6.4: Expectation Values, Observables, and Uncertainty

An electron is trapped in a one-dimensional infinite potential well of length L. Find the expectation values of the electron's position and momentum in the ground state of this well. Show that the uncertainties in these values do not violate the uncertainty principle.

Imagine an electron was trapped in the well described above and we repeatedly measured its location in the well. Due to the wave nature of the electron, we would get different values for these positions but, after many measurements, we could average these values to determine the expectation value of the electron's position.

You may be tempted to just refer to this as the average value of the electron's position, but if you take the wave-like nature of the electron seriously, and you should, the electron does not have a position until it is measured, so it is senseless to refer to the average value of something that doesn't even exist! What you are averaging is your measurements of the electron's position, not its pre-existing position. To avoid this metaphysical conundrum, we will call the value that we most likely expect to measure the expectation value of the variable.

The expectation value of the position (given by the symbol <x>) can be determined by a simple weighted average of the product of the probability of finding the electron at a certain position and the position, or

$$<x>=\int_0^L x\,\mathrm{Prob}(x)dx \tag{6.4.1}$$

$$<x>=\int_0^L (\Psi(x))x(\Psi(x))dx \tag{6.4.2}$$

What may strike you as somewhat strange is why I placed the factor of x between the two factors of the wavefunction. Mathematically, it doesn't matter where I place the x, but it turns out that for other variables the placement of the variable of interest must be "between" the two wavefunctions. Before we explore why this is the case, let's finish the calculation.

$$<x>=\int_0^L \left(\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\right)x\left(\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\right)dx \tag{6.4.3}$$

$$<x>=\frac{2}{L}\int_0^L x\sin^2\left(\frac{\pi x}{L}\right)dx$$

This integral begs for a u-substitution of:

$$u=\frac{\pi x}{L} \tag{6.4.4}$$

$$<x>=\frac{2}{L}\int_0^\pi \left(\frac{2}{L}u\right)\sin^2(u)\left(\frac{L}{\pi}du\right) \tag{6.4.5}$$

$$<x>=\frac{2L}{\pi^2}\int_0^\pi u\sin^2(u)du$$

$$<x>=\frac{2L}{\pi^2}\frac{\pi^2}{4}$$

$$<x>=\frac{L}{2}$$

I'll agree that this seems like a stupid amount of work just to determine that the expectation value of a particle's position in an infinite well is in the center of the well, but it's always nice when learning a new mathematical technique to apply it to a situation in which you know the answer.

Now let's move on to the expectation value of the electron's momentum. You should be tempted to write:

$$<p>=\int_0^L (\Psi(x))p(\Psi(x))dx \tag{6.4.6}$$

The only problem with this, of course, is that we have to express the momentum of the electron in terms of its position in order to do the integral. How can we do that? Well, the momentum of the electron is related (by DeBroglie) to its wavelength, and the wavelength is dependent on how "curvy" the wavefunction is at any point, and the "curviness" of the wavefunction is related to the spatial derivative of the wavefunction. Thus,

$$p \propto \frac{d}{dx} \tag{6.4.7}$$

Not to get overly philosophical here, but in quantum mechanics all that exists is the wavefunction. Everything that is observable in nature must somehow be extracted from the wavefunction. This means that quantities like momentum can only be determined by manipulating the wavefunction is some way, in this case by taking a spatial derivative. Thus, quantities like momentum (or kinetic energy) are represented not by the "formulas" you are familiar with from classical mechanics but by mathematical operators, basically actions that must be taken on the wavefunction in order to squeeze from it the information you are interested in. This is why the placement of the variable in the formula for expectation values is so important. The operator for momentum acts on one "copy" of the wavefunction, and then the result is multiplied by the other "copy" and then integrated over all of space. We are almost ready to do this, but first we need to complete the description of the momentum operator.

If you recall from above, I showed that Schrödinger's equation is consistent with the idea of energy conservation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x)+U(x)\Psi(x)=E\Psi(x) \tag{6.4.8}$$

$$\frac{p^2}{2m}+U(x)=E \tag{6.4.9}$$

Carefully comparing these two relationships leads to the conclusion that the operator representing momentum may be,

$$p=i\hbar ddx \tag{6.4.10}$$

where

$$i=\sqrt{-1} \tag{6.4.11}$$

Thus, if you want to determine the momentum of a wavefunction, you must take a spatial derivative and then multiply the result by –ih. Should you be concerned that this implies that momentum is not "real"? The short answer is no.

Let's determine the expectation value of the momentum of the electron:

$$\begin{aligned}
&<p>=\int_0^L\left(\sqrt{\frac{2}{L}}\sin(\frac{\pi x}{L})\right)\left(-i\hbar\frac{d}{dx}\left(\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\right)dx\right. \\
&<p>=-i\hbar\frac{2}{L}\int_0^L\sin\left(\frac{\pi x}{L}\right)\left(\frac{\pi}{L}\cos\left(\frac{\pi x}{L}\right)\right)dx \\
&<p>=-i\hbar 2\pi\frac{2}{L}\int_0^L\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)dx \\
&<p>=-ih\int_0^\pi\sin(u)\cos(u)\left(\frac{L}{\pi}du\right) \\
&<p>=-ih\frac{L}{\pi}\int_0^\pi\sin(u)\cos(u)du \\
&<p>=-ih\frac{L}{\pi}\int_0^\pi\frac{1}{2}\sin(2u)du \\
&<p>=-ih\frac{L}{\pi}(0) \\
&<p>=0
\end{aligned} \tag{6.4.12}$$

So the expectation value of the momentum of a particle in an infinite square well is zero? Of course it is! The allowed energy levels in a well can be thought of as the standing waves that “fit” in the well. The whole idea of a standing wave is that there is no net flow of energy (or momentum) in either direction. That’s why we call it a standing wave!

Now what about the uncertainties in these values? Obviously, every time we measure the position of the electron it won’t be in the center of the well (just equally likely on the right and the left) and every time we measure the momentum of the particle it won’t be at rest (just equally likely “moving” to the right or the left). The uncertainty in these values gives you an idea of the spread in possible measurements you should expect if you made a large number of measurements. This idea of the spread in a collection of data is simply the idea of the standard deviation.

Mathematically, the standard deviation of a set of position data is determined by

$$\sigma_x = \sqrt{<x^2> - <x>^2} \tag{6.4.13}$$

i.e., the difference between the expectation value of the square of x and the expectation value of x squared. Thus, to find the uncertainty in position, we need the expectation value of x2:

$$\begin{aligned} <x^2> &= \int_0^L \left(\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\right) x^2 \left(\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\right) dx \\ <x^2> &= \frac{2}{L}\int_0^L x^2 \sin^2\left(\frac{\pi x}{L}\right) dx \\ <x^2> &= \frac{2}{L}\int_0^\pi \left(\frac{L}{\pi}u\right)^2 \sin^2(u)\left(\frac{L}{\pi}du\right) \\ <x^2> &= \frac{2L^2}{\pi^3}\int_0^\pi u^2 \sin^2(u) du \\ <x^2> &= \frac{2L^2}{\pi^3}\left(\frac{\pi^3}{6} - \frac{\pi}{4}\right) \\ <x^2> &= 0.283L^2 \end{aligned} \tag{6.4.14}$$

So the uncertainty in position is:

$$\begin{aligned} \sigma_x &= \sqrt{0.283L^2 - (0.5L)^2} \\ \sigma_x &= \sqrt{0.283L^2 - 0.25L^2} \\ \sigma_x &= 0.182L \end{aligned} \tag{6.4.15}$$

The uncertainty in momentum is:

$$\sigma_p = \sqrt{<p^2> - <p>^2} \tag{6.4.16}$$

and the expectation value of p2 is:

$$< p^2 >= \int_0^L \left(\sqrt{\frac{2}{L}}\right) \sin bigg(\frac{\pi x}{L})\bigg) \left(-\hbar^2 \frac{d^2}{dx^2}\left(\sqrt{\frac{2}{L}}\right) \sin bigg(\frac{\pi x}{L})\right) \tag{6.4.17}$$

$$< p^2 >= -\hbar^2 \frac{2}{L} \int_0^L \sin\left(\frac{\pi x}{L}\right)\left(-\frac{\pi^2}{L^2}\sin\left(\frac{\pi x}{L}\right)\right) dx$$

$$< p^2 >= \frac{2\pi^2\hbar^2}{L^3} \int_0^L \sin^2\left(\frac{\pi x}{L}\right) dx$$

$$< p^2 >= \frac{2\pi\hbar^2}{L^2} \int_0^\pi \sin^2(u)\left(\frac{L}{\pi} du\right)$$

$$< p^2 >=< p^2 >= \frac{2\pi\hbar^2}{L^2} \int_0^\pi \sin^2(u) du$$

$$< p^> = \frac{2\pi\hbar^2}{L^2}\left(\frac{\pi}{2}\right)$$

$$< p^2 >= \frac{\pi^2\hbar^2}{L^2}$$

$$< p^2 >= \frac{h^2}{4L^2}$$

Does this result look familiar? If not, compare it to the ground state energy …

So the uncertainty in momentum is:

$$\sigma_p = \sqrt{\left(\frac{h^2}{4L^2}\right) - (0)^2} \tag{6.4.18}$$

$$\sigma_p = \frac{h}{2L}$$

Note that the uncertainty in the momentum is actually equal to the absolute value of the momentum. (The electron has a wavelength of 2L, so the above expression is actually just DeBroglie's relationship for the momentum of the electron.) This can be interpreted as the electron having a momentum magnitude of h/2L but having an unknown direction for this momentum. Thus the momentum is:

$$p = 0 \pm \frac{h}{2L} \tag{6.4.19}$$

Finally, we can verify that the uncertainty in position and momentum are consistent with the uncertainty principle:

$$\sigma_x\sigma_p \geq \hbar/2 (0.182 \text{ L})\left(\frac{h}{2L}\right) \geq \frac{h}{4\pi} \tag{6.4.20}$$

$$0.091h \geq 0.080h$$

Heisenberg can sleep easy since the ground state of the infinite well displays no violation of his principle!