Thoughts for the Day
CH301 Fall 2010
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The particle in a box

The particle in a box is a thought problem looking at the wavefunction of a particle that is confined in space in one dimension. We imagine this confinement comes from walls that are infinitely high in energy. As such, this is a thought problem (there are no infinite energy walls). None the less, there are problems with very very high walls so this demonstrates some key ideas that hold for all QM problems.

How will be put infinitely high walls into the problem. We will set the potential energy to infinity in certain regions of space. From x=0 to x=L the potential energy is equal to zero. Everywhere else then potential is infinity. As such we have reduce the whole universe to the space between x=0 and x=L. That is we know the particle cannot exist in the areas of infinite potential, and thus in those regions we say the wavefunction must be equal to zero. What is it between the walls?

For that we have to solve the Schrödinger equation. As this is done in the book and class, I will be brief here.

First let's look at the equation. Since V(x)=0, the equation is much simpler.

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = E\psi(x)$$

Now the problem is simply what function when we take its second derivative is equal to itself times a constant. Our choices are sine and cosine (or the exp, but a generic exponential function is actually sine and cosine).

The generic solution will be

$$A\sin ax + B\cos bx$$

Where *A, B, a, b* are unknown constants.

We can find them using other information we have. At x=0 and L=0 the wavefunction must be zero. Why? Outside the box the wavefucntion is zero and it must be continuous at these points. Thus we know

$$\psi(o) = \psi(L) = 0$$

This is true for sine but not cosine. Thus $B = 0$ and we can drop the cos part (and not worry about b)

Then what about A & a? Well a needs to be a special value for the wavefunction to be zero when x = L. In fact is must be that $a = n\pi L$ where n is an integer n=1,2,3,…. Wow! We have quantized discrete solutions just from the boundary conditions for the wave. This will give us discrete energies just like we saw in the H-atom line spectra.

What about A? If we look at the integral of the square of the wavefunction we can figure this out.

$$1 = \int_0^L A^2 \sin^2(n\pi x/L)dx = A^2\left(\frac{L}{2}\right)$$

So A = sqrt(2/L)

Now we have a set of wavefunctions

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

For each of these wavefunction we can find an energy using the Schrödinger equation. Plug in the wavefucntion and find E_n.

$$E_n = \frac{n^2h^2}{8mL^2}$$

Look in the book at these solutions and their energies? The wavefunctions as n increases have more times that they change sign (nodes). Where are you most likely to find the particle in the n=1 state? The n=2 state?

Note there are places where the wavefunction changes sign. These are called nodes. When we square the wavefunction these will still be zero and the particle has no probability of being located in these regions. It is very important to note that the sign of the wavefunction is important when two waves are interacting as this will affect how they interfere. However under no circumstance should you ever interpret the sign of the wavefunction to be related to charge or something like that. If it is negative it is just because the function is negative. Positive and negative are merely opposites when you are comparing them. The important thing to compare with two waves is do they have the same sign or opposite signs.

Question: How many nodes are their in the n=4 state?

What do we see about the energy.

1. Energy is inversely proportional to the mass. Therefore when the mass is large, the energy levels (and their spacings) become very very small. Thus we don't have to worry about the quantum energy levels of a baseball in a box.

2. Energy is proportional to $1/L^2$. Thus as the box gets large the energy levels get small (even faster than with respect to the mass). Again a big box will have essentially continuous energy levels since they are so close together. As the box length gets small and the particle is confined then the energies increase. This is an important general idea. Confinement leads to higher energies (and energy spacings).

3. The energy levels increase as n^2. Therefore as we go up in energy the spacing between the levels is getting larger and larger.

4. Finally, the lowest energy is not zero, but finite. This is the idea of *zeropoint energy*. This is the lowest energy possible.

Other questions to ponder.

What is the probability the particle is on the left hand side of the box? The right hand side of the box?

In the n=1 state there is a node in the middle of the box where the probability of finding the particle is zero. If this is the case, how does the particle get from one side of the box to the other? This is a "bad" question. The particle is on both sides of the box at the same time. It is not a particle or a wave despite the fact that we cannot escape that language in talking about it. It is a QM object that is described by the wavefunction.