned}$$

hence

$$\boxed{\langle E \rangle = \frac{6\hbar^2}{ma^2}}.$$

4. At time t we have

$$\boxed{\Psi(x, t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar} = \sum_k \frac{8}{\pi^2 (2k+1)^2} \sqrt{\frac{3}{a}} \sin\left(\frac{\pi (2k+1)x}{a}\right) e^{-iE_{2k+1} t/\hbar}}.$$

Question 2:

Consider a particle of mass m confined in a symmetric one-dimensional potential well as in the previous question. The initial state of the particle is given by the wave function

$$\Psi(x, 0) = A(\varphi_1 - \varphi_2),$$

where φ_n are the eigenstates of the symmetric infinite well.

1. Find A .
2. Find the state of the system at time t .
3. Calculate the probability current density $J(x, t)$.
4. Calculate the mean value of the particles position $\langle x \rangle$ at time t .
5. Calculate the mean value of the particles momentum $\langle p \rangle$ at time t .

Solution:

1. Using normalization condition we find

$$\langle \Psi(x, 0) | \Psi(x, 0) \rangle = |A|^2 (\langle \varphi_1 | \varphi_1 \rangle - \langle \varphi_1 | \varphi_2 \rangle - \langle \varphi_2 | \varphi_1 \rangle + \langle \varphi_2 | \varphi_2 \rangle) = 2|A|^2 = 1,$$

hence

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

2. As before,

$$\Psi(x, t) = \sum c_n \varphi_n(x) e^{-iE_n t/\hbar}, \quad \text{where } E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2} \quad \text{and } \varphi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x + \frac{n\pi}{2}\right)$$

and

$$c_n = \langle \varphi_n | \Psi(x, 0) \rangle = \begin{cases} \frac{1}{\sqrt{2}}, & n = 1, \\ -\frac{1}{\sqrt{2}}, & n = 2. \end{cases}$$

Therefore

$$\Psi(x, t) = \frac{1}{\sqrt{2}} (\varphi_1 e^{-iE_1 t/\hbar} - \varphi_2 e^{-iE_2 t/\hbar}) = \frac{1}{\sqrt{a}} \left(\cos\left(\frac{\pi}{a}x\right) e^{-iE_1 t/\hbar} + \sin\left(\frac{2\pi}{a}x\right) e^{-iE_2 t/\hbar} \right).$$

3. Recalling that

$$J(x, t) = \frac{\hbar}{m} \text{Im} \left[\Psi^* \frac{\partial \Psi}{\partial x} \right],$$

where

$$\frac{\partial \Psi}{\partial x} = \frac{1}{\sqrt{2}} (\varphi_1' e^{-iE_1 t/\hbar} - \varphi_2' e^{-iE_2 t/\hbar}) = \frac{\pi}{a^{3/2}} \left(-\sin\left(\frac{\pi}{a}x\right) e^{-iE_1 t/\hbar} + 2 \cos\left(\frac{2\pi}{a}x\right) e^{-iE_2 t/\hbar} \right),$$

thus

$$\Psi^* \frac{\partial \Psi}{\partial x} = -\frac{i\pi}{a^2} \left[\sin\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi}{a}x\right) + 2 \cos\left(\frac{2\pi}{a}x\right) \cos\left(\frac{\pi}{a}x\right) \right] \sin\left(\frac{E_2 - E_1}{\hbar}t\right) + \text{real terms.}$$

$$J(x, t) = -\frac{\hbar\pi}{2ma^2} \left[3 \cos\left(\frac{\pi x}{a}\right) + \cos\left(\frac{3\pi x}{a}\right) \right] \sin\left(\frac{3\hbar\pi^2}{2ma^2}t\right),$$

where we used the fact that $E_2 - E_1 = \frac{3\hbar^2\pi^2}{2ma^2}$.

4. The mean value of the position is

$$\begin{aligned}
 \langle x \rangle &= \langle \Psi | \hat{x} \Psi \rangle \\
 &= \frac{1}{a} \int_{-a/2}^{a/2} \left(\cos\left(\frac{\pi}{a}x\right) e^{iE_1 t/\hbar} + \sin\left(\frac{2\pi}{a}x\right) e^{iE_2 t/\hbar} \right) x \left(\cos\left(\frac{\pi}{a}x\right) e^{-iE_1 t/\hbar} + \sin\left(\frac{2\pi}{a}x\right) e^{-iE_2 t/\hbar} \right) dx \\
 &= \frac{1}{a} \int_{-a/2}^{a/2} x \cos\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi}{a}x\right) \left(e^{i(E_2-E_1)t/\hbar} + e^{-i(E_2-E_1)t/\hbar} \right) dx \\
 &= \frac{1}{a} \cos\left(\frac{3\hbar\pi^2}{2ma^2}t\right) \int_{-a/2}^{a/2} x \left[\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{3\pi x}{a}\right) \right] dx,
 \end{aligned}$$

where we dropped all the odd terms in the integral. Using the integral

$$\int_{-a/2}^{a/2} x \sin\left(\frac{n\pi x}{a}\right) dx = \frac{a^2}{(n\pi)^2} \left[2 \sin\left(\frac{n\pi}{2}\right) - n\pi \cos\left(\frac{n\pi}{2}\right) \right],$$

we find

$$\boxed{\langle x \rangle = \frac{16a}{9\pi^2} \cos\left(\frac{3\hbar\pi^2}{2ma^2}t\right)}.$$

5. We can calculate $\langle p \rangle = \langle \Psi | \hat{p} \Psi \rangle$, but it is easier to invoke Ehrenfest theorem and use the previous result,

$$\boxed{\langle p \rangle = m \frac{d}{dt} \langle x \rangle = -\frac{8\hbar}{3a} \sin\left(\frac{3\hbar\pi^2}{2ma^2}t\right)}.$$

Question 3:

Consider a particle in an infinite square well of width a ,

1. Show that the wave function returns to its original form after a quantum revival time T and find what is its value. That is: $\Psi(x, t) = \Psi(x, t + T)$ for any state (not just a stationary state).
2. What is the classical revival time, for a particle of energy E bouncing back and forth between the walls?
3. For what energy are the two revival times equal?

Solution:

1. The general solution for a particle in an infinite square well is

$$\Psi(x, t) = \sum_n c_n \psi_n(x) e^{-i \frac{\hbar\pi^2 n^2}{2ma^2} t},$$

hence we must require

$$\frac{\hbar\pi^2 n^2}{2ma^2} T = 2\pi \times \underbrace{\text{integer}}_{n^2} \rightarrow \boxed{T = \frac{4ma^2}{\hbar\pi}}.$$

2. The classical revival time is the time it takes the particle to go the distance $2a$, thus

$$T_c = \frac{2a}{v},$$

where

$$v = \sqrt{\frac{2E}{m}} \rightarrow \boxed{T_c = a\sqrt{\frac{2m}{E}}}.$$

3. The two are the same if the energy of the particle equals

$$T_c = T \rightarrow \boxed{E = \frac{\hbar^2 \pi^2}{8ma^2} = \frac{E_1}{4}}.$$

Question 4:

Consider an infinite square well of width L , with a particle of mass m moving in it ($-L/2 < x < L/2$). At time $t = 0$, the state of the particle is described by the wave function

$$\psi(x) = A [3\varphi_1(x) + 4\varphi_2(x)].$$

1. Find $|A|$.
2. Find $\Psi(x, t)$.
3. We measure the particle's position at time t . What is the probability of finding the particle at the right half of the well?
4. Find $\langle x \rangle(t)$ and $\langle p \rangle(t)$. Notice that while these are periodic, they are very different from the classical results. Discuss the reasons for this difference.

Solution:

For the ease of calculations let us shift our coordinate to $x \rightarrow x + L/2$, where the solution for an infinite square well potential in $(0, L)$ is

$$\varphi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right), \quad \text{with } E_n = \frac{\pi^2 \hbar^2 n^2}{2mL^2}.$$

1. Using the normalization condition

$$\langle \psi | \psi \rangle = |A|^2 (9 + 16) = 1 \quad \rightarrow \quad \boxed{|A| = \frac{1}{5}}.$$

2. Since the only eigenstates in the initial state are $n = 1, 2$ we have

$$\boxed{\Psi(x, t) = \frac{3}{5}\varphi_1(x) e^{-iE_1 t/\hbar} + \frac{4}{5}\varphi_2(x) e^{-iE_2 t/\hbar}}.$$

3. The probability for finding the particle at $x \in (L/2, L)$ is

$$\begin{aligned} P\left(\frac{L}{2} < x < L\right) &= \int_{L/2}^L \Psi^* \Psi dx \\ &= \frac{1}{25} \int_{L/2}^L \left[9|\varphi_1|^2 + 12\varphi_2^* \varphi_1 e^{i(E_2 - E_1)t/\hbar} + 12\varphi_1^* \varphi_2 e^{-i(E_2 - E_1)t/\hbar} + 16|\varphi_2|^2 \right] dx \\ &= \frac{1}{25} \left[\frac{9}{2} - 12 \frac{4}{3\pi} \cos \omega t + \frac{16}{2} \right], \end{aligned}$$

$$\boxed{P\left(\frac{L}{2} < x < L\right) = \frac{1}{2} - \frac{16}{25\pi} \cos \omega t, \quad \text{with } \omega \equiv \frac{E_2 - E_1}{\hbar} = \frac{3\pi^2 \hbar^2}{2mL^2}},$$

where we used the integrals

$$\frac{2}{L} \int_{L/2}^L \sin^2\left(\frac{\pi x}{L}\right) dx = \frac{2}{L} \int_{L/2}^L \sin^2\left(\frac{2\pi x}{L}\right) dx = \frac{1}{2} \quad \text{and} \quad \frac{2}{L} \int_{L/2}^L \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi x}{L}\right) dx = -\frac{4}{3\pi}.$$

4. The expectation value of \hat{x} is

$$\begin{aligned} \langle x \rangle(t) &= \langle \Psi | \hat{x} \Psi \rangle = \left\langle \frac{3}{5}\varphi_1 e^{-iE_1 t/\hbar} + \frac{4}{5}\varphi_2 e^{-iE_2 t/\hbar} \middle| \hat{x} \left(\frac{3}{5}\varphi_1 e^{-iE_1 t/\hbar} + \frac{4}{5}\varphi_2 e^{-iE_2 t/\hbar} \right) \right\rangle \\ &= \frac{9}{25} \langle \varphi_1 | \hat{x} \varphi_1 \rangle + \frac{12}{25} e^{-i\omega t} \langle \varphi_1 | \hat{x} \varphi_2 \rangle + \frac{12}{25} e^{i\omega t} \langle \varphi_2 | \hat{x} \varphi_1 \rangle + \frac{16}{25} \langle \varphi_2 | \hat{x} \varphi_2 \rangle \end{aligned}$$

thus, let us first calculate

$$\begin{aligned}\langle \varphi_1 | \hat{x} \varphi_1 \rangle &= \int_0^L \varphi_1^* x \varphi_1 dx = \frac{L}{2}, \\ \langle \varphi_1 | \hat{x} \varphi_2 \rangle &= \int_0^L \varphi_1^* x \varphi_2 dx = -\frac{16L}{9\pi^2}, \\ \langle \varphi_2 | \hat{x} \varphi_2 \rangle &= \int_0^L \varphi_2^* x \varphi_2 dx = \frac{L}{2}.\end{aligned}$$

Plugging these into the expression for $\langle \hat{x} \rangle$ we get

$$\langle x \rangle (t) = \frac{9}{25} \frac{L}{2} - \frac{24}{25} \frac{16L}{9\pi^2} \cos \omega t + \frac{16}{25} \frac{L}{2} = L \left(\frac{1}{2} - \frac{128}{75\pi^2} \cos \omega t \right).$$

Using Ehrenfest theorem,

$$\langle p \rangle (t) = m \frac{d \langle x \rangle}{dt} = \frac{128}{75\pi^2} mL\omega \sin \omega t = \frac{64\hbar^2}{25L} \sin \omega t.$$