2 Infinite Well Motion and Quantum Tunneling

1/19: **1.** In class, we demonstrated that given a certain time-independent potential, one can find solutions to the Schrödinger equation such that

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_n(\vec{r}) + V(\vec{r})\psi_n(\vec{r}) = E_n\psi_n(\vec{r}) \tag{2.1}$$

Assume now that we are in one dimension, with the potential being a square well:

$$\begin{aligned} &V(x)\to\infty &&\text{for } x\le 0 \text{ and } x\ge a\\ &V(x)\to 0 &&\text{for } 0<x<a \end{aligned} \tag{2.2}$$

Show that in such a case, the solutions are given by

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \tag{2.3}$$

due to the fact that in order to get a finite mean energy value, the wave function must vanish at $x = 0, a$. The energy eigenstates are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{2.4}$$

The factor $\sqrt{2/a}$ comes from the requirement of a good normalized solution, i.e., one with $\langle\psi_n|\psi_n\rangle = 1$. Now, imagine that at $t = 0$, the particle is in the state

$$\psi(x,0) = \frac{A}{\sqrt{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right) \tag{2.5}$$

where A is a real constant.

a) Find the value of A such that $\psi(x,0)$ is normalized. (Hint: Use $\langle\psi_n|\psi_m\rangle = \delta_{nm}$.)

Answer. For $\psi(x,0)$ to be normalized, it must satisfy

$$\langle\psi(x,0)|\psi(x,0)\rangle = 1$$

Now recognize that $\psi(x,0)$ is of the form

$$\psi = c_1\psi_1 + c_3\psi_3 + c_5\psi_5$$

Thus, we have that

$$\begin{aligned} 1 &= \langle\psi|\psi\rangle\\ &= \langle c_1\psi_1 + c_3\psi_3 + c_5\psi_5|c_1\psi_1 + c_3\psi_3 + c_5\psi_5\rangle\\ &= \langle c_1\psi_1|c_1\psi_1\rangle + \langle c_3\psi_3|c_3\psi_3\rangle + \langle c_5\psi_5|c_5\psi_5\rangle + 2\underbrace{\langle c_1\psi_1|c_3\psi_3\rangle}_{0} + 2\underbrace{\langle c_1\psi_1|c_5\psi_5\rangle}_{0} + 2\underbrace{\langle c_3\psi_3|c_5\psi_5\rangle}_{0}\\ &= \langle c_1\psi_1|c_1\psi_1\rangle + \langle c_3\psi_3|c_3\psi_3\rangle + \langle c_5\psi_5|c_5\psi_5\rangle\\ &= \int_0^a \frac{A^2}{a}\sin^2\left(\frac{\pi x}{a}\right)\mathrm{d}x + \int_0^a \frac{3}{5a}\sin^2\left(\frac{3\pi x}{a}\right)\mathrm{d}x + \int_0^a \frac{1}{5a}\sin^2\left(\frac{5\pi x}{a}\right)\mathrm{d}x\\ &= \frac{A^2}{2} + \frac{3}{10} + \frac{1}{10}\\ &= \frac{5A^2+4}{10} \end{aligned}$$

$$\boxed{A = \sqrt{\frac{6}{5}}}$$

$\square$

b) If measurements of the energy are carried out, what are the values that will be found and what are the probabilities of measuring such energies? Calculate the average energy.

Answer. As mentioned above, $\psi(x,0)$ is of the form

$$\psi(x,0) = c_1\psi_1(x) + c_3\psi_3(x) + c_5\psi_5(x)$$

Thus, the energies that will be found are

$$\boxed{E_1 = \frac{\hbar^2\pi^2}{2ma^2} \qquad E_3 = \frac{3^2\hbar^2\pi^2}{2ma^2} \qquad E_5 = \frac{5^2\hbar^2\pi^2}{2ma^2}}$$

Moreover, the probabilities of measuring such energies are given by the integrals calculated in part (a). In other words, the probabilities P_i of measuring energy E_i are

$$\boxed{P_1 = \frac{6}{10} \qquad P_3 = \frac{3}{10} \qquad P_5 = \frac{1}{10}}$$

The average energy could be calculated by evaluating $\langle\psi|\hat{H}|\psi\rangle$, or by calculating

$$\langle E\rangle = E_1P_1 + E_3P_3 + E_5P_5$$

$$\boxed{\langle E\rangle = \frac{29\hbar^2\pi^2}{10ma^2}}$$

□

c) Find the expression of the wave function at a later time t. (Hint: What is $\psi_n(x,t)$?)

Answer. Taking the hint, we know that

$$\psi_n(x,t) = \psi_n(x)\mathrm{e}^{-iE_nt/\hbar} = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\mathrm{e}^{-iE_nt/\hbar}$$

We can rewrite $\psi(x,0)$ in a form relatable to the above as follows.

$$\begin{aligned}
\psi(x,0) &= \sqrt{\frac{6}{5a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right)\\
&= \sqrt{\frac{3}{5}}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{5\pi x}{a}\right)\\
&= \sqrt{\frac{3}{5}}\psi_1(x,0) + \sqrt{\frac{3}{10}}\psi_3(x,0) + \frac{1}{\sqrt{10}}\psi_5(x,0)
\end{aligned}$$

Therefore,

$$\begin{aligned}
\psi(x,t) &= \sqrt{\frac{3}{5}}\psi_1(x,t) + \sqrt{\frac{3}{10}}\psi_3(x,t) + \frac{1}{\sqrt{10}}\psi_5(x,t)\\
&= \sqrt{\frac{3}{5}}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\mathrm{e}^{-iE_1t/\hbar} + \sqrt{\frac{3}{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right)\mathrm{e}^{-iE_3t/\hbar}\\
&\quad + \frac{1}{\sqrt{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{5\pi x}{a}\right)\mathrm{e}^{-iE_5t/\hbar}
\end{aligned}$$

$$\boxed{\psi(x,t) = \sqrt{\frac{6}{5a}}\sin\left(\frac{\pi x}{a}\right)\mathrm{e}^{-iE_1t/\hbar} + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right)\mathrm{e}^{-iE_3t/\hbar} + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right)\mathrm{e}^{-iE_5t/\hbar}}$$

□

d) Is the mean value of the position operator independent of time? What about the mean value of the momentum? (Hint: Use symmetry properties with respect to the central point of the well.)

Answer. To determine whether or not the position operator is independent of time, it will suffice to evaluate

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\langle\psi(x,t)|\hat{\vec{x}}|\psi(x,t)\rangle\Big)$$

If the above expression is equal to zero, then the position operator is independent of time, and if it is not equal to zero, then the position operator is not independent of time. Let's begin.
We have that

$$\begin{aligned}
&\langle\psi(x,t)|\hat{\vec{x}}|\psi(x,t)\rangle \\
&= \left\langle \frac{3}{5}\psi_1 \mathrm{e}^{-iE_1t/\hbar} + \frac{3}{10}\psi_3 \mathrm{e}^{-iE_3t/\hbar} + \frac{1}{10}\psi_5 \mathrm{e}^{-iE_5t/\hbar} \middle| \hat{\vec{x}} \middle| \frac{3}{5}\psi_1 \mathrm{e}^{-iE_1t/\hbar} + \frac{3}{10}\psi_3 \mathrm{e}^{-iE_3t/\hbar} + \frac{1}{10}\psi_5 \mathrm{e}^{-iE_5t/\hbar} \right\rangle \\
&= \frac{9}{25}\mathrm{e}^{-2iE_1t/\hbar}\langle\psi_1|\hat{\vec{x}}|\psi_1\rangle + \frac{9}{100}\mathrm{e}^{-2iE_3t/\hbar}\langle\psi_3|\hat{\vec{x}}|\psi_3\rangle + \frac{1}{100}\mathrm{e}^{-2iE_5t/\hbar}\langle\psi_5|\hat{\vec{x}}|\psi_5\rangle \\
&\quad + \frac{9}{50}\mathrm{e}^{-i(E_1+E_3)t/\hbar}\langle\psi_1|\hat{\vec{x}}|\psi_3\rangle + \frac{3}{50}\mathrm{e}^{-i(E_1+E_5)t/\hbar}\langle\psi_1|\hat{\vec{x}}|\psi_5\rangle + \frac{3}{100}\mathrm{e}^{-i(E_3+E_5)t/\hbar}\langle\psi_3|\hat{\vec{x}}|\psi_5\rangle
\end{aligned}$$

Now, computing integrals, we have the following.

$$\langle\psi_1|\hat{\vec{x}}|\psi_3\rangle = \langle\psi_1|\hat{\vec{x}}|\psi_5\rangle = \langle\psi_3|\hat{\vec{x}}|\psi_5\rangle = 0$$

One easy way to see this without direct computation is to observe, per the hint, that $(x-0.5a)\psi_1\psi_3$ and $0.5a\psi_1\psi_3$ are both odd about the central point of the well and hence evaluate to zero. Thus,

$$\langle\psi_1|\hat{\vec{x}}|\psi_3\rangle = \int_0^a x\psi_1\psi_3\,\mathrm{d}x = \int_0^a (x-0.5a)\psi_1\psi_3\,\mathrm{d}x + \int_0^a 0.5a\psi_1\psi_3\,\mathrm{d}x = 0+0=0$$

On the other hand, we may observe that $x\psi_i^2$ $(i=1,3,5)$ are all strictly positive on $(0,a)$ and hence evaluate to positive constants c_i. Consequently,

$$\langle\psi(x,t)|\hat{\vec{x}}|\psi(x,t)\rangle = \frac{9}{25}c_1\mathrm{e}^{-2iE_1t/\hbar} + \frac{9}{100}c_3\mathrm{e}^{-2iE_3t/\hbar} + \frac{1}{100}c_5\mathrm{e}^{-2iE_5t/\hbar}$$

This function clearly has a nonzero derivative with respect to time, meaning that the mean value of the position operator $\boxed{\text{is not}}$ independent of time.
As to the second part of the question, we have that

$$\frac{\mathrm{d}\langle\hat{\vec{p}}\rangle}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(m\frac{\mathrm{d}\langle\hat{\vec{x}}\rangle}{\mathrm{d}t}\right) \neq 0$$

Therefore, the mean value of the momentum operator $\boxed{\text{is not}}$ independent of time, either. □

e) Would the result of part (d) be different if we replaced ψ_3 by ψ_2 in Eq. 2.5?

Answer. If we replaced ψ_3 by ψ_2, then we would additionally have

$$\langle\psi_1|\hat{\vec{x}}|\psi_2\rangle \neq 0 \qquad\qquad \langle\psi_2|\hat{\vec{x}}|\psi_5\rangle \neq 0$$

However, $\boxed{\text{this would change neither result overall.}}$ □

2. a) Consider now the wave function $\Psi(x,t)$ of a particle moving in one dimension in a potential $V(x)$ such that

$$\begin{aligned} &V(x) \to \infty && \text{for } |x| \geq a/2 \\ &V(x) = 0 && \text{for } -a/2 < x < 0 \\ &V(x) = V_0 && \text{for } 0 \leq x < a/2 \end{aligned} \tag{2.6}$$

Considering that the wave function and its derivative are continuous at $x = 0$, and that the wave function vanishes at $x = \pm a/2$, try to find the equation that gives the possible energy states assuming $E_n > V_0$.

Hint: There are different combinations of sine and cosine functions for positive and negative values of x.

Answer. Taking the hint, split the total wave function $\psi(x)$ into the sum of two parts, $\psi_1(x)$ and $\psi_2(x)$, where $\psi_1(x) = 0$ for $x \geq 0$ and $\psi_2(x) = 0$ for $x \leq 0$. In general, we have

$$\psi_1(x) = A\sin(kx) + B\cos(kx) \qquad\qquad \psi_2(x) = C\sin(k_2x) + D\cos(k_2x)$$

If $\psi = \psi_1 + \psi_2$ is to be continuous at $x = 0$, then we must have

$$\begin{aligned} \psi_1(0) &= \psi_2(0) \\ B &= D \end{aligned}$$

If $\psi = \psi_1 + \psi_2$ is to have a continuous first derivative at $x = 0$, then we must have

$$\begin{aligned} \psi_1'(0) &= \psi_2'(0) \\ kA &= k_2C \end{aligned}$$

Thus, altogether, we have that

$$\psi(x) = \begin{cases} A\sin(kx) + B\cos(kx) & x \leq 0 \\ \frac{kA}{k_2}\sin(k_2x) + B\cos(k_2x) & x > 0 \end{cases} \qquad \text{for } |x| \leq a/2$$

The boundary condition is met when either...

i. $B = 0$, $k = n\pi$, and $k_2 = m\pi/a$;
ii. $A = 0$, $k = n\pi/2$, and $k_2 = m\pi/2a$.

$\square$