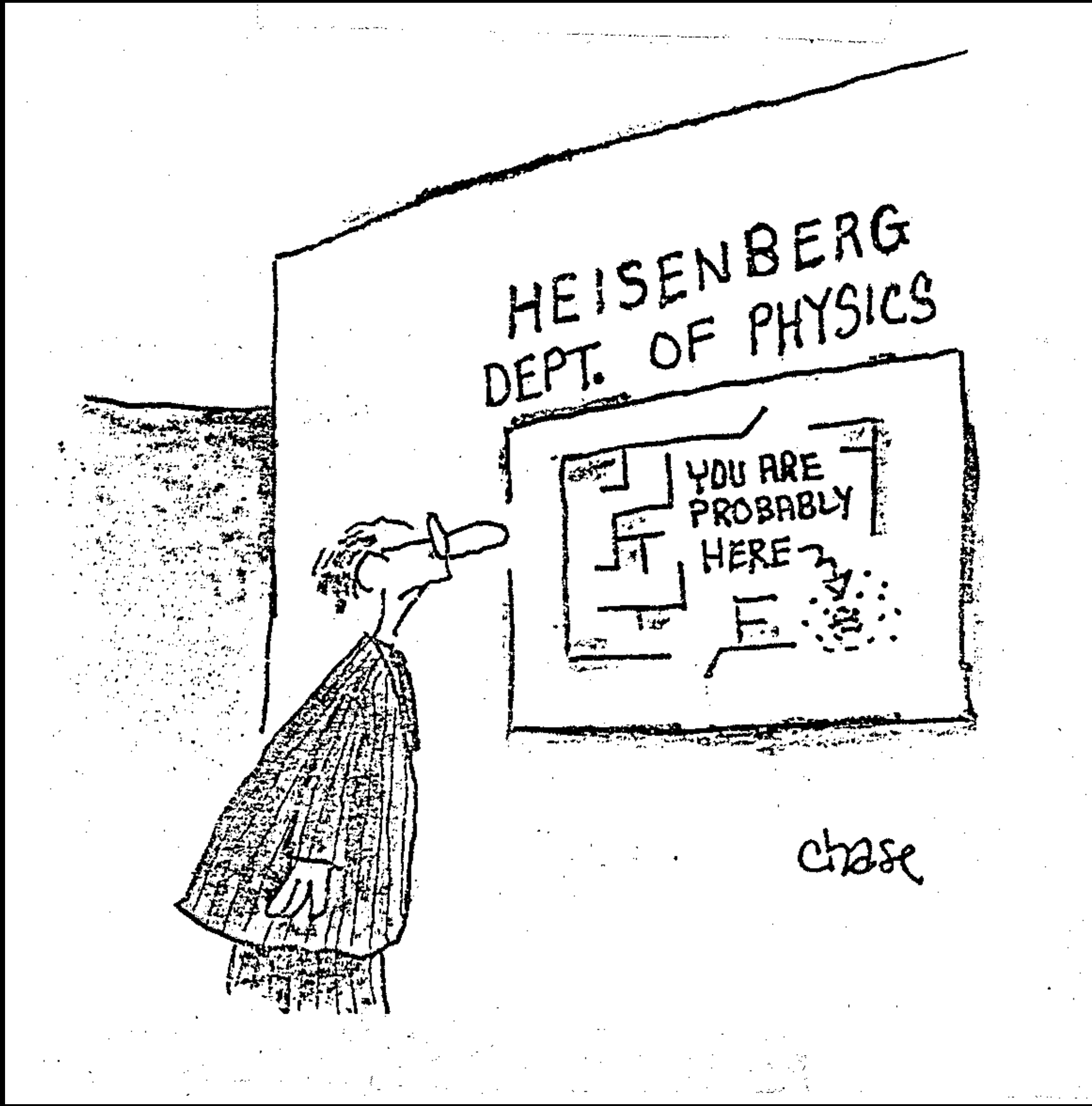


Schrödinger's Equation

Agenda today

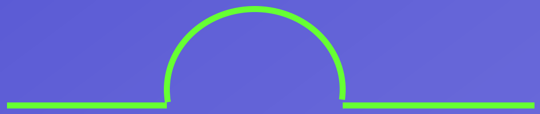
1. Wave function
2. Schrödinger's equation
3. One dimensional trap
4. Tunnel effect

Wave function(波函数）

What is it really?

Guide wave?

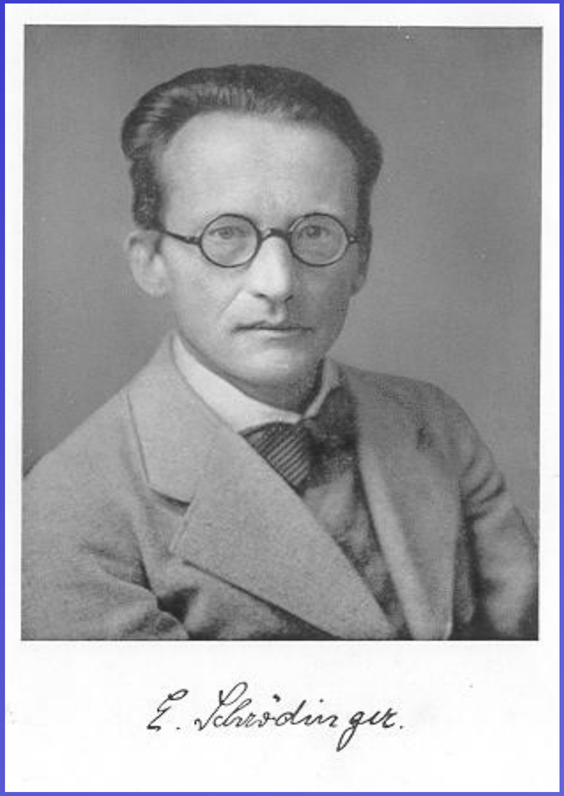
Wave packet?



Density wave?

Schrodinger's equation（薛定谔方程）:(1926)

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t)=[-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r},t)]\ \Psi(\vec{r},t)$$



Where U is the potential energy for the particle.

Laplace operator:

$$\nabla^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$$

Time-independent Schodinger equation:

定态薛定谔方程）

$$\nabla^2\Psi + \frac{2m}{\hbar^2}(E-U)\Psi = 0$$

Where Ψ is called time-independent wave function, E is the total energy of the system

In one dimensional case

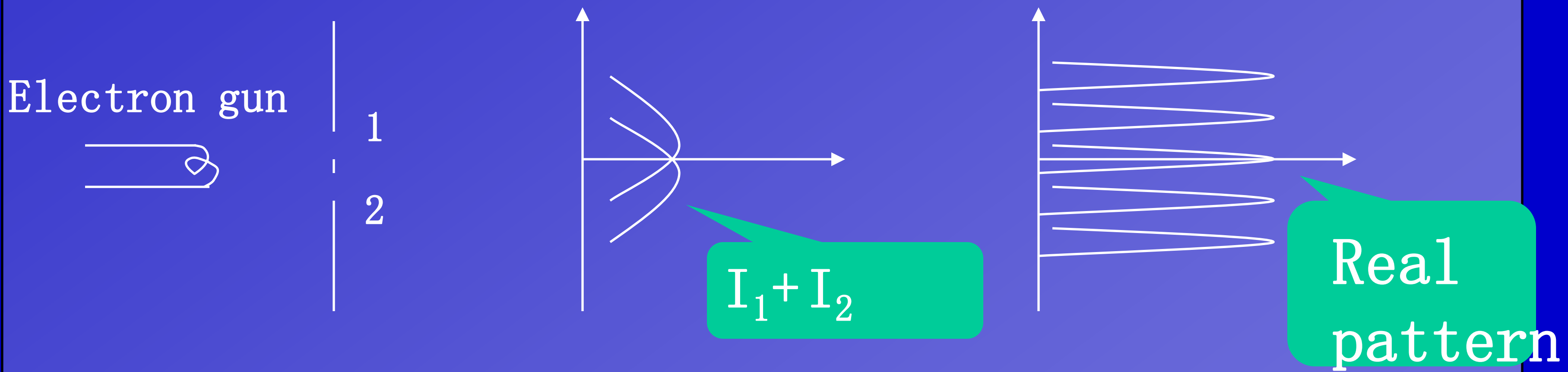
$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-U)\psi = 0$$

Born's interpretation:(1928)

Like electric field, wave function can satisfy wave equation in quantum physics.

Unlike electric field, wave function does not mean anything itself in quantum physics

Double slits experiment revisited.



The pattern of electron interference is just like that of the light, so we can use a property like E in optics whose square stands for the probability of electron appearing at certain position.

But the square of wave function's module is call probability density:

If Ψ represents a single particle, then $|\Psi|^2$ is the probability per unit volume that the particle will be found within the infinitesimal volume containing the point.

$$P(x,y,z)\,dV = |\Psi(x,y,z)|^2\,dV$$

The property of wave function:

Single-valued, limited-valued, continuous.

Normalization condition:

$$\boxed{\int_{\infty} |\Psi|^2 dV = 1}$$

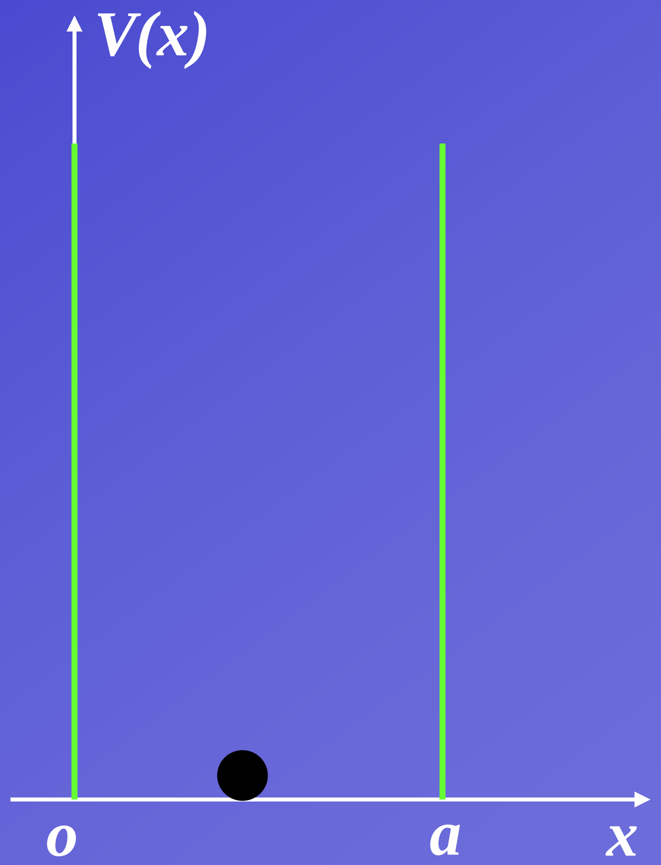
Expectation value:

$$\langle x \rangle = \int_{\infty} x |\Psi|^2 dV$$

One-dimensional trap（一维势阱）

A particle in a box

$$U(x)=\begin{cases}0 & 0<x<a\\ \infty & x\le 0,\ x\ge a\end{cases}$$



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

(1） x < 0 , x > a

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

Let: $(V-E)=\lambda^2$

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

We have $\psi=Ae^{\lambda x}+Be^{-\lambda x}$

Since Ψ(x) only have limit value

A=0 B=0

That is to say: $\psi = 0 \quad (x < 0 , x > a)$

(2)

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

0 < x < a , V = 0

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

$$Let \quad k^2 = \frac{2mE}{\hbar^2} \qquad wehave \quad \frac{d^2\psi}{dx^2} = -k^2\psi$$

$$\psi = C\sin kx + D\cos kx$$

Wave function must be continuous

$$\psi(0) = \psi(a) = 0$$

$$\psi(x) = C\sin kx + D\cos kx$$

$$\psi(0) = 0 \rightarrow D = 0$$

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

$$\psi(a) = 0 \rightarrow C\sin ka = 0$$

$$\sin ka = 0 \quad \rightarrow \quad ka = n\pi \quad (n = 1.2.\cdots)$$

$$k = \frac{n\pi}{a} \qquad \because \quad k^2 = \frac{2mE}{\hbar^2}$$

$$\frac{n^2\pi^2}{a^2} = \frac{2mE}{\hbar^2}$$

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2} \quad (n = 1, 2, 3, \cdots)$$

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

$$\psi_n(x) = C_n \sin \frac{n\pi}{a} x$$

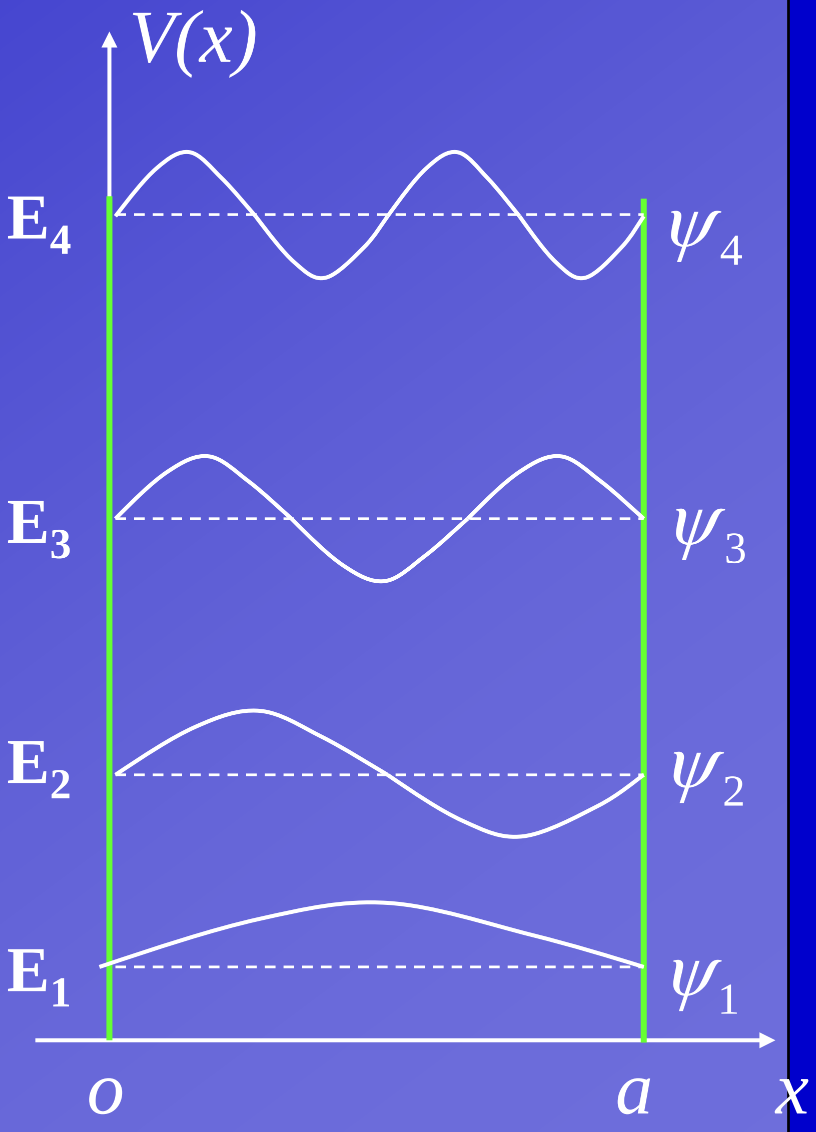
By normalization condition

$$\int_0^a \left| \psi_n(x) \right|^2 dx = 1$$

$$\int_0^a C_n^2 \sin^2 \frac{n\pi x}{a} dx = \frac{1}{2} C_n^2 a = 1 \qquad C_n = \sqrt{\frac{2}{a}}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x$$

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$$



Since the solution of the equation is stationary wave, the states are stationary state

The solution only exists in the region of $0<x<a$,

the states are called bounding state

For $n=1$ the state is called ground state;

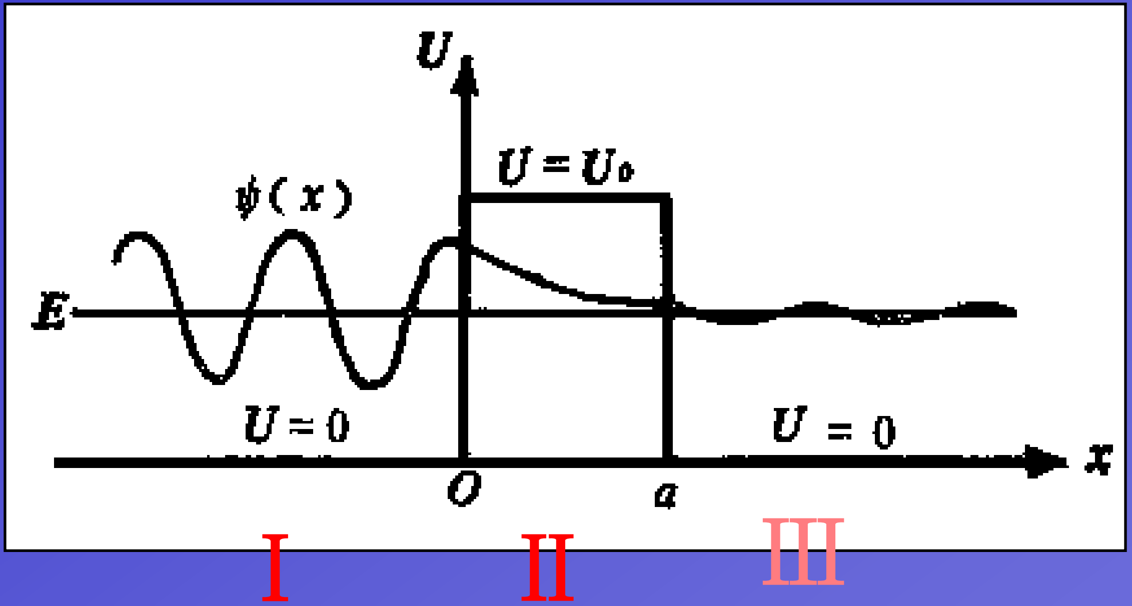
the energy is called the zero-point energy

Size effect of nanocrystallites

Quantum dots

Tunnel effect（隧道效应）

Energy barrier



The particle could pass through the barrier, even its kinetic energy is smaller than the height of the barrier.

Scanning tunneling microscope

G.Binnig

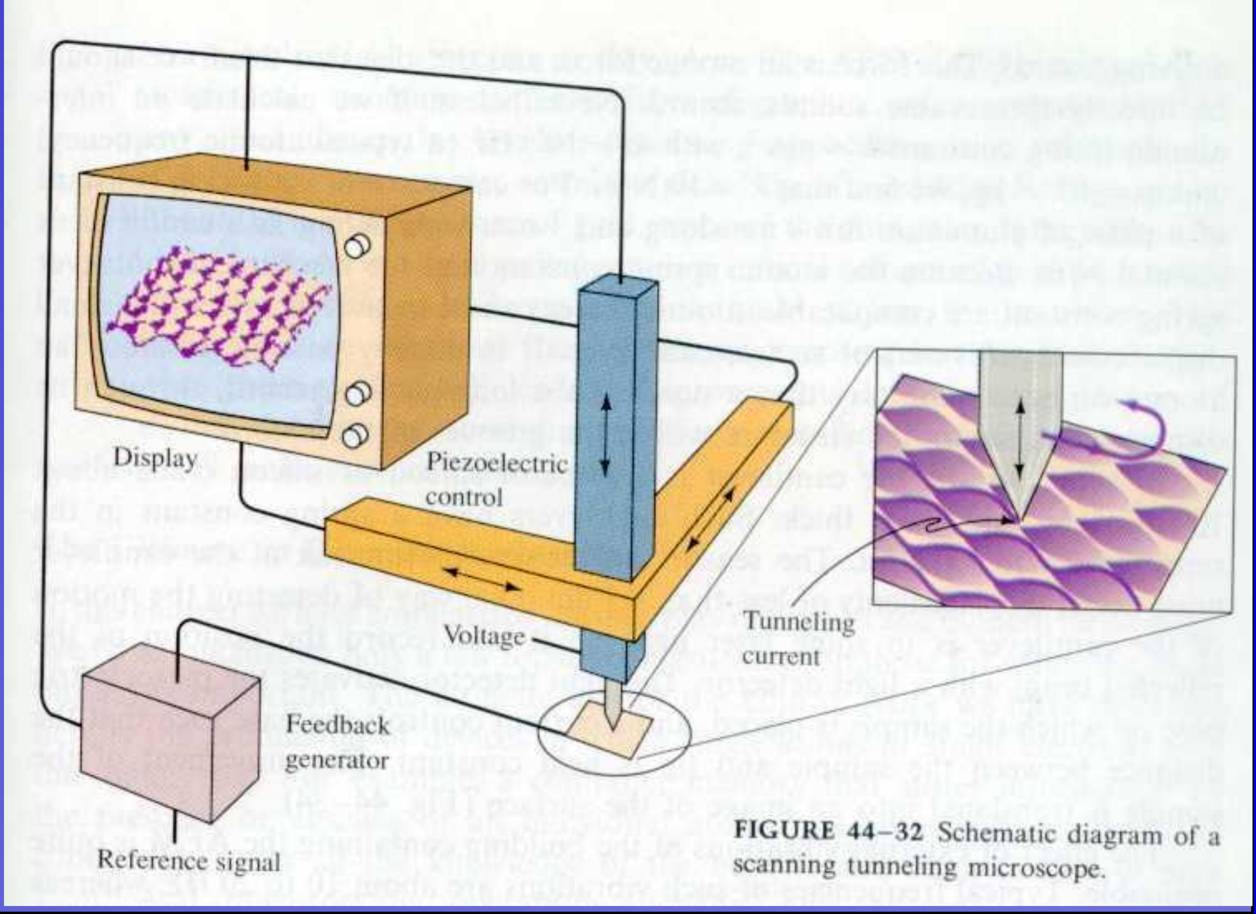


FIGURE 44–32 Schematic diagram of a scanning tunneling microscope.

Quantum corral