The Schrödinger Equation

First, let's review, because repetition is good for understanding.

- First, we saw that light has particle-like properties, consisting of individual quanta of energy, \( E = hf \).

That was motivated by the blackbody emission spectrum and supported by the photo-electric effect.

- Second, we saw that atoms absorb and emit light only at specific, discrete frequencies and hence energies.

This was explained by the Bohr model of the atom, in which the assumption that angular momentum is quantized led to quantized energy levels for the atom. That explained the emission spectra, but there was no explanation for why or how -- and the model had limited application.

We will now see a way to predict these.

- Third, we saw that particles have wave-like properties, 
  \[ p = \frac{h}{\lambda} \]

Electron interference demonstrated this.
This forced us to change our view of a particle's position as being some specific point. We now need to think of a particle as a wavepacket. As such, it has a range of positions and a range of wavelengths. We cannot simultaneously determine both position and wavelength, so the uncertainty in them is related by $\Delta p \Delta x \geq \hbar$.

Similarly, a wavepacket has a range of time and a range of frequency, so $\Delta t \Delta \omega \geq \hbar$.

Fourth, we changed our description of a particle from being able to specify its position, to only being able to specify its probability density at that position.

This is done with the wavefunction, $\psi(x)$, where

$$ P(x) = |\psi(x)|^2 $$

and

$$ \int_{a}^{b} P(x) \, dx = \int_{a}^{b} |\psi(x)|^2 \, dx $$

is the probability to find the particle between $x = a$ and $x = b$. 
Now, we need to figure out how to predict the wavefunction.

You may recall that way back at the beginning of the course we first described motion; $x(t)$, $v(t)$, vectors, etc. Then we described Newton’s laws that allowed the motion to be predicted.

In the same way, we described electric and magnetic fields, then Maxwell’s equations that allowed us to predict the fields.

In neither case could we derive Newton’s law or Maxwell’s equations; they just work. (Other ideas could have been tried, but if they don’t properly explain/predict experiments they fade away.)

Now, we’ll discuss Schrödinger’s equation that allows us to calculate the wavefunction for a physical system. As before, we can’t derive it; we can only verify that it is theoretically sensible and experimentally verified.
Schrödinger equation: time-independent for now.

\[-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U(x) \psi(x) = E \psi(x)\]

or, if you prefer

\[\frac{d^2 \psi(x)}{dx^2} = -\frac{2m}{\hbar^2} \left[ E - U(x) \right] \psi(x)\]

where the second way is just to show more explicitly that it is \( E - U(x) \) = kinetic energy at its foundation.

To help understand what it means, and later, how to use it, let’s spend a minute “justifying” this equation. (Not a derivation or a proof, just playing with it…)

\[P = \frac{\hbar}{i} \text{ is what pushed us here.}\]

In terms of energy, \( P = \sqrt{2amK} \) because,

\[P = mv = \sqrt{2am\left(\frac{1}{2}mv^2\right)} = \sqrt{amK}\]

So, we want to describe the wave-function of a particle with \( K \)...
Since we have a "wavefunction" with wavelength \( \lambda \), let's use a simple guess:

\[
\psi(x) = \psi_0 \sin\left(\frac{2\pi x}{\lambda}\right)
\]

\[= \psi_0 \sin kx \text{ Note: This is little } k. \]

\[k = \frac{2\pi}{\lambda} = \frac{2\pi}{\hbar/P} = \frac{P}{\hbar} \text{ while we are at it.} \]

\[\omega = 2\pi f = 2\pi \frac{E}{\hbar} = \frac{E}{\hbar} \text{ Nice symmetry!} \]

So, \( \frac{d\psi}{dx} = \frac{2\pi}{\lambda} \psi_0 \cos\left(\frac{2\pi x}{\lambda}\right) \)

\[
\frac{d^2\psi}{dx^2} = -\left(\frac{2\pi}{\lambda}\right)^2 \psi_0 \sin \frac{2\pi x}{\lambda} = -\left(\frac{2\pi}{\lambda}\right)^2 \psi(x)
\]

\[
\frac{d^2\psi}{dx^2} = -\left(\frac{P}{\hbar}\right)^2 \psi(x) \]

\[
= -\frac{2m\hbar^2}{\hbar^2} \psi(x)
\]

\[
= -\frac{2m}{\hbar^2} [E-U(x)] \psi(x)
\]

Note, again. This is not a proof, just a demonstration of reasonableness for a very simple case.

It turns out to hold in all tested cases.
The Schrödinger equation describes the wave function in terms of energy:

\[ E = \text{total energy.} \]
\[ U(x) = \text{potential} \]

It doesn't use force. Potentials are much more convenient.

Let's review.

\[ U(x) = -\int_{-\infty}^{x} F(x') \, dx' \implies \text{work to get it there} \]
\[ = \int_{x}^{\infty} F(x') \, dx' \implies \text{work that could potentially be done once you have it there.} \]

Choice of \( U=0 \) is arbitrary.

A simple example:

Where is \( k \) greatest, for constant \( E \)?
Where is it least?
Note that nothing changes if I redefine the point where \( U = 0 \).

\[
E = U + K \text{ still.}
\]

For \( U(r) = \frac{q^2}{4\pi \varepsilon_0 r} \) it makes mathematical sense (convenience) to make \( U(\infty) = 0 \).

Here, it is convenient to make \( U(0) = 0 \).

\( K \) changes with \( x \), so does \( p \).

\( \lambda \) changes with position.
As in the past, the problem solving approach will be to:

1. Determine the physical setup
   Find $\xi \xi' \rightarrow$ Find $U(x)$

2. Plug and chug

3. Apply ancillary information to solve for constants.
   E.g. initial position, or other
   "BOUNDARY CONDITIONS"

   This can include things such as continuity
   (a ball bouncing off the floor does so with a continuous position).

   It also includes intuition: (a ball bounces off the floor, not into and out).

1 0 3 is going to be arbitrary since real problems have hard realities.

2 0 3 is guess and check for our problems.

3 Boundary conditions are key! We'll see some oddities though. Also normalization.
A few sample problems on uncertainty:

What is the velocity uncertainty for a dust particle confined to a region \( \approx 10 \mu \text{m} \) long? If you see one sitting on a CD (for example) under a microscope, is it really at rest?

\[
\Delta p \Delta x = \hbar \\
\downarrow \quad 10 \mu \text{m}
\]

\[
m \Delta v = \frac{\hbar}{\Delta x}
\]

\[
\Delta v = \frac{\hbar}{m \Delta x} = \frac{1 \times 10^{-34} \text{ J s}}{10^{-15} \text{ kg} \times 10^{-5}} = 1 \times 10^{-14} \text{ m/s}
\]

At a speed of \( 10^{-14} \text{ m/s} \), it would take \( 10^8 \) s to move one micron. Undetectable.

Good... I've never seen dust spontaneously move... but I've never watched for 10 years straight.
Now, let's do the same for an electron, contained in an atom. $\Delta x = 0.1$ nm

$$\Delta p = \frac{\hbar}{\Delta x}$$

$$\Delta v = \frac{\hbar}{m \Delta x} \approx \frac{1 \times 10^{-34}}{10^{-30} \cdot 10^{-10}} = 10^6 \text{ m/s}$$

So, it (the uncertainty principle) begins to matter only on very small scales.

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Estimate the lifetime of a state with a mass that is $\sim 100 \text{ MeV}$, $\frac{1}{2}$, and $20 \text{ MeV}$ wide.

$$E = mc^2 = 100 \text{ MeV}$$

$$\Delta E = 20 \text{ MeV}$$

$$\Delta t = \frac{\hbar}{\Delta E} = \frac{1 \times 10^{-34}}{20 \text{ MeV}} \cdot \frac{5.4 \times 10^{-16} \text{ eV s}}{2 \times 10^2 \text{ eV}}$$

$$= 3 \times 10^{-23} \text{ s}$$