Physics 228

Today:

Infinite Square Well
Tunneling
Harmonic Oscillator
Stationary States

A particle with a fixed energy $E = \hbar \omega$ (zero uncertainty in the energy) is described by a wave function $\Psi(x,t) = \psi(x) e^{-i\omega t}$.

For example, if $U(x) = 0$: plane waves $\Psi(x,t) = A e^{i(kx - \omega t)} = A e^{ikx} e^{-i\omega t}$

The probability density is then given by $|\psi(x)|^2$. This is constant in time. Therefore, a state with well-defined energy is also called a "stationary state".

Plugging $\Psi(x,t)$ into the Schrödinger Equation we obtain the time-independent Schrödinger Equation:

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x) \Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

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

Let’s trap a particle in a box. The potential \( U(x) \) is infinite except in the region \( 0 < x < L \). Therefore, the particle is confined to the box and \( \psi(x) = 0 \) for \( x \) outside the box. But in the box \( U(x) = 0 \), so here the Schrödinger Equation is simply:

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

What wave function solves this equation?
What wave function solves this differential equation? We use the “method of the known solution”:

Let's try $\psi(x) = C \sin(kx)$.

The Schrödinger Equation becomes $\left(\frac{\hbar^2 k^2}{2m}\right)\psi = E\psi$, so $E = \frac{\hbar^2 k^2}{2m}$.

For our sine function, $\psi(0) = 0$, as it should. To ensure that $\psi(L) = 0$, we require that $kL = n\pi$ with $n = 1, 2, 3, ...$

Thus $k = \frac{n\pi}{L}$, $\psi(x) = C \sin(n\pi x/L)$, and $E_n = \frac{n^2\hbar^2\pi^2}{2mL^2}$.

As in the Bohr atom, the integer $n$ is a quantum number. For each quantum number $n$, there exists an energy level $E_n$. Other values of the energy are not possible. The energy is “quantized”. 
Infinite Square Well

\[ \psi(x) = C \sin(kx) \]

with \( k = \frac{n\pi}{L} \)

and \( n = 1, 2, 3, \ldots \)

Here are the wave functions and energies corresponding to the five lowest quantum numbers:
Wavefunction Normalization

- For the particle in the box we have $\psi(x) = C \sin(kx)$ for $x$ inside the box, and $\psi(x) = 0$ outside.
- Allowed wave vectors: $k = n\pi/L$ ($n = 1, 2, 3, ...$)

But what is the factor $C$?

Remember that $|\psi(x)|^2$ is the probability density at point $x$.

The total probability of finding the particle somewhere is the probability density integrated over all space. This total probability must clearly be one, since the particle must be somewhere:

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1$$

This is called the normalization condition. Applying it to our particle-in-the-box wavefunction, we find $C = \sqrt{\frac{2}{L}}$. 
Suppose you can measure the position of a particle in the ground state of an infinite square well, by shooting a beam of photons at it and seeing one scatter. Where are you likely to find the particle?

a) near the edges
b) near the center
c) equally likely anywhere in the well
d) the photon gives it energy, so it escapes and is found outside the well
e) Because the particle has a definite momentum, the uncertainty principle, $\Delta p \Delta x \geq \hbar/2$, says its position uncertainty is infinite. So it can be found anywhere in space, even far from the well.
Clicker Question

The first five wave functions for a particle in a box are shown.

The probability of finding the particle near $x = L/2$ is

A) least for $n = 1$.

B) least for $n = 2$ and $n = 4$.

C) least for $n = 5$.

D) the same (and nonzero) for $n = 1, 2, 3, 4$, and 5.

E) zero for $n = 1, 2, 3, 4$, and 5.
When there is a potential barrier, and the particle has energy $E$ less than the top of the barrier, classically we expect the particle to be reflected. But in quantum mechanics the wave function penetrates into the barrier as an exponential function, $e^{-\kappa x}$.

As a result, there can be a traveling wave on the far side of the barrier, and particles can "tunnel" through it!

This behavior is of enormous importance. It explains phenomena ranging from circuit elements (Josephson junctions in superconductors, tunnel diodes) to scanning tunneling microscopes, to radioactive alpha decays of nuclei, and nuclear fusion that powers the sun.
Tunneling

The math techniques are the same (solve S. E. inside and outside the barrier, and match the solutions at the edges). The textbook gives the result for the transmission probability $T$ through a square barrier:  

$$T \propto e^{-2\kappa L}, \text{ where } \kappa = \left[\frac{2m(U_0-E)}{\hbar}\right]^{1/2}$$

The wave function is exponential within the barrier ($0 \leq x \leq L$) ...

... and sinusoidal outside the barrier.

The function and its derivative (slope) are continuous at $x = 0$ and $x = L$ so that the sinusoidal and exponential functions join smoothly.
A mass on a spring is called a harmonic oscillator, with potential $U = \frac{1}{2} k' x^2$. Solving the S. E. for this potential leads to energy levels are evenly spaced, with $E_n = (n + \frac{1}{2}) \hbar \omega$, with $\omega^2 = k'/m$.

Note that the ground state energy is non-zero: $E_0 = \frac{1}{2} \hbar \omega$ ("zero-point energy", and "zero-point motion").
The harmonic oscillator wave functions involve "Hermite" polynomials. The four lowest energy wave functions are shown above.

Note that the “odd n” solutions are antisymmetric about the origin, and for them the particle cannot be found at $x = 0$ where the potential is deepest.