

# Particle in a Box (continued)

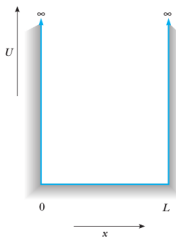
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# Particle in an Infinite Potential Well

We consider the potential

$$\begin{aligned} V(x) &= 0 \text{ for } 0 < x < L \\ &= \infty \text{ for all other } x. \end{aligned}$$



We solve time independent Schroedinger's equation

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x),$$

for this potential.

# Particle in an Infinite Potential Well

- Solution of this equation gives us the **energy eigenvalues and the corresponding eigenfunctions**.
- The boundary conditions lead to the quantization condition  $kL = n\pi$ .
- The energy eigenfunctions and eigenvalues are

$$\phi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right), \quad E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$

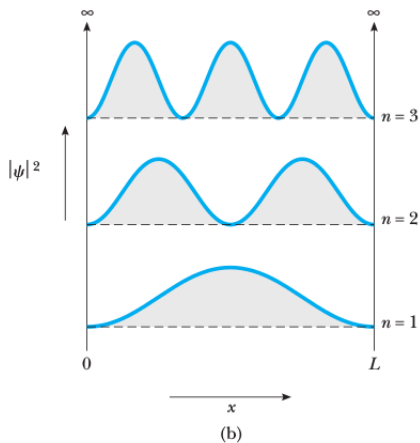
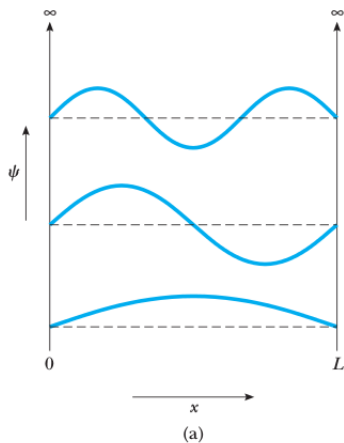
$$\phi_2(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right), \quad E_2 = \frac{4\pi^2 \hbar^2}{2mL^2} \dots$$

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

- These eigenfunctions form an **orthonormal** set.

$$\int_0^L \phi_m(x)^* \phi_n(x) dx = \delta_{mn}$$

# Graphs of Energy Eigenstates



# Properties of Energy Eigenstates

- Suppose the particle is in the ground state of the infinite potential well.

$$\psi(x, t) = \phi_1(x) \exp\left(\frac{-iE_1 t}{\hbar}\right).$$

I do an experiment where I measure the energy of the particle.

- What result do I get? Since the particle is in the ground state, my measurement gives the result  $E_1$ .
- What happens to the particle, after I have made the measurement? In this case, **nothing**.
- Why? An energy measurement makes the wave function **collapse** into one of the energy eigenstates. Since the original state is an energy eigenstate, it remains in the same state after the energy measurement.

# Properties of Energy Eigenstates

- Once again I start with the particle in the ground state, but this time I measure its momentum.
- The ground state can be written as the linear combination linear combination

$$\phi_1(x) = \sqrt{2/L} \sin(\pi x/L) = \frac{\sqrt{2/L}}{2i} [\exp(i\pi x/L) - \exp(-i\pi x/L)].$$

- So the ground state (and every other state in this problem) are linear combinations of two momentum states  $\hbar k$  and  $-\hbar k$ . So the momentum measurement gives one of these two values as a result.
- Suppose we got the answer  $\hbar k$ . The momentum measurement makes the ground state collapse into a momentum eigenstate. If we immediately make another momentum measurement, we get the result  $\hbar k$  again.

# Properties of Energy Eigenstates

- Suppose we wait for a bit and then make the momentum measurement. Now it is possible to get either of the results  $\hbar k$  or  $-\hbar k$ .
- Why is that? Did not our first momentum measurement force the particle into a momentum eigenstate?
- Yes. But then we left the particle alone. The only influence on the particle is only the potential. It is this potential and the kinetic energy which guide the further time evolution of the wave function.
- Our first momentum measurement has forced the particle into one of the two momentum eigenstates of the ground state. Later, this state becomes the usual ground state. When there is no external influence on the particle, the wave function of the particle should be either an energy eigenstate or a linear combination of energy eigenstates.
- Here the momentum measurement never took it out of the ground state. Hence at later times, the wave function is the general ground state, not just the  $\hbar k$  part of the ground state.

# Properties of Energy Eigenstates

- Suppose we put the particle in the ground ( $n = 1$ ) state of the box. We measure its position and find  $x = L/2$ . What happens to particle after this measurement?
- The measurement changes the wave function of the particle from  $\phi_1(x)$  into a function which is strongly peaked at  $x = L/2$ . This wave function can be written as a superposition of  $\phi_n$ s,

$$\psi(x) = \sum_n c_n \phi_n(x),$$

with  $\sum_n |c_n|^2 = 1$ , as the normalization condition.

- This is possible because the the energy eigenfunctions form a **complete set**. Because of this **completeness** property, any arbitrary wave function, which vanishes at  $x = 0$  and at  $x = L$ , can be written as a superposition (or linear combination) of the energy eigenfunctions.
- This is true not only for the infinite square well potential but for any potential.



# Properties of Energy Eigenstates

- Immediately after measuring the position and getting the answer  $x = L/2$ , I measure the energy of the particle. What answer do I get?
- Energy measurement can only probe the energy and it collapses the wave function into one of the energy eigenstates. Before the energy measurement, the particle is in the state

$$\psi(x) = \sum_n c_n \phi_n(x).$$

For a particle with this wave function, the **amplitude** of finding the particle in the energy eigenstate  $\phi_m(x)$  is given by

$$\int_0^L \phi_m^*(x) \psi(x) dx = \sum_n c_n \int_0^L \phi_m^*(x) \phi_n(x) dx = c_m.$$

The probability of finding it in the energy eigenstate  $\phi_m(x)$  is  $|c_m|^2$ .

# Properties of Energy Eigenstates

- In the above example, I said that my measurement gave the result  $x = L/2$ . But  $\phi_n(x = L/2) = 0$  for all even  $n$ .
- Therefore, in the superposition, the coefficients  $c_n = 0$  for all even  $n$ , because for these wave functions the probability of finding the particle in the neighbourhood of  $L/2$  is zero.
- Let us now consider a different situation. After measuring the position, suppose I do nothing. What happens to the wave function? How does it **evolve** in time?
- I define the moment of position measurement to be  $t = 0$ . Therefore

$$\psi(x, 0) = \sum_n c_n \phi_n(x).$$

- $\psi(x, t)$  should satisfy time dependent Schrodinger's equation. In time, that equation is a first order differential equation.
- Therefore, given the initial condition  $\psi(x, 0)$ , we should get a unique solution to this equation.

# Time Evolution of the Superposition of Eigenstates

- Unlike an energy eigenstate,  $\psi(x, 0)$  does not have a well defined energy. So we can't just say that the time evolution is given by the multiplication of the factor  $\exp(-iEt/\hbar)$ .
- The time dependent Schroedinger's equation is

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x, t).$$

- Let us try the old technique of separation of variables, but with the awareness that the initial wave function is a superposition.

$$\psi(x, t) = \sum_n c_n \phi_n(x) \xi_n(t),$$

where the functions  $\xi_n(t)$  carry only the time dependence and they are different for different values of  $n$ .

# Time Evolution of the Superposition of Eigenstates

- Substituting this form of  $\psi(x, t)$  in the time dependent Schroedinger's equation, we get

$$\sum_n c_n \phi_n(x) i\hbar \frac{\partial \xi_n(t)}{\partial t} = \sum_n c_n \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \phi_n(x) \xi_n(t).$$

- Given that

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \phi_n(x) = E_n \phi_n(x),$$

we get

$$\sum_n c_n \phi_n(x) i\hbar \frac{\partial \xi_n(t)}{\partial t} = \sum_n c_n E_n \phi_n(x) \xi_n(t).$$

- Since  $\phi_n(x)$  are orthonormal, their coefficients on both sides should be equal.

# Time Evolution of the Superposition of Eigenstates

- Equating coefficients of  $\phi_n(x)$  on either side, we get

$$i\hbar c_n \frac{\partial \xi_n(t)}{\partial t} = c_n E_n \xi_n(t)$$

Hence  $\xi_n(t)$  are given by

$$\xi_n(t) = \exp(-iE_n t/\hbar),$$

leading to

$$\psi(x, t) = \sum_n c_n \exp(-iE_n t/\hbar) \phi_n(x).$$

- The time evolution of an energy eigenstate is always given by the factor  $\exp(-iE_n t/\hbar)$ .
- If the wave function consists of a single energy eigenstate  $\phi_n(x)$ , then  $\psi(x, t) = \exp(-iE_n t/\hbar) \phi_n(x)$ .
- If the wave function is a superposition of energy eigenstates, each different eigenstate evolves in its own way, completely unaware of the existence of the other energy eigenstates in the superposition.

# Probability of Localizing the Particle

- Let us consider a somewhat different problem. Consider the a classical particle, trapped in a box of width  $L$ . The probability density for finding it at any point is the same. So the probability of finding finding it between  $L/4$  and  $3L/4$  is 0.5.
- Let us calculate this probability for finding a quantum particle in a box. This is given by

$$\int_{L/4}^{3L/4} |\psi(x)|^2 dx.$$

If we assume that the particle is in the ground state this probability is equal to

$$\begin{aligned} P &= \frac{2}{L} \int_{L/4}^{3L/4} \sin^2 \left( \frac{\pi x}{L} \right) dx \\ &= \frac{1}{L} \int_{L/4}^{3L/4} \left[ 1 - \cos \left( \frac{2\pi x}{L} \right) \right] dx \end{aligned}$$

# Probability of Localizing the Particle

$$\begin{aligned} P &= \int_{1/4}^{3/4} [1 - \cos(2\pi y)] dy \text{ where } y = x/L \\ &= \left[ \frac{1}{2} - \frac{1}{2\pi} (\sin(3\pi/2) - \sin(\pi/2)) \right] = 0.818. \end{aligned}$$

The quantum particle, in the ground state, spends most of its time in the middle of the box!

Let us repeat this calculation for the particle in the state  $\phi_n(x)$ .

$$\begin{aligned} P_n &= \frac{2}{L} \int_{L/4}^{3L/4} \sin^2 \left( \frac{n\pi x}{L} \right) dx \\ &= \frac{1}{L} \int_{L/4}^{3L/4} \left[ 1 - \cos \left( \frac{2n\pi x}{L} \right) \right] dx \end{aligned}$$

# Probability of Localizing the Particle

- Doing the integrations, we get

$$P_n = \left[ \frac{1}{2} - \frac{1}{2\pi n} (\sin(3n\pi/2) - \sin(n\pi/2)) \right]$$

- $P_n = 0.5$  for eigenstates with  $n$  even. This is just a reflection of the fact that  $|\phi_n(x)|^2$  is symmetric about  $x = L/4$  and about  $x = 3L/4$  for these states.
- For odd  $n$  states, the probability keeps swinging above and below 0.5. But for large  $n$ , because of the  $1/n$  factor in the second term, these swings are less and less important and the quantum probability approaches the classical probability of 0.5.