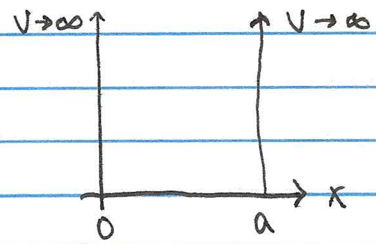
prop 1

Lecture 14 Physics 342

Welcome to more quantum mechanics! On Monday, we had began our study of the infinite square well for which its potential is:



or $V(x) = \begin{cases} 0, & 0<x<a \\ \infty, & \text{else} \end{cases}$

We found the energy eigenstates of the ∞-□ well to be indexed by a natural number $n \in \mathbb{N}$:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a},$$ with corresponding energy eigenvalues of:

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}.$$ Note that n is at least 1, so the energy of the particle is always non-zero. Because the potential energy in the ~~b~~ box is 0, this means that the particle must have a non-zero kinetic energy. Quantum mechanically, the particle must be moving, while classically, of course, such a "ball in a box" could just sit there at rest. This minimal energy that a quantum mechanical particle can have is often called the "zero-point" energy. In this lecture we will explore other strange properties of these eigenstates.

We'll focus our discussion in this lecture around interpreting these eigenstates through the Heisenberg uncertainty relation:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}.$$

To calculate the standard deviations/variances, we first need to calculate the expectation values of $\hat{x}$ and $\hat{p}$ operators on the energy eigenstates. This is actually trivial. For the expectation value of $\hat{x}$; we have

$$\langle \psi_n | \hat{x} | \psi_n \rangle = \int_0^a dx \, \frac{2}{a} \sin^2 \frac{n\pi x}{a} \cdot x$$

The function $\sin^2 \frac{n\pi x}{a}$ is symmetric in the well about $a/2$. That is, we can replace $x \to a - x$, and the integral is identical:

$$y = a - x, \, x = a - y \Rightarrow \int_0^a dy \, \frac{2}{a} \sin^2 \frac{n\pi (a-y)}{a} (a-y)$$

$$= \int_0^a dy \, \frac{2}{a} \sin^2 \frac{n\pi y}{a} \left(a - y\right) = a - \langle \hat{x} \rangle .$$

If this is to equal $\langle \hat{x} \rangle$, then we must have that $\langle \hat{x} \rangle = a/2$, the center of the well.

This result is natural when we consider $\langle \hat{p} \rangle$. In constructing the energy eigenvalues, we had noted that an energy eigenvalue corresponds to a fixed magnitude of momentum. There is no preference for moving right or left in the well, so the momentum p and its opposite $-p$ occure with the <u>same</u> probability in an energy eigenstate. If a particle moves right just as much as left, its average net motion is 0, and so $\langle \hat{p} \rangle = 0$, in an energy eigenstate.

The more nontrivial things to calculate are the second moments $\langle \hat{x}^2 \rangle$ and $\langle \hat{p}^2 \rangle$. For the second moment of position, we must calculate the integral:

$$\langle \hat{x}^2 \rangle = \int_0^a dx\, x^2 \frac{2}{a} \sin^2 \frac{n\pi x}{a}$$

This can be done by integration by parts, which I won't do here. The answer is:

$$\langle \hat{x}^2 \rangle = \frac{a^2}{6}\left(2 - \frac{3}{n^2\pi^2}\right)$$

For the second moment of momentum $\langle \hat{p}^2 \rangle$, we can use a trick. We want to calculate:

$$\langle \hat{p}^2 \rangle = \int_0^a dx\, \psi_n(x)\, \hat{p}^2\, \psi_n(x),$$

but the Schrödinger equation states that:

$$\hat{H}\psi_n = \frac{\hat{p}^2}{2m}\psi_n = E_n\psi_n, \text{ or that } \hat{p}^2\psi_n = 2mE_n\psi_n = \frac{n^2\pi^2\hbar^2}{a^2}\psi_n.$$

So, the second moment of $\hat{p}$ on an energy eigenstate is:

$$\langle \hat{p}^2 \rangle = \int_0^a dx\, \psi_n(x)\, \hat{p}^2\, \psi_n(x) = \int_0^a dx\, \psi_n(x)\, \frac{n^2\pi^2\hbar^2}{a^2}\psi_n(x)$$

$$= \frac{n^2\pi^2\hbar^2}{a^2}, \text{ because } \langle \psi_n | \psi_n \rangle = 1.$$

With these results then, the variances of position and momentum are:

$$\sigma_x^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2 = a^2\left(\frac{1}{12} - \frac{1}{2n^2\pi^2}\right)$$

$$\sigma_p^2 = \langle \hat{p}^2 \rangle = \frac{n^2\pi^2\hbar^2}{a^2}.$$

Now, the uncertainty relation of these quantities is:

$$\sigma_x^2 \sigma_p^2 = \frac{n^2\pi^2\hbar^2}{12} - \frac{\hbar^2}{2} = \frac{\hbar^2}{4}\left(\frac{n^2\pi^2}{3} - 2\right)$$

Note that $n^2\pi^2/3 - 2$ is positive for all $n \in \mathbb{N}$, and so we see that the Heisenberg uncertainty relation indeed holds:

$$\sigma_x^2 \sigma_p^2 \geq \frac{\hbar^2}{4}.$$

Indeed, this multiplicative factor, $\frac{n^2\pi^2}{3} - 2$, is minimized when $n=1$. In that case, we find:

$$\frac{\pi^2}{3} - 2 = 1.289868\ldots$$

One way to interpret the $n=1$ energy eigenstate is as the most "quantum" of the states of the infinite square well: it gets as close as it can in the well to saturating the Heisenberg uncertainty principle.

The opposite limit is also interesting. As $n \to \infty$, the product of variances becomes:

$$\sigma_x^2 \sigma_p^2 \to \frac{\hbar^2 n^2 \pi^2}{12} = \frac{ma^2}{6} E_n$$

Recall that m and a are just some constants for a given particle and well; only E_n here is changing. The Heisenberg uncertainty relation in this $n \to \infty$ limit is then:

$$\sigma_x^2 \sigma_p^2 = \frac{ma^2}{6} E_n \geq \frac{\hbar^2}{4} \quad \text{or} \quad E_n \geq \frac{3}{2}\frac{\hbar^2}{ma^2}.$$

For large n, $E_n \to \infty$, so this relation is trivially satisfied.

In fact, for large energies and small $\hbar$, this is nothing more than stating that $E \geq 0$, which must be true because the particle only has kinetic energy.

Let's belabor this point a bit and attempt to understand what this $E \to \infty$ ($\hbar \to 0$) limit means. To do this, let's figure out what the classical probability distributions for a particle in a box would be. Classically, an "infinite square well" just means a box with pefectly elastic walls: a ball hits the wall and only its direction of velocity is changed, not its magnitude. So, this pefect elastivity means that such a ball has a fixed magnitude of momentum, exactly as it did in the quantum case. So, if a ball has momentum magnitude $|p_0| > 0$ in the box, if you wait long enough, it will have bounced back and forth many times. Between each hit of the wall, it is traveling at constant speed, so its probability distribution of position is uniform over the box. That is, you are equally likely to find the ball anywhere in the box when you open it.

These data are sufficient to define the classical probability distributions of position and momentum, $p(x), p(p)$. Uniform in x means that $p(x)$ is independent of x and must integrate to 1 over the box:

$$1 = \int_0^a dx\, p(x) = p(x) \int_0^a dx = a\, p(x) \Rightarrow p(x) = \frac{1}{a}.$$

For the momentum distribution, there is only non-zero probability at p_0 or $-p_0$; every other value of momentum has 0 probability. Further, the probability of finding the ball going left or right is equal: leftness and rightness are not special. So, we can express the probability distribution of momentum with δ-functions:

$$\rho(p) = \frac{1}{2}\delta(p-p_0) + \frac{1}{2}\delta(p+p_0).$$

Recall that $\delta(x) = 0$ if $x \neq 0$. So, $\rho(p) = 0$ for $p \neq p_0$ or $-p_0$. ~~Additional~~ Additionally, note that the coefficients of the δ-functions are both 1/2, reflecting their equal probability. Finally, this distribution is normalized:

$$\int_{-\infty}^{\infty} dp \left[\frac{1}{2}\delta(p-p_0) + \frac{1}{2}\delta(p+p_0)\right] = \frac{1}{2} + \frac{1}{2} = 1,$$

as

$$\int_{-\infty}^{\infty} dx\, \delta(x) = 1.$$

So, with these classical distributions, we can then calculate their variances. For position, we have:

$$\langle x \rangle_{class} = \int_0^a dx\, \frac{x}{a} = \frac{a}{2}, \quad \langle x^2 \rangle_{class} = \int_0^a dx\, \frac{x^2}{a} = \frac{a^2}{3},$$

so that $\sigma^2_{x,class} = \langle x^2 \rangle_{class} - \langle x \rangle^2_{class} = \frac{a^2}{3} - \frac{a^2}{4} = \frac{a^2}{12}.$

For momentum, we have:

$$\langle p \rangle_{class} = \int_{-\infty}^{\infty} dp\, \frac{p}{2}\left[\delta(p-p_0) + \delta(p+p_0)\right] = \frac{p_0 - p_0}{2} = 0$$

and: $\langle p^2 \rangle_{class} = \int_{-\infty}^{\infty} dp\, \frac{p^2}{2} \left[\delta(p-p_0) + \delta(p+p_0) \right] = p_0^2.$

So, the classical variance in momentum is:

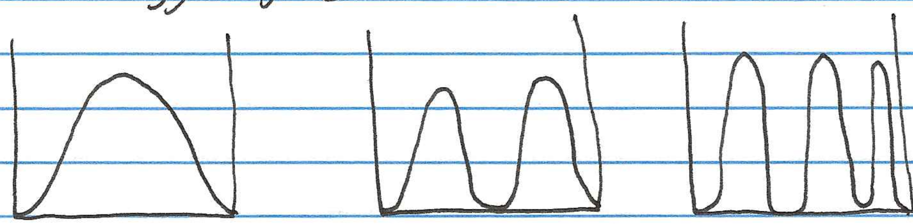
$$\sigma^2_{p,class} = \langle p^2 \rangle_{class} - \langle p \rangle^2_{class} = p_0^2.$$

Now, the product of these classical variances are:

$$\sigma^2_{x,class}\, \sigma^2_{p,class} = \frac{a^2}{12} \cdot p_0^2 = \frac{a^2 m}{6} \frac{p_0^2}{2m} = \frac{ma^2}{6} E,$$

where we identify the particle's energy as $E = \frac{p_0^2}{2m}$. If you recall, this is exactly the same relationship we found quantum mechanically, as $n \to \infty$! Precisely, then, for large quantum mechanical energies/high-n states, their properties correspond to classical states. This "correspondence principle" is one of the mysteries of quantum mechanics but must be true if the universe, all of it, is fundamentally quantum mechanical.

Another, graphical way, to think ~~a~~ about this is as follows: let's draw the absolute square of a few energy eigenstates:



$n=1$ $\quad$ $n=2$ $\quad$ $n=3$ $\quad$ ...

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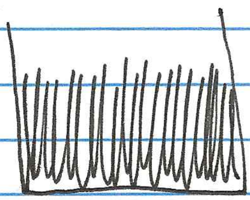

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$n=100$

as n increases, the probability oscillates more and more rapidly over smaller and smaller distances. for the n^{th} state, there are n humps in $\psi_n^* \psi_n$ over the well. Over any small distance Δx, we can calculate the probability that the particle lies between x and $x + \Delta x$. We have:

$$p_n(x, x+\Delta x) = \int_x^{x+\Delta x} dx \, \frac{2}{a} \sin^2 \frac{n\pi x}{a}$$

$$= \frac{\Delta x}{a} + \frac{\sin \frac{2\pi n x}{a} - \sin \frac{2\pi n (x+\Delta x)}{a}}{2n\pi}.$$

Let's take the $n \to \infty$ limit now. The sin factors vanish, as they are never larger than ± 1 individually. Thus, we have:

$$\lim_{n\to\infty} p_n(x, x+\Delta x) = \frac{\Delta x}{a}.$$

This just corresponds to a probability distribution for position of $\frac{1}{a}$, exactly as we identified classically. That is, fast oscillations average out: as $n \to \infty$, we can just take the average of $\sin^2$:

$$\lim_{n\to\infty} p_n(x) = \lim_{n\to\infty} \frac{2}{a} \underbrace{\sin^2 \frac{n\pi x}{a}}_{\text{averages to } 1/2} = \frac{1}{a}.$$

So, another way to state the correspondence principle is that at high energies, quantum fluctuations average out to classical behavior.

More on Friday...