

# Chapter 34

## Quantum Mechanics

- The Wave Function and Its Interpretation
- The Heisenberg Uncertainty Principle
- The Schrödinger Equation
- Particle in an Infinitely Deep Square Well Potential
- \*Finite Potential Well
- \*Tunneling Through a Barrier

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1927 Solvay Conference

## § 31-1 The Wave Function and Its Interpretation

### 1. The wave function $\Psi(x, y, z, t)$

de Broglie matter wave:  $\lambda = h / p$

**Wave function  $\Psi$ :** wave displacement of a matter wave.

### 2. Interpretation of $\Psi(x, y, z, t)$

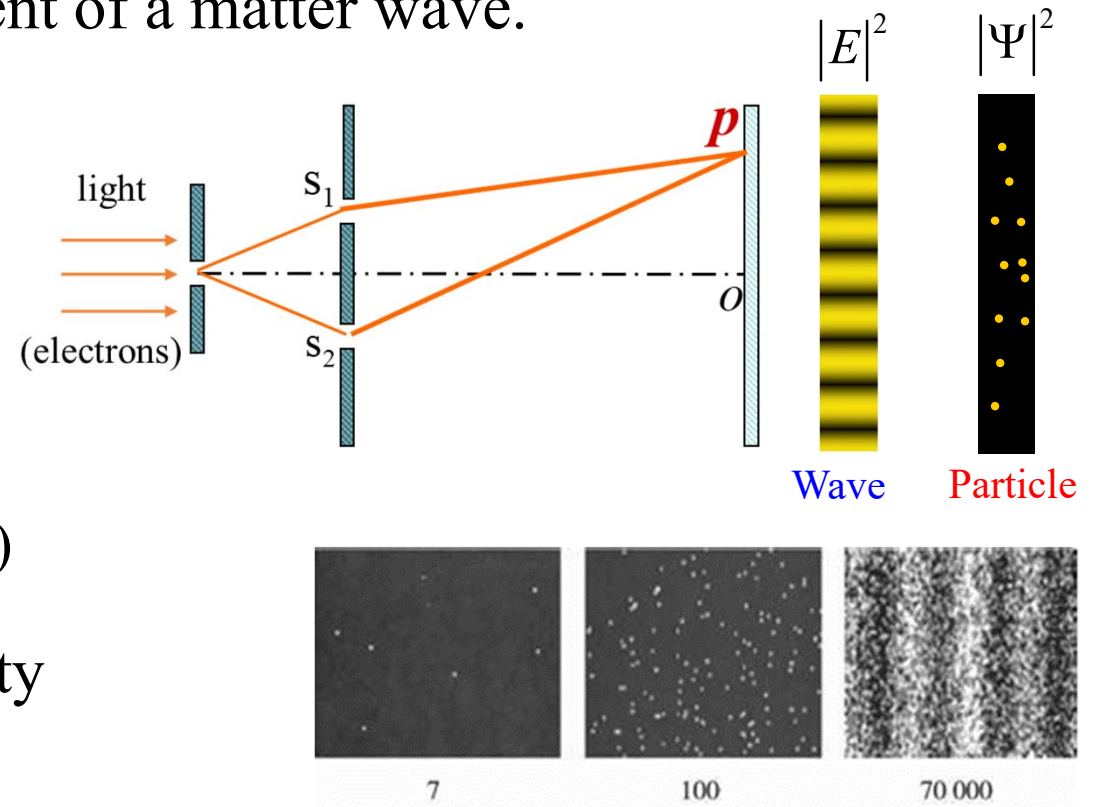
#### (1) View of wave

$$I \propto |E|^2$$

#### (2) View of particle

$$I \propto |\Psi|^2 \propto N \text{ (number of particles)}$$

$N$ : proportional to the probability of particle occurrence.



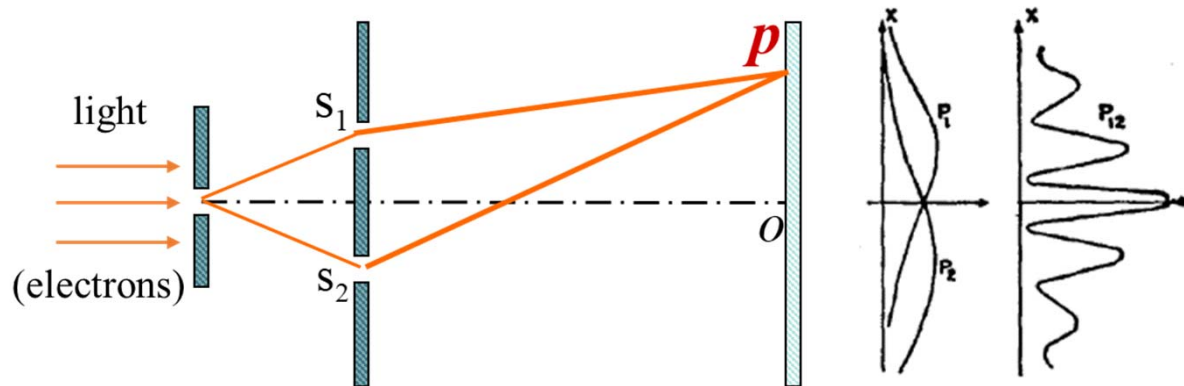
## Interpretation of $\Psi(x, y, z, t)$ (Max Born, Nobel 1954):

$|\Psi(x, y, z, t)|^2$  represents the probability of finding the particle **in a unit volume** at the given position and time.

$|\Psi(x, y, z, t)|^2$  ——— **probability density**:

$$\int |\Psi(x, y, z, t)|^2 dV = \int |\Psi(x, y, z, t)|^2 dx dy dz = 1$$

**Normalization condition**

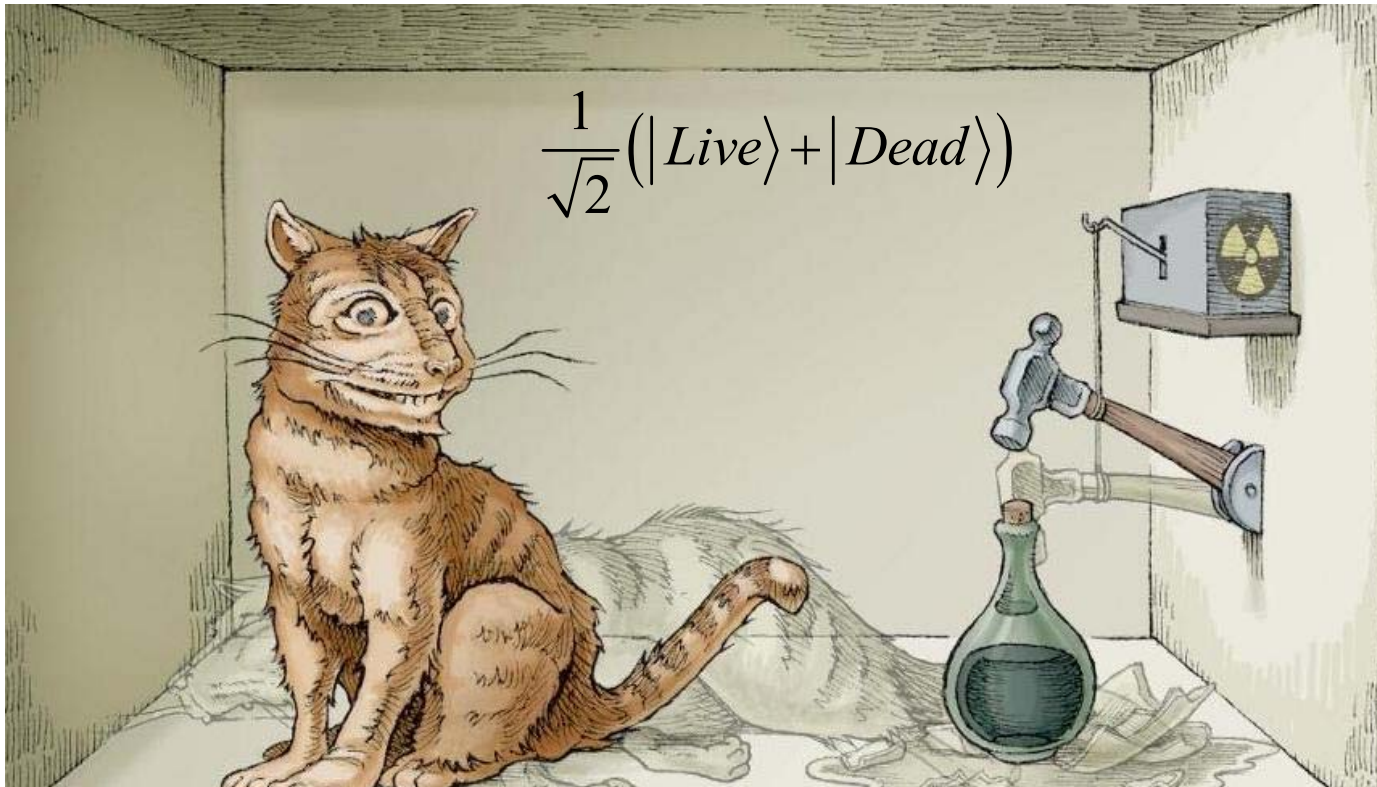


$$P_{12} = |\Psi_1 + \Psi_2|^2 \neq P_1 + P_2$$
$$(P_1 = |\Psi_1|^2, P_2 = |\Psi_2|^2)$$

**Note:** We cannot predict-or even follow-the path of a single particle precisely through space and time.

The particle passed through both slits at the same time, interfering with itself.

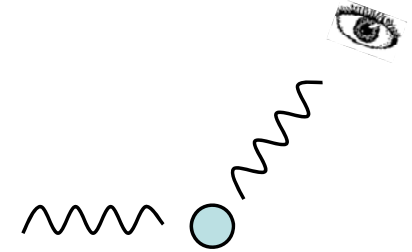
## Superposition state & Schrödinger cat:



For double-slit experiment, if we can **measure** which slit the particle passes, the measurement disturbs the state of particle.

## § 31-2 The Heisenberg Uncertainty Principle

- ◆ We measure (observe) objects by using waves;
- ◆ Measurement disturbs the state of the object;



**position uncertainty  
(resolution):**

$$\Delta x \approx \lambda$$

**momentum  
uncertainty:**

$$\Delta p_x = \frac{h}{\lambda}$$

- ◆ Always an uncertainty in position or momentum, their relation:

$$(\Delta x)(\Delta p_x) \approx h$$

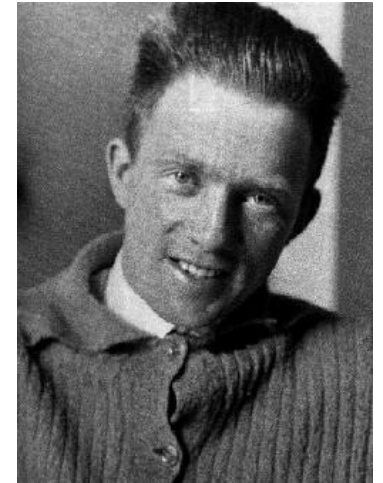
The precise relationship:  $(\Delta x)(\Delta p_x) \geq \hbar = \frac{h}{2\pi}$

**The uncertainty  
principle**

## Heisenberg uncertainty principle:

The position and the momentum of a particle can not be precisely determined simultaneously.

$$(\Delta x)(\Delta p_x) \geq \hbar = \frac{h}{2\pi}$$



W. K. Heisenberg  
Nobel 1932

- (1) It is a natural result of **duality**;
- (2) A **criterion** of classical and quantum physics;
- (3) The uncertainty is **inherent** rather than caused by the limitation of instruments or methods;
- (4) Microscopic particle does not have a precise position and momentum at the same time.

## Other forms of uncertainty principle:

$$(\Delta E)(\Delta t) \geq \hbar = \frac{h}{2\pi}$$

$$(\Delta L_z)(\Delta \phi) \geq \hbar = \frac{h}{2\pi}$$

- Inherent principles in quantum mechanics;
- Microscopic particles will not stay at rest;
- Zero point energy (at 0K).

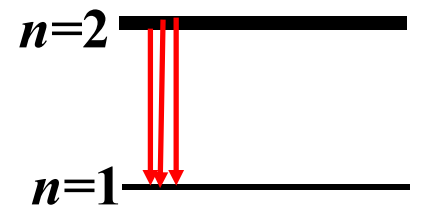
**Note:** quantum mechanics allow simultaneous precise measurements of  $P_x$  and  $y$ :

$$(\Delta y)(\Delta p_x) \gtrsim 0$$

**例：**原子激发态的平均寿命 $\Delta t=10^{-8}\text{s}$ ，求激发态能级能量的不确定量和谱线的自然宽度。

解：  $\Delta E \cdot \Delta t \geq \hbar \Rightarrow \Delta E \geq \frac{\hbar}{\Delta t} \approx 2 \times 10^{-8} \text{ eV}$

$$\Delta E = h\Delta\nu \Rightarrow \Delta\nu \approx \Delta E/h = 1.59 \times 10^7 \text{ Hz}$$



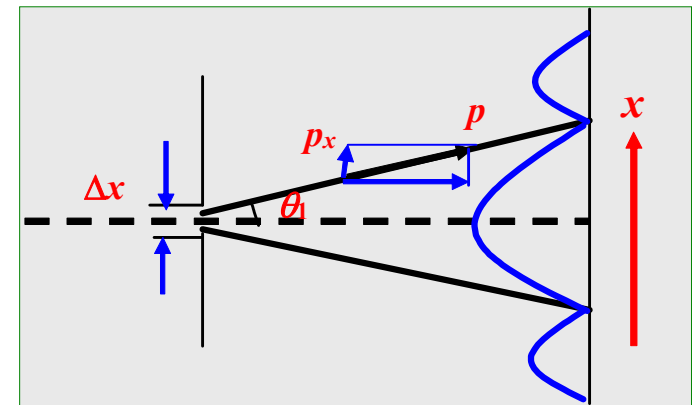
所以原子光谱存在自然宽度。

**案例分析：**单电子单缝衍射

忽略次极大，电子在  $x$  方向动量范围

$$0 \leq p_x \leq p \sin \theta_1$$

电子在  $x$  方向动量不确定度  $\Delta p_x \geq p \sin \theta_1$



单缝衍射第一级暗条纹出现位置的条件  $\Delta x \sin \theta_1 = \lambda$

$$\left. \begin{array}{l} \Delta x \sin \theta_1 = \lambda \\ \lambda = \frac{h}{p} \end{array} \right\} \Delta x \cdot \Delta p_x \geq h$$

## A quantum criterion:

**Example1:** Calculate the uncertainty in position for (a) a 150-g baseball and (b) an electron both measured with 50 m/s to a precision of 0.3%.

**Solution:** (a) 
$$\Delta x \geq \frac{\hbar}{\Delta p} = \frac{1.055 \times 10^{-34}}{0.15 \times 50 \times 0.3\%} = 4.7 \times 10^{-33} \text{ m}$$

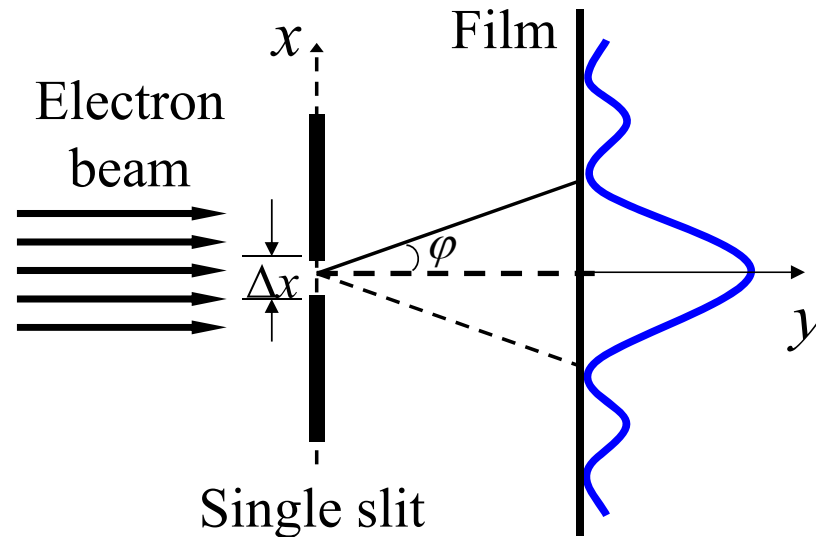
It's too small, so we can ignore the limitation

(b) 
$$\Delta x \geq \frac{\hbar}{\Delta p} = \frac{1.055 \times 10^{-34}}{9.11 \times 10^{-31} \times 50 \times 0.3\%} = 7.7 \times 10^{-4} \text{ m}$$

Quantum mechanics is necessary!

## Diffraction of electron:

**Thinking:** An electron beam (each with  $p$ ) falls on a single slit, show that the central bright fringe satisfies the uncertainty relation:  $\Delta x \Delta p_x = h$



## **Probability vs determinism:**

**Probability is inherent in nature, not a limitation on our abilities to calculate or to measure**

**——Copenhagen interpretation of quantum mechanics**

**“God does not play dice. ”                      —— A. Einstein**

**“Anyone who is not shocked by quantum theory has not understood it”                      —— N. Bohr**

## § 31-3 The Schrödinger Equation

A **free particle** (energy  $E$ , momentum  $p$ ) moves along  $x$  axis.

It can also be treated as a wave:

$$\lambda = \frac{h}{p}, \quad f = \frac{E}{h}$$

The simple harmonic form of the wave function:

$$\Psi(x, t) = A \cos(2\pi ft - \frac{2\pi}{\lambda} x) = A \cos(\frac{E}{\hbar} t - \frac{p}{\hbar} x)$$

Wave function in general form (**complex value**) :

$$\Psi(x, t) = A e^{-\frac{i}{\hbar}(Et - px)}$$



E. Schrödinger  
Nobel 1933

$$i\hbar \frac{\partial \Psi}{\partial t} = E \cdot \Psi(x, t), \quad -i\hbar \frac{\partial \Psi}{\partial x} = p \cdot \Psi(x, t)$$

**Energy operator:**  $i\hbar \frac{\partial}{\partial t}$ ; **Momentum operator:**  $-i\hbar \frac{\partial}{\partial x}$

**Nonrelativistic free particle:**  $E = p^2 / 2m$

$$\Rightarrow i\hbar \frac{\partial \Psi}{\partial t} = E\Psi = \frac{p^2}{2m} \Psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

**Schrödinger equation  
for free particle**

For particle moves in a potential  $U(x)$ , considering the **potential energy**:

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

**1-dimensional  
Schrödinger equation**

## Conclusion

1D time-dependent Schrödinger equation:

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

3D time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + U\right)\Psi = \hat{H}\Psi$$

**Hamilton operator:**  $\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + U$

**Note:** Schrödinger equation can't be derived; it is valid only because it was checked by experiments for a wide range of situations.

If potential  $U$  is independent of time  $t$ , time  $t$  can be separated from wave function  $\Psi(x, y, z, t)$ :

$$\Psi(x, y, z, t) = \psi(x, y, z)f(t)$$

$$\Rightarrow \frac{\hat{H}\psi(x, y, z)}{\psi(x, y, z)} = i\hbar \frac{1}{f(t)} \frac{df(t)}{dt} = E \quad \Rightarrow \quad f(t) = e^{-\frac{i}{\hbar}Et}$$

Time-independent Schrödinger equation:

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + U \right) \psi = E \cdot \psi \quad \text{or} \quad \hat{H}\psi = E \cdot \psi$$

(1)  $E$ : eigen energy;    (2)  $\psi$ : stationary state / eigenstate.

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + U\right)\psi = E\psi$$

Solve the Schrödinger equation to analyze quantum systems:

- (1) Find the potential energy  $U$  of the system, and substitute it into the Schrödinger equation of the system;
- (2) Solve the Schrödinger equation, and find the wave function solutions with physical meanings:

$\Psi$  ——— **continuous, normalized, finite, and single-valued**

- (3) Each solution represents a stationary state;
- (4) The system may be in a **superposition state**:

$$\text{solution : } \Psi_1, \Psi_2 \quad \Rightarrow \quad \text{solution : } \Psi = c_1\Psi_1 + c_2\Psi_2$$

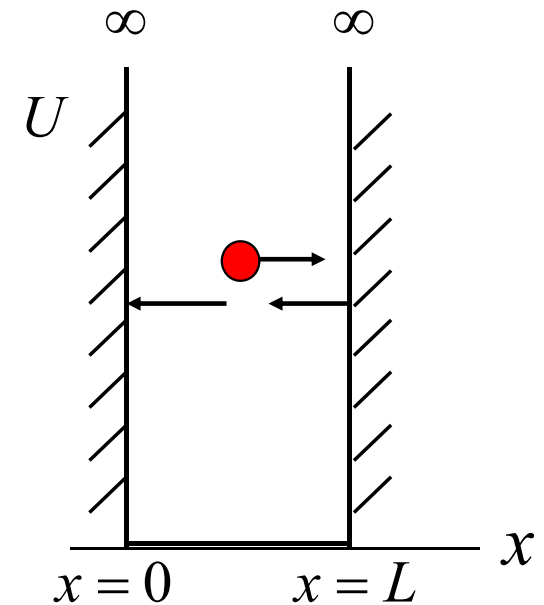
## § 31-4 Particle in an Infinitely Deep Square Well Potential

A particle is trapped in an infinitely deep square well potential or “rigid box”:

$$U(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & x \leq 0 \text{ and } x \geq L \end{cases}$$

### 1. View from classical mechanics

- The particle is trapped in the well, can't escape;
- The particle can move freely in the well until collides with the wall elastically;
- The particle has equal probability at any point;
- The particle's energy is continuous, and can vary from 0 to  $\infty$ .



## 2. View from quantum mechanics

Infinitely deep potential well means the probability that the particle appears out of the well is 0, so:

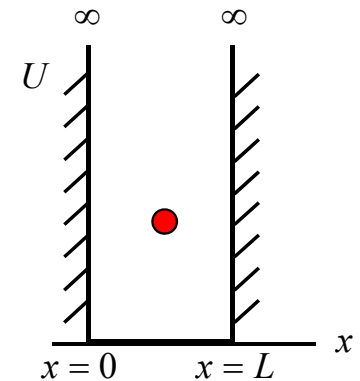
$$\psi(x) = 0, \quad (x \leq 0, \quad x \geq L)$$

Schrödinger equation in the region  $0 \leq x \leq L$  ( $U=0$ ):

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$$

or: 
$$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad \left( k^2 = \frac{2mE}{\hbar^2} \right)$$

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



$$\psi(x) = 0 \\ (x = 0, L)$$

$$\left. \begin{aligned} \psi(0) &= A \sin kx + B \cos kx \Big|_{x=0} = 0 \\ \psi(L) &= A \sin kx + B \cos kx \Big|_{x=L} = 0 \end{aligned} \right\} \Rightarrow \begin{cases} B = 0 \\ \sin(kL) = 0 \end{cases}$$

$$\sin(KL) = 0 \Rightarrow kL = n\pi, \quad (n = \pm 1, \pm 2, \dots)$$

(1) The energy of the particle is quantized

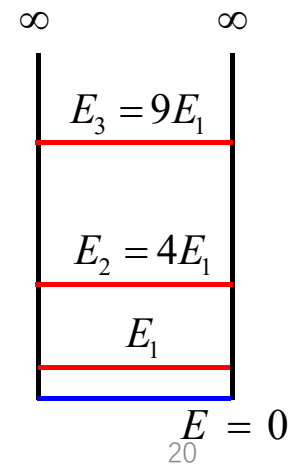
$$k = \frac{n\pi}{L}, \quad k^2 = \frac{2mE}{\hbar^2} \Rightarrow E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2}, \quad (n = \pm 1, \pm 2, \dots)$$

$E_n$ : the eigen energy;  $n$ : quantum number.

➤ The minimum energy of the particle is not zero;

$$E_1 = \pi^2 \hbar^2 / 2mL^2 \neq 0 \rightarrow \text{zero point energy}$$

➤ Microscopic particles will not stay at rest!



## (2) Standing wave form of the wave function $\psi$

$$\psi_n(x) = A \sin\left(\frac{n\pi}{L}x\right), \quad \int_0^L |\psi|^2 dx = 1 \quad \Rightarrow \quad A = \sqrt{\frac{2}{L}}$$

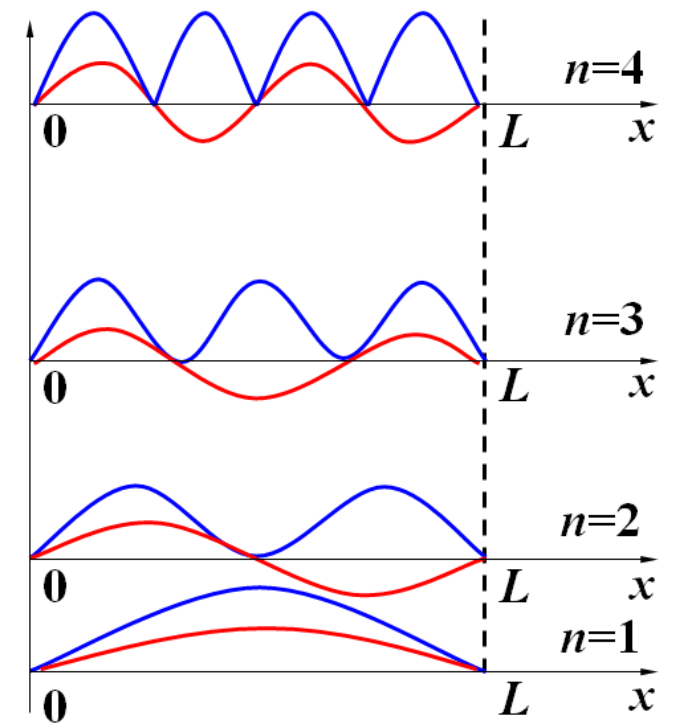
Eigen function  $\psi_n(x)$ :

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right), \quad (n = \pm 1, \pm 2, \dots)$$

The probability density of the particles appearing within the potential well is:

$$|\psi_n(x)|^2 = \frac{2}{L} \sin^2\left(\frac{n\pi}{L}x\right), \quad (n = \pm 1, \pm 2, \dots)$$

**Notice:** The probability is not uniform!



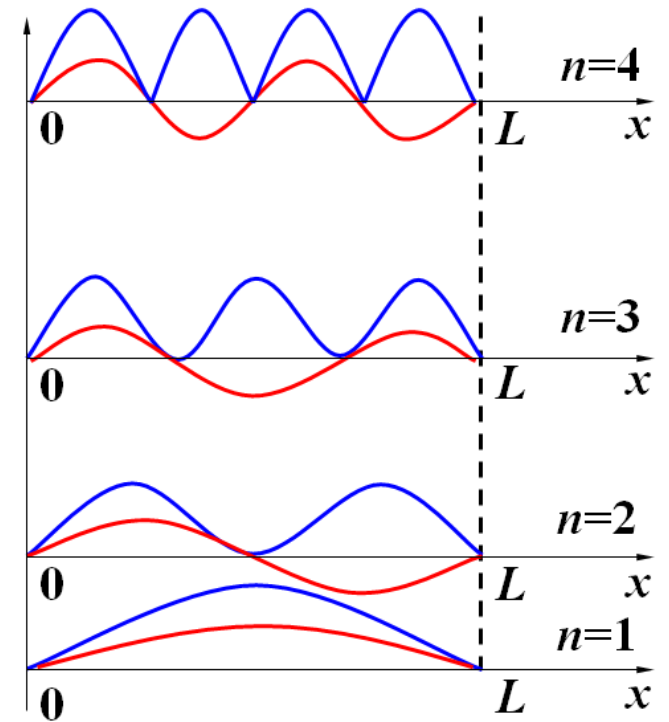
### (3) de Broglie wavelength

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} = n^2 \frac{h^2}{8mL^2} = \frac{p_n^2}{2m}, \quad p_n = \frac{h}{\lambda_n}$$
$$\Rightarrow \lambda_n = \frac{2L}{n}$$

It is consistent with the wave function  $\psi_n(x)$ .

### (4) Uncertainty principle

$$\Delta x \cdot \Delta p = L \times \frac{nh}{2L} = \frac{nh}{2} \geq \hbar$$



## Electron in the well

**Example2:** Calculate the energy of ground state and first excited state for an electron trapped in an IDSWP of width  $L = 0.1\text{nm}$ .

**Solution:** The ground state ( $n=1$ ) has energy

$$E_1 = \frac{h^2}{8mL^2} = 6.03 \times 10^{-18} \text{ J} = 37.7 \text{ eV}$$

First excited state:  $E_2 = 4E_1 = 151 \text{ eV}$

$\lambda$  of photon if jumping from  $n = 2$  to  $n = 1$  ?

## Probability in well

Example3: In the state of

$$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi}{L}x\right)$$

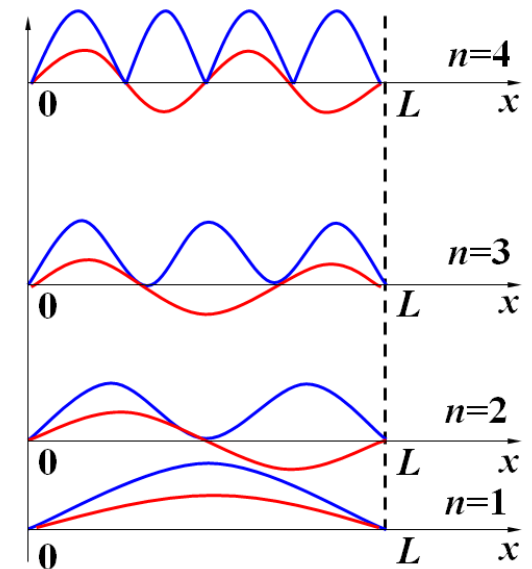
(a) Where does the particle have maximum probability densities? (b) What is the probability to find the particle in region  $0 < x < L/4$  ?

Solution: (a)

$$|\psi|^2 = \frac{2}{L} \sin^2\left(\frac{3\pi}{L}x\right)$$

$$\frac{d}{dx}|\psi|^2 = 0 \quad \text{and} \quad \frac{d^2}{dx^2}|\psi|^2 < 0$$

So:  $x = \frac{L}{6}, \frac{L}{2}, \frac{5L}{6}$

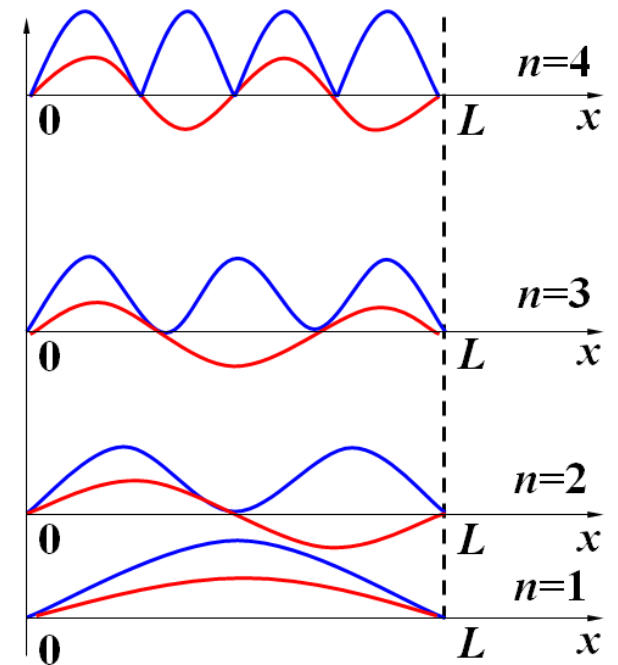


(b) What is the probability to find the particle in region  $0 < x < L/4$  ?

$$P = \int_0^{\frac{L}{4}} |\psi|^2 dx = \int_0^{\frac{L}{4}} \frac{2}{L} \sin^2\left(\frac{3\pi}{L}x\right) dx \quad \psi = \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi}{L}x\right)$$

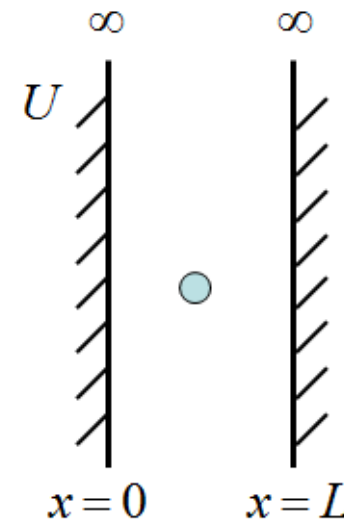
$$= \int_0^{\frac{L}{4}} \frac{1}{L} [1 - \cos\left(\frac{6\pi}{L}x\right)] dx$$

$$= \frac{1}{4} + \frac{1}{6\pi} = 0.303$$



## Probability for other $\psi$

**Homework:** A particle trapped in a special well has a wave function  $\psi=Cx(L-x)$ ,  $0 < x < L/3$ , and  $C$  is a constant. What is the probability to find the particle in region  $0 < x < L/3$  ?



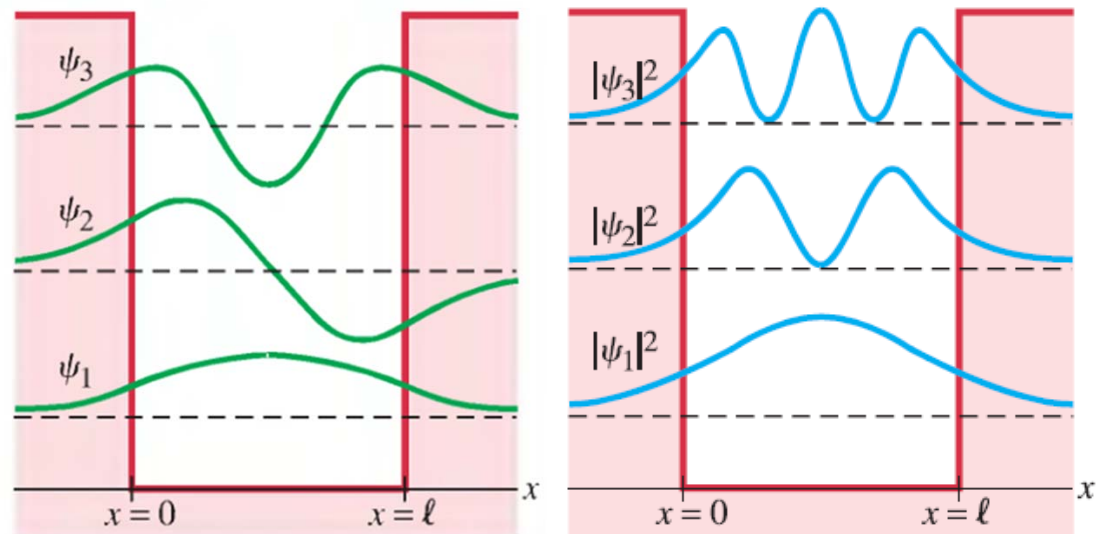
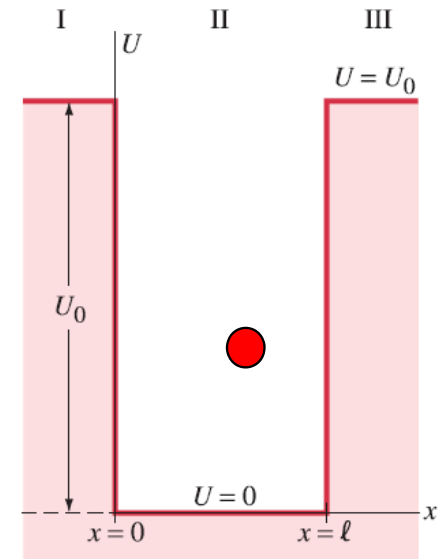
## § 31-5 \*Finite Potential Well

A particle is trapped in an finitely deep potential well:

$$U(x) = \begin{cases} 0, & 0 < x < L \\ U_0, & x \leq 0 \text{ and } x \geq l \end{cases}$$

If its energy  $E < U_0$ , can the particle jump out of the potential well?

By solving Schrödinger equation, it is found that the particle can appear out of the well.



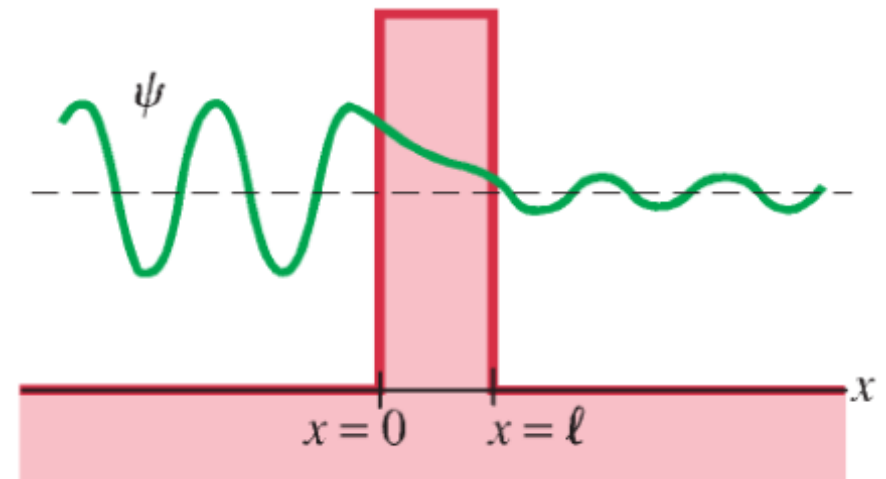
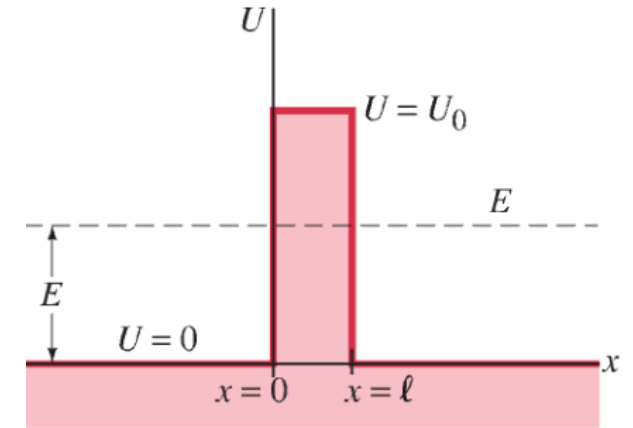
## § 31-6 \*Tunneling Through a Barrier

A particle moves from left to right encountering a thin potential barrier higher than its energy ( $U_0 > E$ ).

By solving Schrödinger equation, the results show that the particle has probability to penetrate the barrier:

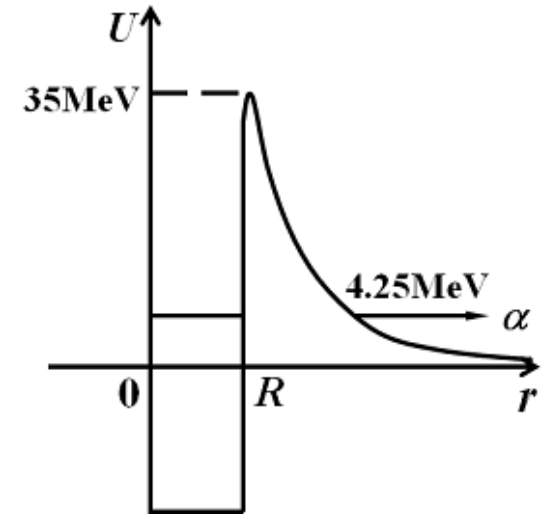
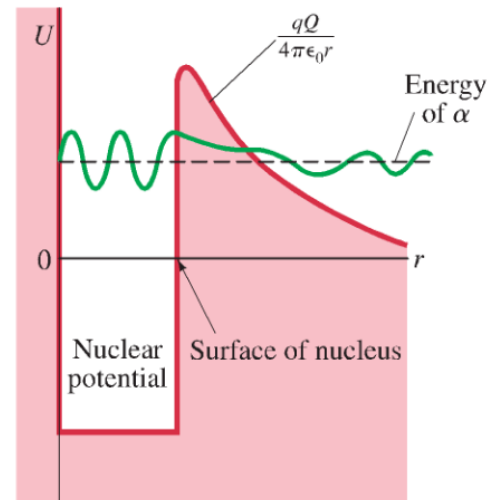
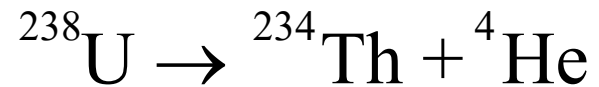
$$T \approx e^{-2Gl}, \quad \left( G = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}} \right)$$

This process is called **tunneling** through the barrier, or **barrier penetration**.

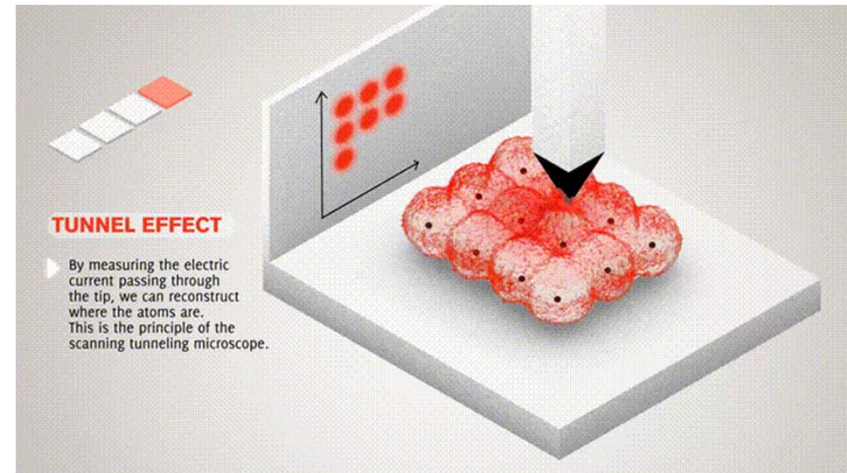
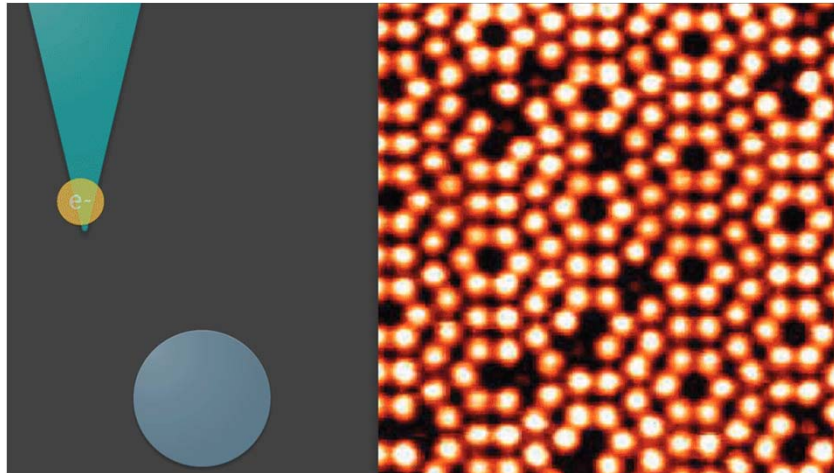


## \*Applications of tunneling

### (1) Radioactive decay



### (2) Scanning Tunneling Microscope (STM), (Invented 1981, Nobel 1986)



# Summary

## 1. Interpretation of $\Psi(x, y, z, t)$

$|\Psi(x, y, z, t)|^2$  represents the probability of finding the particle **in a unit volume** at the given position and time.

probability finding the  
particle in the region  $x_a \rightarrow x_b$ :

$$P_{x_a \rightarrow x_b} = \int_{x_a}^{x_b} |\Psi(x, t)|^2 dx$$

## 2. Normalization condition

$$\int |\Psi(x, y, z, t)|^2 dV = \int |\Psi(x, y, z, t)|^2 dx dy dz = 1$$

## 3. Heisenberg uncertainty principle

$$(\Delta x)(\Delta p_x) \geq \hbar = \frac{h}{2\pi}, \quad (\Delta E)(\Delta t) \geq \hbar = \frac{h}{2\pi}, \quad (\Delta L_z)(\Delta \phi) \geq \hbar = \frac{h}{2\pi}$$

## 4. Schrödinger equation

1D time-dependent Schrödinger equation:

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

3D time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + U\right)\Psi = \hat{H}\Psi$$

**Hamilton operator:**

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + U$$

Time-independent Schrödinger equation:

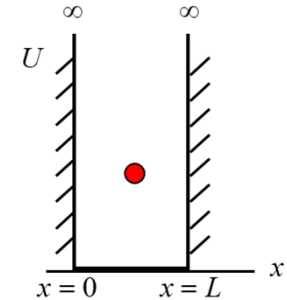
$$\left(-\frac{\hbar^2}{2m} \nabla^2 + U\right)\psi = E \cdot \psi \quad \text{or} \quad \hat{H}\psi = E \cdot \psi$$

(1)  $E$ : eigen energy;      (2)  $\psi$ : stationary state / eigenstate.

## 5. Particle in an Infinitely Deep Square Well Potential

$$U(x) = \begin{cases} 0, & 0 < x < L \\ \infty, & x \leq 0 \text{ and } x \geq L \end{cases}$$

$$\psi(x) = 0, \quad (x \leq 0, \quad x \geq L)$$



$$0 \leq x \leq L: \quad -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi, \quad \text{or:} \quad \frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad \left( k^2 = \frac{2mE}{\hbar^2} \right)$$

$$k = \frac{n\pi}{L} \Rightarrow E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2}, \quad (n = \pm 1, \pm 2, \dots)$$

$$E_1 = \pi^2 \hbar^2 / 2mL^2 \neq 0 \rightarrow \text{zero point energy}$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right), \quad (n = \pm 1, \pm 2, \dots)$$

