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DEPARTMENT OF PHYSICS

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Particle in a Box

Schrödinger's equation to a particle bound to a one-dimensional box. This special case provides lessons for understanding quantum mechanics in more complex systems. The energy of the particle is quantized as a consequence of a standing wave condition inside the box.

Consider a particle of mass m that is allowed to move only along the *x*-direction and its motion is confined to the region between hard and rigid walls located at x=0 and at x=L . Between the walls, the particle moves freely.

- This physical situation is called the infinite square well, described by the potential energy function
- $$U(x) = \begin{cases} 0, & 0 \leq x \leq L, \\ \infty, & \text{otherwise.} \end{cases}$$

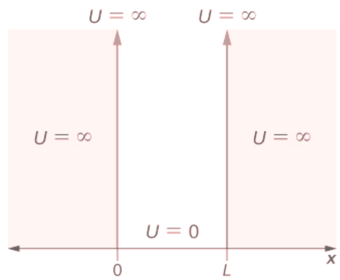
Combining this equation with Schrödinger's time-independent wave equation gives

- $$\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)\,, \text{for } 0 \leq x \leq L$$

where *E* is the total energy of the particle. What types of solutions do we expect? The energy of the particle is a positive number,

- The value of the wave function is positive (right side of the equation), the curvature of the wave function is negative, or concave down (left side of the equation).
- Similarly, if the value of the wave function is negative (right side of the equation), the curvature of the wave function is positive or concave up (left side of equation).
- This condition is met by an oscillating wave function, such as a Sine or Cosine wave. Since these waves are confined to the box, we envision standing waves with fixed endpoints at x=0 and x=L.

The potential energy function that confines the particle in a one-dimensional box.



Solutions $\psi(x)$ to this equation have a probabilistic interpretation.

- In particular, the square $|\psi(x)|^2$ represents the probability density of finding the particle at a particular location *x*.
- This function must be integrated to determine the probability of finding the particle in some interval of space.
- Therefore looking for a normalizable solution that satisfies the following normalization condition:

➢ $$\int_0^L dx|\psi(x)|^2 = 1.$$

The walls are rigid and impenetrable, which means that the particle is never found beyond the wall. Mathematically, this means that the solution must vanish at the walls:

➢ $$\psi(0) = \psi(L) = 0.$$

We expect oscillating solutions, so the most general solution to this equation is

➢ $$\psi_k(x) = A_k \cos kx + B_k \sin kx$$

where *k* is the wave number, and A_k and B_k are constants. Applying the boundary condition expressed by figure gives

$$\psi_k(0) = A_k \cos(k0) + B_k \sin(k0) = A_k = 0.$$

$A_k=0$, the solution must be

$$\psi_k(x) = B_k \sin kx.$$

If B_k is zero for all values of *x* and the normalization condition, cannot be satisfied. Assuming B_k=/0, figure for x=L then gives

$$0 = B_k \sin(kL) \sin(kL) = 0 kL = n\pi, n = 1, 2, 3, ...$$

The discard the n=0 solution because $\psi(x)$ for this quantum number would be zero every where—an un-normalizable and therefore unphysical solution. Substituting into figure gives

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}(B_k \sin(kx)) = E(B_k \sin(kx)).$$

Computing these derivatives leads to

- $E = E_k = \frac{\hbar^2 k^2}{2m}$.

According to de Broglie, p=ħk so this expression implies that the total energy is equal to the kinetic energy, consistent with our assumption that the "particle moves freely." Combining the results of figure.

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2},\ n = 1, 2, 3, ...$$

A particle bound to a one-dimensional box can only have certain discrete (quantized) values of energy. Further, the particle cannot have a zero kinetic energy—it is impossible for a particle bound to a box to be "at rest."

- To evaluate the allowed wave functions that correspond to these energies, we must find the normalization constant B_n. We impose the normalization condition figure on the wave function

$$\psi_n(x) = B_n \sin n\pi x/L$$

$$1 = \int_0^L dx |\psi_n(x)|^2 = \int_0^L dx B_n^2 \sin^2 \frac{n\pi}{L} x = B_n^2 \int_0^L dx \sin^2 \frac{n\pi}{L} x = B_n^2 \frac{L}{2} B_n = \sqrt{\frac{2}{L}}.$$

Hence, the wave functions that correspond to the energy values given in (figure.) are

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, n = 1, 2, 3, ...$$

For the lowest energy state or ground state energy, we have

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2},\ \psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right).$$

All other energy states can be expressed as

$$E_n = n^2 E_1, \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right).$$

The index *n* is called the energy quantum number or principal quantum number.

- The state for n=2 is the first excited state, the state for n=3 is the second excited state, and so on. The first three quantum states (for n=1,2and3 of a particle in a box are shown in figure.
- The wave functions in (fig) are sometimes referred to as the "states of definite energy." Particles in these states are said to occupy energy levels, which are represented by the horizontal lines. Energy levels are analogous to rungs of a ladder that the particle can "climb" as it gains or loses energy.
- The wave functions in (figure.) are also called stationary states and standing wave states. These functions are "stationary," because their probability density functions, $|(x,t)|^2$, do not vary in time, and "standing waves" because their real and imaginary parts oscillate up and down like a standing wave—like a rope waving between two children on a playground. Stationary states are states of definite energy.
- Energy quantization is a consequence of the boundary conditions. If the particle is not confined to a box but wanders freely, the allowed energies are continuous. However, in this case, only certain energies(E_1,$4E_1$,$9E_1$…) are allowed. The energy difference between adjacent energy levels is given by
  - $E_{n+1,n} = E_{n+1} - E_n = (n+1)^2 E_1 - n^2 E_1 = (2n+1) E_1.$

Conservation of energy demands that if the energy of the system changes, the energy difference is carried in some other form of energy. The expectation value of the position for a particle in a box is given by

- $x = \int_0^L dx \psi_n^*(x) x \psi_n(x) = \int_0^L dx x |\psi_n^*(x)|^2 = \int_0^L dx x \frac{2}{L} \sin^2 \frac{n\pi x}{L} = \frac{L}{2}.$

We can also find the expectation value of the momentum or average momentum of a large number of particles in a given state:

$$
\begin{aligned}
p &= \int_0^L dx\psi_n^*(x)\left[i\hbar\tfrac{d}{dx}\psi_n(x)\right] \\
&= i\hbar\int_0^L dx\sqrt{\tfrac{2}{L}}\sin\tfrac{n\pi x}{L}\left[\tfrac{d}{dx}\sqrt{\tfrac{2}{L}}\sin\tfrac{n\pi x}{L}\right] = i\tfrac{2\hbar}{L}\int_0^L dx\sin\tfrac{n\pi x}{L}\left[\tfrac{n\pi}{L}\cos\tfrac{n\pi x}{L}\right] \\
&= i\tfrac{2n\pi\hbar}{L^2}\int_0^L dx\tfrac{1}{2}\sin\tfrac{2n\pi x}{L} = i\tfrac{n\pi\hbar}{L^2}\,\tfrac{L}{2n\pi}\int_0^{2n} d\phi\sin\phi = i\tfrac{\hbar}{2L}0 = 0.
\end{aligned}
$$

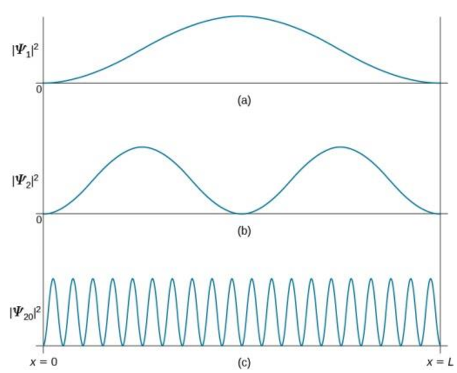
The average particle energy in the *nth* quantum state—its expectation value of energy—is

➢ $E_n = E = n^2\frac{\pi^2\hbar^2}{2m}.$

The result is not surprising because the standing wave state is a state of definite energy. Any energy measurement of this system must return a value equal to one of these allowed energies. Illustrate how this principle works for a quantum particle in a box, we plot the probability density distribution

➢ $|\psi_n(x)|^2 = \frac{2}{L}\sin^2(nx/L)$

for finding the particle around location *x* between the walls when the particle is in quantum state ψ_n. figure.The probability density distribution $|\psi_n(x)|^2$ for a quantum particle in a box for: (a) the ground state, n=1; (b) the first excited state, n=2; and, (c) the nineteenth excited state, n=20.



The probability density of finding a classical particle between *x* and x+x depends on how much time the particle spends in this region.