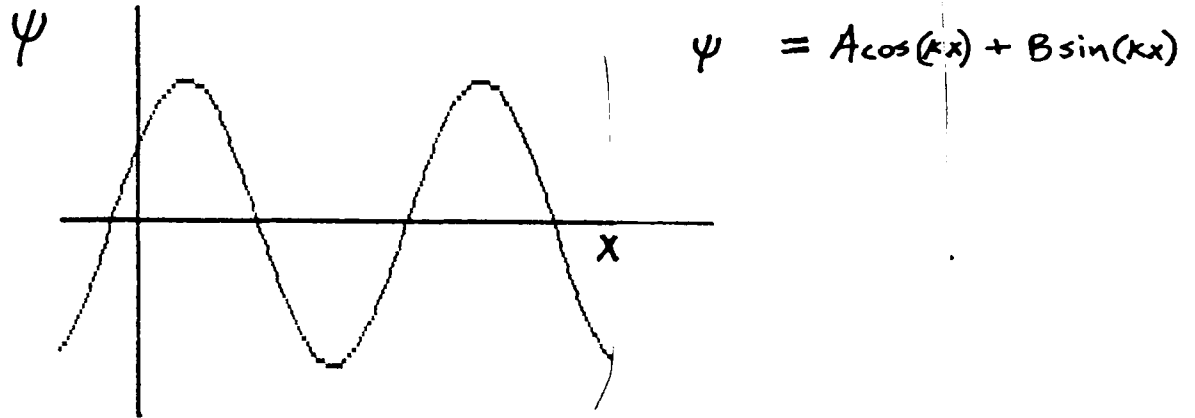


APPENDIX A THE GENERALIZED WAVE EQUATION

Waves are oscillations in space and time. The most general mathematical description of the spatial distribution of a wave is a superposition of sine and cosine functions.

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

where Ψ , the "wavefunction," represents the wave amplitude at some point in space, or in the case of the deBroglie waves associated with particles, the amplitude to find the particle at that point. A is the amplitude of the component cosine wave, and B is the amplitude of the component sine wave. k , the wavenumber (which = h/λ), measures how rapidly the wave oscillates in space, i.e. how many complete oscillations per unit distance.



We must add another factor to our equation to describe the wave's oscillation in time.

$$\Psi = e^{-i\omega t} (A \cos(kx) + B \sin(kx))$$

where $e^{-i\omega t}$ is a time-varying function equal to

$$\cos(\omega t) + i \sin(\omega t)$$

and $i = \sqrt{-1}$. ω (omega) stands for the angular frequency, that is how rapidly the sine and cosine functions are changing over time.

By inserting the appropriate variables, A , B , ω , and k , and by superposing waves with different parameters (see section on Fourier analysis in Ch.5), we can describe any wave.

APPENDIX B
THE SCHRODINGER EQUATION *

We would like to be able to describe the behavior of an electron (or any other particle) mathematically. For example, we would like to analyze the distribution and energies of electrons around atomic nuclei, and we would like to be able to describe the flow of electrons through semiconductor devices.

To do so, we can combine our understanding of waves and the quantum nature of energy and momentum. Erwin Schrodinger and Werner Heisenberg separately discovered mathematical descriptions of quantum behavior in 1926. We will derive the Schrodinger equation here, as it is the most straightforward.

To begin our wave description of the electron, we borrow from classical physics: $E = p^2/2m + V$. That is, a particle's total energy equals its kinetic energy plus its potential energy (symbolized by V). Into this equation we substitute the quantum relations of energy and momentum,

$$E = hf = \hbar\omega$$

$$p = h/\lambda = \hbar k$$

$$\text{where } \hbar = h/2\pi$$

Therefore

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V$$

We proceed by deriving ω and k^2 in terms of the general wave equation:

$$\psi = e^{-i\omega t} [A \cos(kx) + B \sin(kx)]$$

$$\frac{d\psi}{dt} = -i\omega \psi \quad \text{so} \quad \omega = \frac{d\psi/dt}{-i\psi}$$

$$\frac{d^2\psi}{dx^2} = -k^2 \psi \quad \text{so} \quad k^2 = \frac{d^2\psi/dx^2}{-\psi}$$

Substituting into the energy equation,

$$\frac{\hbar}{-i} \left(\frac{d\psi/dt}{\psi} \right) = -\frac{\hbar^2}{2m} \left(\frac{d^2\psi/dx^2}{\psi} \right) + V$$

Finally, multiplying both sides of the equation by ψ and by i/i gives

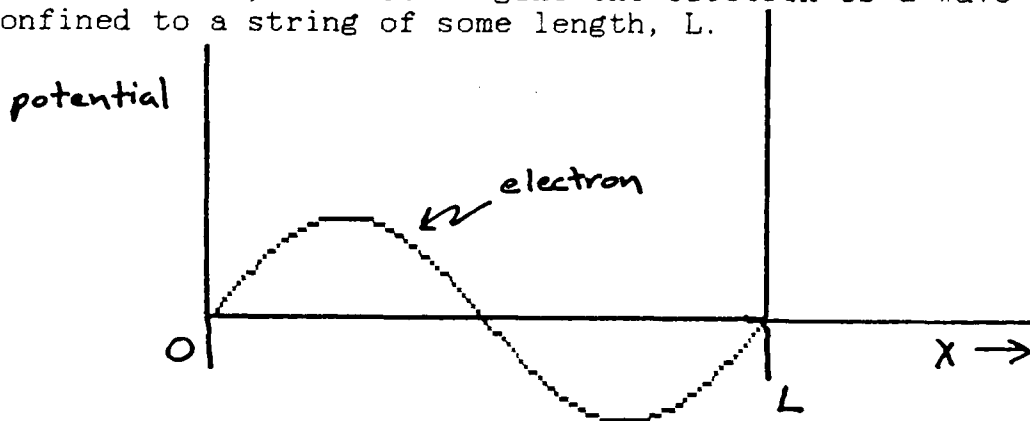
$$i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \left(\frac{d^2\psi}{dx^2} \right) + V\psi$$

* adapted from Crawford, Waves (Berkeley Physics Course)

This is the Schrodinger equation. As we will illustrate in the next section, it allows us to calculate the amplitude to find an electron at any point in time and space.

APPENDIX C QUANTIZED ENERGY STATES OF ATOMS *

We will consider the case of an electron trapped in a "potential well," and, for purposes of illustration, we will assume the well is infinitely deep. In a real atom, the electron is confined to the potential well of the positively charged nucleus, attracted by the protons, and in a real atom the electrons can be stripped away from the nucleus. For simplicity, too, we will only consider the one-dimensional case: that is, we will imagine the electron is a wave confined to a string of some length, L .



By the Schrodinger equation,

$$i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \left(\frac{d^2\psi}{dx^2} \right) + V\psi$$

But

$$\begin{aligned} \psi &= e^{-i\omega t} [A \cos(kx) + B \sin(kx)] \\ &= e^{-i(E/\hbar)t} [A \cos(kx) + B \sin(kx)] \end{aligned}$$

$$\text{and } \frac{d\psi}{dt} = -\left(\frac{i}{\hbar}\right) E \psi$$

So the Schrodinger equation becomes

$$i\hbar \left(-\frac{i}{\hbar}\right) E \psi = E \psi = -\frac{\hbar^2}{2m} \left(\frac{d^2\psi}{dx^2} \right) + V\psi$$

* adapted from Crawford, Waves (Berkeley Physics Course)

If, as we assume, the electron is confined, we can set $V = 0$. So

$$E\psi = -\frac{\hbar^2}{2m} \left(\frac{d^2\psi}{dx^2} \right)$$

Solving this equation for ψ will tell us the wave distribution in the well and allow us to evaluate its energy.

To simplify the algebra, let $k^2 = 2mE/\hbar^2$

so
$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

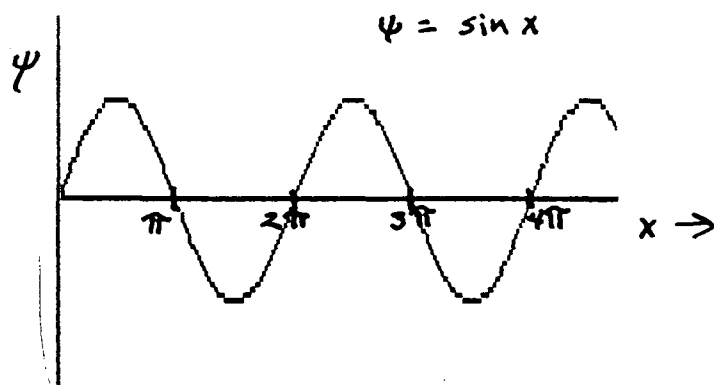
This looks familiar: we have the second derivative of a function, ψ , equal to some constant times the function itself. An obvious solution is

$$\psi(x) = A \cos(kx) + B \sin(kx)$$

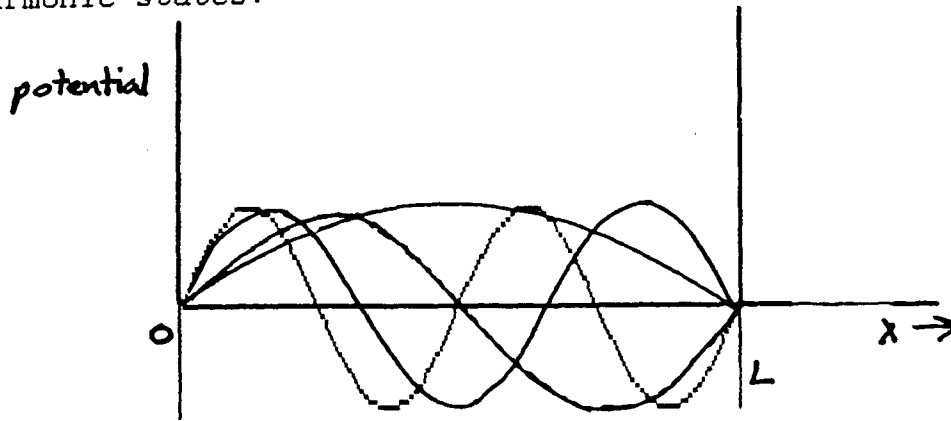
If the electron is confined, ψ must = 0 at $x = 0$ (the left end of the string) and at $x = L$ (the right end of the string). Therefore, ψ can have no cosine component ($\cos(0) = 1$), and A must = 0. ψ then only has sine components, and our solution reduces to

$$\psi(x) = B \sin(kx)$$

This equation satisfies our condition for $x = 0$, since $\sin(0) = 0$. If $\psi = 0$ at $x = L$, we must have that $kL = n\pi$ and, therefore, $k = n\pi/L$, where $n = \text{any integer}$. This is true because $\sin(n\pi)$ always = 0, since the sine function returns to 0 at multiples of π .



The electron wave, then, can exist only in certain harmonic states:



Some electron waves that may be confined in potential well of width L

We can show that its energy must be quantized. Solving for E :

$$E \psi(x) = \frac{-\hbar^2}{2m} \left[\frac{d^2 B \sin\left(\frac{n\pi}{L}x\right)}{dx^2} \right]$$

$$= \frac{-\hbar^2}{2m} \left[-\frac{n^2 \pi^2}{L^2} \psi(x) \right]$$

$$E = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

Since n is an integer, the electron can exist only in certain discrete energy states: the energy is quantized.