Quantum Mechanics I - Session 9

May 25, 2015

1 Infinite potential well

In class, you discussed the infinite potential well, i.e.

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{else} \end{cases} \tag{1}$$

You found the permitted energies are discrete:

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

and you found the corresponding wave functions:

$$\phi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} sin(\frac{n\pi x}{L}) & \text{if } 0 < x < L \\ 0 & \text{else} \end{cases} \tag{3}$$

1.1 time evolution

Each of the states $|\phi_n\rangle$ describes a stationary state, which leads to time-independent physical predictions. Time evolution appears only when the state vector is a linear combination of several kets $|\phi_n\rangle$. We shall consider here the situation where at $t = 0$ the state vector is:

$$|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}[|\phi_1\rangle + |\phi_2\rangle] \tag{4}$$

Since $|\phi_1\rangle, |\phi_2\rangle$ are energy eigen-states, the state at $t > 0$ will be:

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}[e^{-i\frac{\pi^2\hbar}{2mL^2}t} |\phi_1\rangle + e^{-2i\frac{\pi^2\hbar}{mL^2}t} |\phi_2\rangle] \tag{5}$$

we can omit the global phase and re-write this as:

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}[|\phi_1\rangle + e^{-i\omega_{12}t} |\phi_2\rangle] \tag{6}$$

where:

$$\omega_{12} = \frac{E_2 - E_1}{\hbar} = \frac{3\pi^2\hbar}{2mL^2} \tag{7}$$

The shape of the wave packet is given by the probability density:

$$|\psi(x,t)|^2 = \frac{1}{2}\phi_1(x)^2 + \frac{1}{2}\phi_2(x)^2 + \phi_1(x)\phi_2(x)cos(\omega_{12}t) \tag{8}$$

We see that the time variation of the probability density is due to the interference term in $\phi_1\phi_2$. The typical time it takes the probability density to travel from left to right and back again is of order $T = \frac{2\pi}{\omega_{12}}$.

Let us calculate the mean position of the particle at time t: $\langle X(t)\rangle$. It is convenient to define: $X' = X - \frac{L}{2}$. since the diagonal matrix elements of X' are zero:

$$\begin{aligned} \langle\phi_1| X' |\phi_1\rangle &\propto \int_0^L (x - \frac{L}{2}) sin^2(\pi x/L) dx = 0 \\ \langle\phi_2| X' |\phi_2\rangle &\propto \int_0^L (x - \frac{L}{2}) sin^2(2\pi x/L) dx = 0 \end{aligned} \tag{9}$$

We are left with:

$$\begin{aligned} \langle X'(t)\rangle &= Re\{e^{-i\omega_{12}t} \langle\phi_1| X' |\phi_2\rangle\} = Re\{e^{-i\omega_{12}t}[\langle\phi_1| X |\phi_2\rangle - \frac{L}{2}\langle\phi_1|\phi_2\rangle]\} \\ &= Re\{e^{-i\omega_{12}t}\frac{2}{L}\int_0^L x sin(\frac{\pi x}{L}) sin(\frac{2\pi x}{L}) dx\} = -cos(\omega_{12}t)\frac{16L}{9\pi^2} \end{aligned} \tag{10}$$

From which it follows that:

$$\langle X(t)\rangle = -\frac{16L}{9\pi^2}cos(\omega_{12}t) + \frac{L}{2} \tag{11}$$

The position changes from 0 to L as a cosine function with a period $T = \frac{2\pi}{\omega_{12}}$. compare this to the classical case, where inside the range $[0, L]$ the potential is constant and therefore there is no force and we expect the particle's speed to be constant and the particle to be bouncing between 0 and L with a linear dependence of $\langle X(t)\rangle$ on t within each segment. The center of the quantum wave packet, instead of turning back at the walls of the well, executes a movement of smaller amplitude and retraces its steps before reaching the regions where the potential is not zero. The physical explanation of this phenomenon is that before the center of the wave packet has touched the wall, the action of the potential on the "edges" of this packet is sufficient to make it turn back.

1.2 Perturbation caused by a position measurement

Consider a particle in the state $|\phi_1\rangle$. Assume its position is measured at $t = 0$ and found to be $\frac{L}{2}$.What are the probabilities of the different results that can be obtained in a measurement of the energy, performed immediately after this first measurement? One must beware of the following false argument: after the measurement, the particle is in the eigenstate of X corresponding to the result found, and its wave function is therefore proportional to $\delta(x - \frac{L}{2})$;

if a measurement of the energy is then performed, the various values E_n can be found, with probabilities proportional to:

$$|\int_0^L dx\delta(x-\frac{L}{2})\phi_n^*(x)|^2 = |\phi_n(\frac{L}{2})|^2 = \begin{cases} \frac{2}{L} & \text{if n is odd} \\ 0 & \text{if n is even} \end{cases} \tag{12}$$

Using this incorrect argument, one would find the probabilities of all values of E_n corresponding to odd n to be equal. This is absurd, since the sum of these probabilities would then be infinite. This error results from the fact that we have not taken the norm of the wave function into account. It is necessary to write the wave function as normalized just after the first measurement. However it is not possible to normalize the function $\delta(x-\frac{L}{2})$. The problem posed above must be stated more precisely. An experiment in which the measurement of an observable with a continuous spectrum is performed never yields any result with complete accuracy. For the case with which we are concerned, we can only say that:

$$\frac{L}{2}-\frac{\epsilon}{2} < x < \frac{L}{2}+\frac{\epsilon}{2} \tag{13}$$

If we assume ϵ to be much smaller than the extension of the wave function before the measurement (here L), the wave function after the measurement will be practically: $\sqrt{\epsilon}\delta^{(\epsilon)}(x-\frac{L}{2})$ where $\delta^{(\epsilon)}(x)$ is equal to $1/\epsilon$ for $-\epsilon/2 < x < \epsilon/2$ and zero otherwise. Now if the energy is measured, each E_n can be found with a probability:

$$P(E=E_n) = |\int_0^L dx\sqrt{\epsilon}\delta^\epsilon(x-\frac{L}{2})\phi_n^*(x)|^2 = \begin{cases} \frac{8L}{\epsilon}\left(\frac{1}{n\pi}\right)^2 sin^2\left(\frac{n\pi\epsilon}{2L}\right) & \text{if n is odd} \\ 0 & \text{if n is even} \end{cases} \tag{14}$$

However small ϵ may be, the distribution depends strongly on ϵ. The smaller ϵ is the more the distribution extends to larger energies. The interpretation of this result is the following: according to the uncertainty relations if one measures the position of the particle with great accuracy, one drastically changes its momentum. Thus kinetic energy is transferred to the particle, the amount of which is increasing as ϵ decreases.

2 Half-infinite potential well

Consider a bound particle of mass m in a potential:

$$V(x) = \begin{cases} \infty & \text{if } x<0 \\ -V_0 & \text{if } 0<x<L \\ 0 & \text{if } x>L \end{cases} \tag{15}$$

where $V_0 > 0$. We aim to find the energy levels and corresponding wave functions for this potential. This problem is of particular interest as it can be a zeroth order approximation for many real life potentials, such as the effective two body Coulomb potential or the Van der Waals potential that keeps molecules bound.

The solutions of the Schroedinger equation in the different ranges are:

$$\psi(x) = \begin{cases} Ae^{k_1 x} + Be^{-k_1 x} & x > L \\ De^{ik_2 x} + Ee^{-ik_2 x} & 0 < x < L \\ 0 & x < 0 \end{cases} \tag{16}$$

where $k_1 = \sqrt{-\frac{2mE}{\hbar^2}}$ and $k_2 = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$. Requiring that $\psi(x)$ is continuous at $x = 0$ we get:

$$D + E = 0 \rightarrow D = -E \tag{17}$$

In addition, we know that $A = 0$ otherwise the probability will be un-normalizable and the state unphysical since most of the probability is to find the particle outside the well. Now, requiring that $\psi(x)$ and its first derivative are continuous at $x = L$ we get:

$$Be^{-k_1 L} = De^{ik_2 L} - De^{-ik_2 L} \tag{18}$$

and:

$$-k_1 Be^{-k_1 L} = ik_2 De^{ik_2 L} + ik_2 De^{-ik_2 L} \tag{19}$$

Solving Eq. 18 yiels: $B = 2iD\sin(k_2 L)e^{k_1 L}$. Plugging this result back into Eq. 19:

$$cot(k_2 L) = -\frac{k_1}{k_2}. \tag{20}$$

Since both k_1 and k_2 depend on energy, this is an equation for the allowed energies in the system. This equation cannot be solved explicitly and instead has to be solved graphically or numerically. To obtain a simpler expression, we notice that:

$$k_1^2 = -\frac{2mE}{\hbar^2} \rightarrow E = -\frac{\hbar^2 k_1^2}{2m} \tag{21}$$

and plugging to k_2:

$$k_2^2 = -k_1^2 + \frac{2mV_0}{\hbar^2} \rightarrow k_1 = \sqrt{-k_2^2 + \frac{2mV_0}{\hbar^2}} \tag{22}$$

Returning to Eq. 19 and multiplying by L we have:

$$k_2 Lcot(k_2 L) = -\sqrt{-k_2^2 + \frac{2mV_0}{\hbar^2}}L = -\sqrt{-k_2^2 L^2 + \frac{2mV_0 L^2}{\hbar^2}} \tag{23}$$

We define a dimensionless parameter $z = k_2 L$ and a dimensionless constant: $\alpha = (\frac{2mV_0 L^2}{\hbar^2})^{1/2}$. We can now re-write the equation above as:

$$zcot(z) = -\sqrt{-z^2 + \alpha^2} \tag{24}$$

The number of solutions to this equation depends on the value of α. To have at least one solution the term in the square root should be larger than zero:

$$\alpha^2 > z^2 \rightarrow E < 0 \tag{25}$$

As α increases there are more and more solutions. For $\alpha \to \infty$ the energy equation simplifies to:

$$(zcot(z))^{-1} = 0 \to z = \pi n \to \sqrt{\frac{2m(E+V_0)L^2}{\hbar^2}} = \pi n \tag{26}$$

For large n this yields:

$$E = -V_0 + \frac{\hbar^2 \pi^2 n^2}{2m\hbar^2} \tag{27}$$

as familiar from the solution for the infinite square well.

Normalizing the wave function gives us:

$$1 = \int_0^\infty |\psi|^2 dx = 4|D|^2 (\frac{L}{2} - \frac{\sin(2k_2L)}{4k_2}) + |B|^2 \frac{e^{-2k_1L}}{2k_1} = 4|D|^2 (\frac{L}{2} - \frac{\sin(2k_2L)}{4k_2} + \frac{\sin^2(k_2L)}{2k_1}) \tag{28}$$

Leading to:

$$|D| = \frac{1}{\sqrt{2L - \frac{\sin(2k_2L)}{k_2} + \frac{2\sin^2(k_2L)}{k_1}}} \tag{29}$$