Name:

Physics 200 Tutorial 12:

Bound States in Quantum Mechanics

So far in class, we have talked about the quantum mechanical description of freely propagating (i.e. travelling) electrons (or other particles). We understood that the wavefunctions for these may be written as a superposition of pure waves (momentum eigenstates) with:

wavelength = h / momentum	$\lambda = h/p$
frequency = energy / h	$f = E/h$

where E is the electron's kinetic energy $p^2/(2m)$.

Mathematically, the formula for a complex wave with wavelength λ and frequency f is

$$e^{2\pi i(x/\lambda - ft)}$$

so setting $\lambda = h/p$ and $f = E/h = p^2/(2mh)$, we get

$$\boxed{\psi(x,t) = e^{2\pi i/h\,(px - p^2/(2m)\,t)}}$$

(+ve momentum electron)

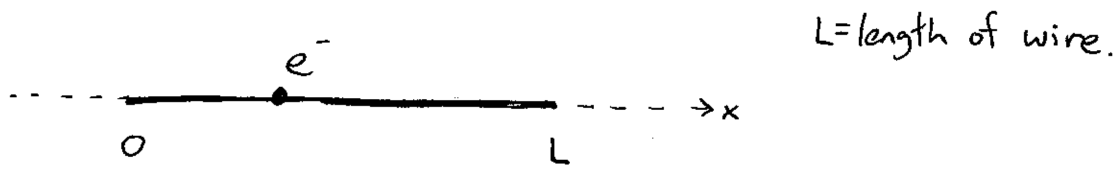
as the wavefunction for a momentum eigenstate. The time dependence is just a simple oscillation, but once we add up these waves in a general wavefunction, we get wavepackets (or more general shapes) that propagate, disperse, etc... . Any superposition of the oscillating pure waves (and therefore any electron wavefunction) satisfies the Schrodinger equation, which is conventionally written as

$$\boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial x^2}}$$

where we define $\hbar = h/(2\pi)$ (pronounced "h-bar").

For most application, the particles are not just freely propagating. Instead, we have forces on the particles (e.g. the Coulomb force between electrons and protons in atoms) ,and often these forces result in electrons or other particles being confined in a particular region of space (e.g. near the nucleus of an atom, or inside a metal). These confined states are known as BOUND STATES, and they exhibit some really interesting features that we will begin to explore today.

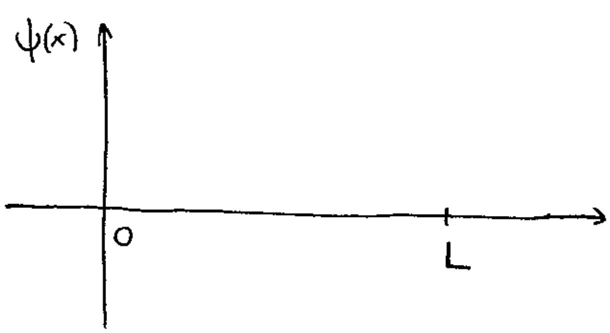
Soon, we will learn how to write down the Schrodinger equation when we have general forces or potentials, but for today, we'll look at a really simple example: an electron moving in a thin (1-dimensional) finite wire:



Question 1

a) If the electron is confined to a wire stretched between x=0 and x=L, what can we say about the wavefunction ψ(x)? How would the possible ψ(x)s differ from the case where the wire is infinite?

b) Sketch a possible wavefunction for the electron.



note: like most physical quantities, wavefunctions must be continuous (i.e. there are no jumps allowed).

Question 2

For wavefunctions of freely propagating electrons, we said that it is always possible to decompose these into superpositions of pure waves. These waves could have any wavelength and any frequency, as long as

$$f = \frac{h}{2\,m\,\lambda^2} \qquad \text{(this follows from } \lambda = h/p \text{ and } hf = p^2/(2m)\text{)}$$

For an electron in a wire of length L, we can think of the electron as being freely propagating inside the wire, but constrained not to move past the ends. In this case, we can thing of the possible wavefunctions as being built up from finite waves (like the waves on a guitar string) rather than "pure" waves that go on forever in both directions.

a) What can you say about the wavelengths/frequencies for the modes of vibration (harmonics) on a guitar string? (*Hint: for a string of fixed length and tension, can you make any sound you want?*)

b) Sketch the profile of a guitar string vibrating at its lowest possible frequency.

c) Based on the analogy with a guitar string, what wavelengths do you think are allowed for an electron in a wire of length L?

d) If we assume that the relationship between wavelength and frequency still holds for the confined electron, what are the allowed frequencies for these finite waves?

e) What does your result in part d imply about the possible energies of an electron moving in a finite wire?

Question 3

Now let's try to verify our guesses using Schrodinger's equation.

a) Our study of free electrons revealed an important connection between energy and frequency for electrons, just like the relation between momentum and wavelength. States of a definite energy E should have wavefunctions that simply oscillate in time with a definite frequency f = E/h. More precisely, we want the time dependence to be $e^{-2\pi i (E/h) t}$, as we had for pure waves. If

$$\psi(x,t) = f(x)\, e^{-2\pi i \frac{E}{h} t}$$

is a solution to the Schrodinger equation in the wire, determine the equation that must be satisfied by f(x).

check your answer with me or a TA before continuing.

b) The equation you just derived is the “time independent Schrodinger equation”. It determines the specific shape that the wavefunction must have at t=0 so that it will just oscillate with frequency E/h as a function of time (and therefore have a definite energy E). It is simpler than the full Schrodinger equation since it only depends on space and not time. Linear equations like this with two derivatives usually have two independent solutions. Show that for your equation, two solutions are

$$f_1(x) = \cos(kx) \qquad \text{and} \qquad f_2(x) = \sin(kx)$$

and determine k in terms of E. (Note: the general solution is just the superposition of these two with arbitrary coefficients).

c) So far, we haven't used the fact that the electron is trapped in a wire. If we demand that ψ(x) = 0 for x outside the wire and that ψ us continuous, the solutions must go to zero at x=0 and x=L. If we want to have a solution of the form

$$A \cos(kx) + B \sin(kx)$$

satisfying this requirement, what can we say about the constants A, B, and/or k? (*note: you don't need to use the relation between k and E for this part.*)

d) Combining your results from part b) and c), what are the possible energies for an electron in a 1D wire of length L? Does this agree with your answer for 2 e)?

e) Sketch f(x) = ψ(x,0) for the state with the lowest possible energy. Is this energy zero? What would the minimum energy be according to classical physics (assuming the potential energy in the wire is 0)?

★ TAKE HOME MESSAGE: ★

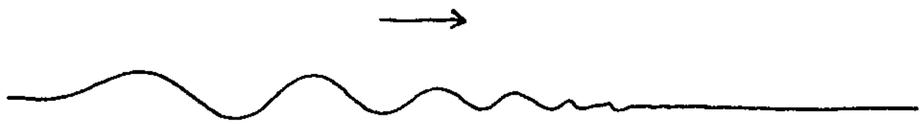
We have seen in our simple example a dramatic general feature of bound states in quantum mechanics: ★ *they can only exist at specific energies.* ★ We will see that this explains the discrete nature of the spectrum from gases of atoms and also resolves the problem of the classical instability of atoms. We have also encountered the phenomenon of ZERO-POINT ENERGY: enen in their lowest energy states, bound particles still have kinetic energy.

Question 4

Referring to your wavefunction from question 3 e, what does the uncertainty principle tell us about the range of velocities we might find if we measure the velocity of the electron in its lowest energy state in a wire of length 10nm?

Question 5

In the simulation of a propagating wavepacket, one feature that we did not discuss is the fact that after some time, the wavepacket becomes asymmetrical



with the wavelength near the front end of the packet appearing shorter than the wavelength near the back. Can you explain this?

Question 6

Verify that the pure waves from page 1 also satisfy the differential equation

$$i\hbar\psi\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial\psi}{\partial x}\right)^2$$

If this equation has the same set of pure wave solutions, how do we know that this isn't the right equation for quantum mechanics instead of the Schrodinger equation?