Notes for Quantum Mechanics I

Richard Seto

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Lecture 2
Getting to the Schroedinger Equation: A guess

Now we need to find some way to incorporate waves and particles into one theory. For the moment it will seem like we are free associating (which we are). But then, we will see if our guesses give us predictions which are in line with experiments. So lets first write down the energy equation for a particle. Let's use the non-relativistic equation to make things easier. Think of electrons:

$$E = \frac{p^2}{2m} + V(r) \quad \text{where V(r) is some potential. This is for particles} \tag{1}$$

Next lets write down a wave equation. Lets do it in 1-D instead of 3D to make it easier.

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u(x,t)}{\partial t^2} \quad \text{for waves} \tag{2}$$

The solutions to (2) are $u(x, t) = \mathrm{A}e^{\pm i(\mathrm{kx}-\omega \mathrm{t})}$ where k is the wavenumber $k = \frac{2\pi}{\lambda}$

remember this comes from the following:

$\omega = 2\pi\nu$ c=$\nu\lambda$ (velocity = distance / time) $\longrightarrow \nu = \frac{c}{\lambda}$ so $\omega = \frac{2\pi \mathrm{c}}{\lambda}$

now lets plug the solutions into (2) we will get

$-k^2 u = \frac{-\omega^2}{c^2} u$ so $k^2 = \frac{1}{c^2}\frac{(2\pi)^2 c^2}{\lambda^2}$ and finally $k = \frac{2\pi}{\lambda}$

Now we will use some of the guesses from the last lecture. First let use eqn (1.7 and 1.8) $p = \frac{h}{\lambda}$ and get $k = \frac{p}{\hbar}$ and E=hν=$\hbar\omega$

and now the solutions are $u(x, t) = \mathrm{A}e^{\pm \frac{i}{\hbar}(\mathrm{px}-\mathrm{Et})}$

if we now plug this into 2 we get

$p^2 c^2 = E^2$ which is good for a massless particles, but not for a particle with mass - what we are hoping to get is something like (1)

(one might think though that this might be encouraging for later when we try to think about massless relativistic particles)

Now let's try to fix this up. Let's try a modified wave equation.

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{1}{c}\frac{\partial u(x,t)}{\partial t}$$

Then we get

$-\frac{1}{\hbar^2}\,p^2 = \mp\frac{i}{\hbar}\,\frac{E}{c}$ OK. Now we are getting warmer since we are getting something line $E \sim p^2$ Lets rescale the p and E and put an i on the RHS as follows

$$-\frac{\hbar^2}{2\,m}\,\frac{\partial^2 u(x,\,t)}{\partial x^2} = -i\hbar\,\frac{\partial u(x,\,t)}{\partial t} \tag{3}$$

Then we will get

$\frac{p^2}{2m} = E$ Which is eqn (1) for a potential V(r)=0. So now if (3) is our new wave eqn then we have satisfied a wave eqn and the equation for the energy of a particle!

Now we will simplify even more. We will imagine that the solution will be of the form $u(x,t)=F(x)e^{\frac{i}{\hbar}Et}$ i..e the the time dependence is just a simple oscillitory form so the RHS of (3) is always equal to Eu(x,t) and we can write

$$-\frac{\hbar^2}{2\,m}\,\frac{\partial^2 u(x,\,t)}{\partial x^2} = E u(x,\,t) \tag{4}$$

Equations 3 and 4 are the Schrodinger's equations. (3) is the time dependent Schrodinger's equation and (4) is the time independent Schrodinger's eqn. Now lets think about (4). Is it somehow equivalent to (1) in our new world of wave/particles? Later when we talk about bra's and ket's this will make more sense. But for now let me continue. The way we can make (4) equivalent to (1) is to first associate p with an "operator" $\hat{p} \to \frac{\hbar}{i}\,\frac{\partial}{\partial x}$. The hat over the p is there to remind us that it is now an operator and not a regular variable. Now typically for matter waves, we will denote them as ψ(x,t) instead of u(x,t) So then we have

$\left(\frac{\hat{p}^2}{2m} + V(r)\right)\psi(x,t)=E\psi(x,t)$ for the time independent equation and (5)

$\left(\frac{\hat{p}^2}{2m} + V(r)\right)\psi(x,t)=-i\hbar\,\frac{\partial}{\partial t}\psi(x,t)$ for the time dependent one. (6)

The V(r) is the potential, and often is just an ordinary function. (not always - sometimes it involves an operator, but for instance in the case of the electric potential, its just $\frac{e^2}{r}$ as *a* multiplicative factor to ψ.

$\hat{p}$ is the momentum operator $\hat{p} \to \frac{\hbar}{i}\,\frac{\partial}{\partial x}$ in 1-D and $\frac{\hbar}{i}\nabla$ in 3D. (7)

the combination on the LHS of (5) and (6) is the Hamiltonian Operator a word taken over from classical mechanics:.

$$\hat{H} = \left(\frac{\hat{p}^2}{2\,m} + V(\vec{r})\right) \tag{8}$$

Then the time independent Schrodinger can just be written as $\hat{H}\psi=E\psi$ (9)

Now at the moment we have no idea if Schodinger's eqn has anything to do with the real world bit for now lets take it as true (it actually holds up under experimental verification pretty well) -.

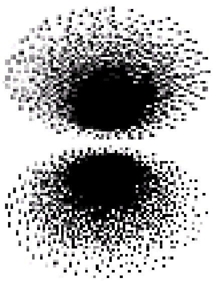
The problem in Quantum mechanics then comes down to solving for ψ which is often a pain, since it is a differential equation. Also, as a general rule, when one does research - the problem is to first to figure out the form of V($\vec{r}$). We will be doing rather simple problems where the form of V(r) is known and the forms of ψ is easy to solve. Hence we will spend time with the "particle in a box" - about the simplest V(r) you can imagine.

Now in principle we could just start right in, and put the potential V($\vec{r}$) = $\frac{e^2}{|\hat{r}|}$ into (5) and solve and we would have done the hydrogen atom, and you could quit. But that is awfully hard at this point. Written out, the diff eq would be

$\frac{1}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,\ y,\ z)-\frac{e^2}{\sqrt{x^2+y^2+z^2}}\psi$(x,y,z)=E$\psi$(x,y,z) - good luck - but in principle it would work.

But now I would like to take up a different line of logic for a while which will make our lives much easier. Let us first ask ourselves what ψ is. You say its a matter wave. Correct - but what is that? (for that matter - what is an electromagnetic wave?-Lets leave that for another time).

One of the common interpretations of ψ is that its square tells you the probability of finding the object there, that is the probability of finding an electron at x is $|\psi(x)|^2$. This is a reasonable way to think about it as long as you don't think too hard. There is a problem when you look at the p orbital in a hydrogen atom which looks like this



$2p_0$

This thing has 2 lobes, and there is a 50% probability of finding the electron in each lobe. BUT there is a zero percent probability of finding it in between. When then how does it get from one lobe to another? What you have to end up believing is that the electron doesn't sort of whiz between the two lobes and spend half of its time there - but rather that it exists with a 50% probability in each lobe - it doesn't really whiz back and forth. This sound crazy - it is crazy - but it seems to be the way it works. If it didn't - your body chemistry would fall apart and you would not exist.

OK - at least to me this idea of thinking of ψ(x) as the thing to think about, has some problems to it. Hence I would now like to introduce you to bra's and ket's and hilbert spaces. What we are going to do is to represent the particle as BEAST - we call a ket.

Its not like anything you have had before. It exists in some realm called a Hilbert space.

First we will spend a little more time with the Schroedinger eqn as we have written today.

