• PROGRAM OF “PHYSICS”

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PHYSICS 4
(Wave, Light, and Atoms)

02 credits (30 periods)

PHYSICS 4

Chapter 3
Introduction to Quantum Physics

- The Wave Property of Electrons
- De Broglie’s Theory - Matter Wave
- The Schrödinger’s Equation
- The Heisenberg’s uncertainty principle
- Particle in a square well
- Tunneling Phenomena

Nature of light

Diffraction, Interference phenomena $\rightarrow$ light has wave nature
Photoelectric, Compton's effects $\rightarrow$ light has particle nature

What is the nature of light?

ANSWER:

From a modern viewpoint,
the light has both wave and particle characteristics

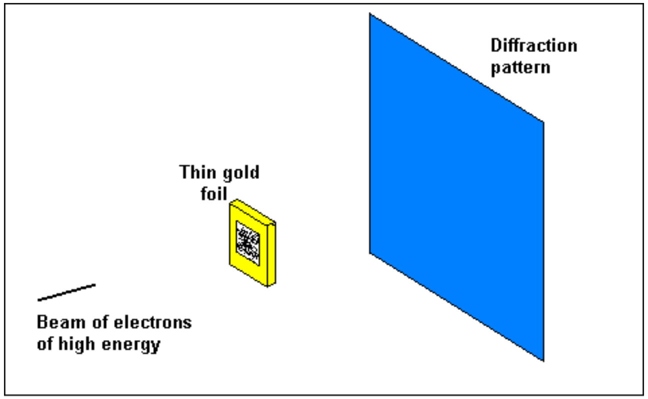
That is **The Wave-Particle Duality of Light**

"… the wave and corpuscular descriptions are only to be regarded as complementary ways of viewing one and the same objective process…" (Pauli, physicist)

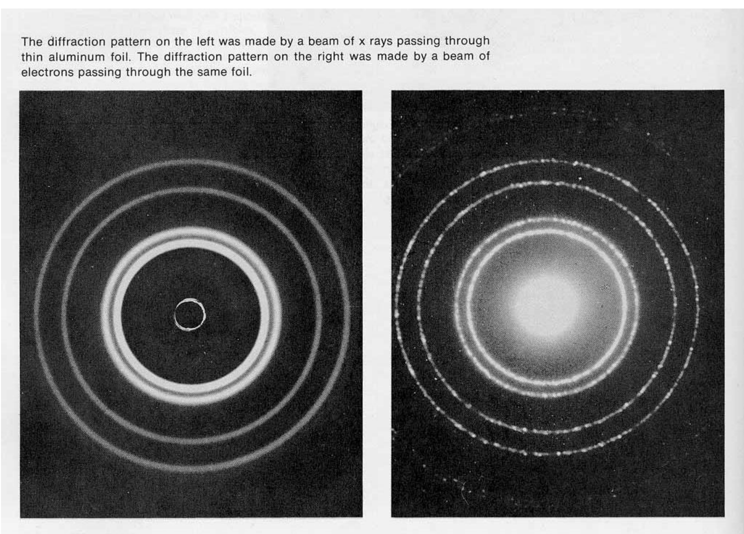
1. The Wave Property of Electrons

a. *Electron diffraction experiment*

(Davisson, Germer, Thomson, 1927)



The beam of electrons of high energy causes the creation of the diffraction pattern on the screen when passing through the thin foil.



A beam of either X rays (wave) or electrons (particle) is directed onto a target which is a gold foil

The scatter of X rays or electrons by the gold crystal produces a circular diffraction pattern on a photographic film

The pattern of the two experiments are the same

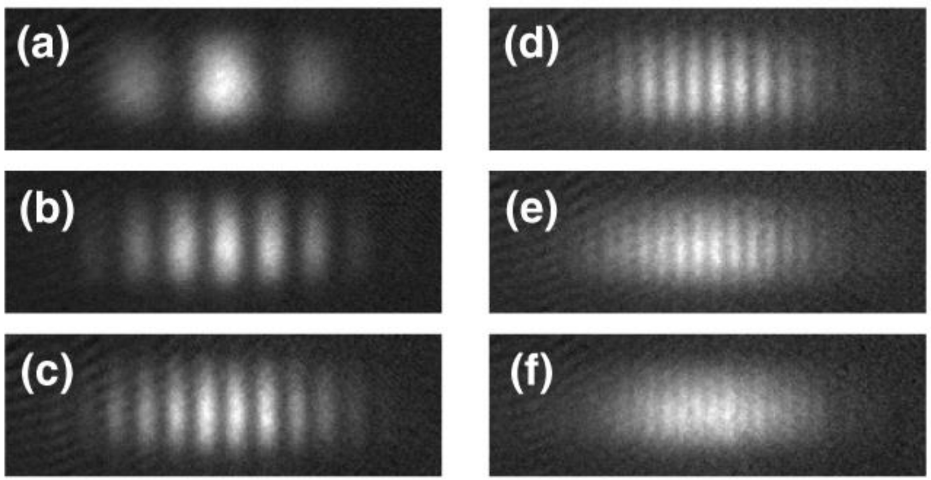
Particle could act like a wave; both X rays and electrons are WAVE

b. *Discussion*

• Similar diffraction and interference experiments have been realized with protons, neutrons, and various atoms

(see "Atomic Interferometer", Xuan Hoi DO, report of practice of Bachelor degree of Physics, University Paris-North, 1993)

In 1994, it was demonstrated with iodine molecules I_2



Wave interference patterns of **atoms**

• Small objects like electrons, protons, neutrons, atoms, and molecules travel as **waves** - we call these waves "**matter waves**"

2. De Broglie's Theory - Matter Wave

a. *De Broglie's relationships*

We recall that
for a photon (E, p) associated to an electromagnetic wave (f, λ):

$$\boxed{E = h\,f}$$

$$\boxed{\underbrace{p}_{particle} = \underbrace{h\frac{1}{\lambda}}_{wave}}$$

De Broglie's hypothesis:

To a **particle** (E, p) is associated a **matter wave**,

which has a frequency f and a wavelength λ

$$\boxed{f = \frac{E}{h}} \qquad \boxed{\lambda = \frac{h}{p}}$$

- From $f = \dfrac{E}{h}$ and $\lambda = \dfrac{h}{p}$

if we put: $\boxed{h = 2\pi\,\hbar}$ $\Rightarrow$ $\boxed{E = 2\pi f\;\hbar}$

$\Rightarrow$ $\boxed{p = \dfrac{2\pi}{\lambda}\hbar}$

$$\left.\begin{array}{l} \boxed{E = \hbar\omega} \\ \boxed{\vec{p} = \hbar\,\vec{K}} \end{array}\right\}$$ **Planck-Einstein's relationship**

λ is called **de Broglie wavelength**

b. *Conclusion. Necessity of a new science*

- When we deal with a wave, there is always some quantity that varies (the coordinate u, the electricity field E)

- For a matter wave, what is varying?

ANSWER: That is the WAVE FUNCTION

→ New brand of physics: **THE QUANTUM MECHANICS**

PROBLEM 1 In a research laboratory, electrons are accelerated to speed of 6.0×10^{6} m/s. Nearby, a 1.0×10^{-9} kg speck of dust falls through the air at a speed of 0.020m/s. Calculate the de Broglie wavelength in both case

SOLUTION

- For the electron:

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.625\times10^{-34}\,J.s}{9.11\times10^{-31}kg\times6.0\times10^{6}\,m/s}$$

$$\lambda = 1.2\times10^{-10}m$$

- For the dust speck:

$$\lambda_d = \frac{h}{p_d} = \frac{h}{mv_d} = \frac{6.625\times10^{-34}\,J.s}{1.0\times10^{-9}kg\times6.0\times0.020\,m/s}$$

$$\lambda_d = 3.3\times10^{-23}m$$

DISCUSSION: The de Broglie wavelength of the dust speck is so small that we do not observe its wavelike behavior

PROBLEM 2 An electron microscope uses 40-keV electrons. Find the wavelength of this electron.

SOLUTION

The velocity of this electron:

$$v = \sqrt{2K/m}$$

$$v = \sqrt{\frac{2\times 40\times 10^{3}\times 1.6\times 10^{-19}}{9.1\times 10^{-31}}} = 1.2\times 10^{8}\, m/s$$

The wavelength of this electron:

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{6.63\times 10^{-34}}{9.1\times 10^{-31}\times 1.2\times 10^{8}} = 6.1\times 10^{-10}\, m = 6.1\, \overset{o}{A}$$

3. The Schrödinger's Equation

a. Wave Function and Probability Density

Matter waves:

A moving particle (electron, photon) with momentum p is described by a **matter wave**; its wavelength is $\lambda = h / p$

A matter wave is described by a **wave function**: $\Psi(x, y, z; t)$

(called *uppercase psi*)

$\Psi(x, y, z; t)$ is a complex number ($a + ib$ with $i^2 = -1$, a, b: real numbers)

$\Psi(x, y, z; t)$ depends on the space (x, y, z) and on the time (t)

The space and the time can be grouped separately:

$$\boxed{\Psi(x, y, z; t) = \psi(x, y, z)\, e^{-i\omega t}}$$

$$\begin{cases} \psi(x, y, z): \text{space-dependent part (lower case psi)} \\ e^{-i\omega t}: \text{time-dependent part } (\omega: \text{angular frequency}) \end{cases}$$

- <u>The meaning of the wave function</u>: $\psi(x, y, z)$

The function $\psi(x, y, z)$ has no meaning

Only $|\psi|^2$ has a physical meaning. That is:

<u>The probability per unit time</u> of detecting a particle in a small volume centered on a given point in the matter wave is **<u>proportional to the value at that point</u>** of $|\psi|^2$

$|\psi|^2$ greater $\rightarrow$ it is easier to find the particle

N.B.: $|\psi|^2 = \psi\,\psi^*$ with ψ^* is the complex conjugate of ψ

If we write $\psi = a + ib \longrightarrow \psi^* = a - ib$ (*a*, *b*: real numbers)

- <u>How can we find the wave equation?</u>

Like sound waves described by Newtonian mechanics, or electromagnetic waves by Maxwell's equation, matter waves are described by an equation called

Schrödinger's equation (1926)

b. The Schrödinger's equation

For the case of one-dimensional motion,
when a particle with the mass *m* has a potential energy $U(x)$
Schrödinger's equation is

$$\boxed{\frac{d^2\psi}{dx^2}+\frac{8\pi^2 m}{h^2}[E-U(x)]\psi=0}$$

where E is total mechanical energy (potential energy plus kinetic energy)

Schrödinger's equation is the **basic principle**
(we cannot derive it from more basic principles)

EXAMPLE: Waves of a **free particle**

For a free particle, there is no net force acting on it, so

$$U(x)=0 \quad \text{and} \quad E=\frac{1}{2}mv^2$$

Schrödinger's equation becomes:

$$\boxed{\frac{d^2\psi}{dx^2}+\frac{8\pi^2 m}{h^2}\left(\frac{1}{2}mv^2\right)\psi=0}$$

By replacing: $mv = p \rightarrow \boxed{\dfrac{d^2\psi}{dx^2} + \left(\dfrac{2\pi\, p}{h}\right)^2 \psi = 0}$

With the de Broglie wavelength: $\dfrac{1}{\lambda} = \dfrac{p}{h}$

and the wave number: $K = \dfrac{2\pi}{\lambda}$

we have the Schrödinger's equation for free particle:

$$\boxed{\frac{d^2\psi}{dx^2} + K^2\psi = 0}$$

This differential equation has the most general solution:

$$\psi(x) = Ae^{iKx} + Be^{-iKx}$$

(A and B are arbitrary constants)

The time-dependent wave function:

$$\Psi(x,t) = \psi(x)\, e^{-i\omega t} = (Ae^{iKx} + Be^{-iKx})\, e^{-i\omega t}$$

$$\boxed{\Psi(x,t) = Ae^{i(Kx-\omega t)} + Be^{-i(Kx+\omega t)}}$$

$$\boxed{\Psi(x,t) = Ae^{i(Kx-\omega t)} + Be^{-i(Kx+\omega t)}}$$: **<u>traveling waves</u>**

- $Ae^{i(Kx-\omega t)}$: wave traveling in the direction of increasing x
- $Be^{-i(kx+\omega t)}$: wave traveling in the negative direction of x

<u>Probability density:</u>

Assume that the free particle travels only in the positive direction

Relabel the constant A as ψ_0 : $\psi(x) = \psi_0 e^{iKx}$

The probability density is:

$$|\psi|^2 = \left|\psi_0 e^{iKx}\right|^2 = (\psi_0)^2 \left|e^{iKx}\right|^2$$

Because:

$$\left|e^{iKx}\right|^2 = (e^{iKx})(e^{iKx})^* = (e^{iKx})(e^{-iKx}) = e^0 = 1$$

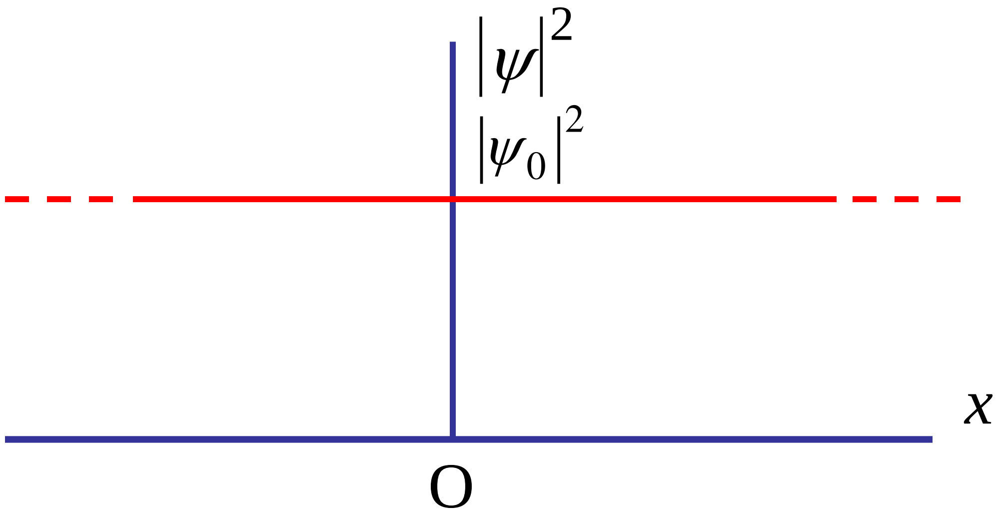
we have:

$$|\psi|^2 = (\psi_0)^2 = const$$

What is the meaning of a constant probability? $\boxed{\left|\psi\right|^2 = (\psi_0)^2 = const}$

The plot of $\left|\psi\right|^2 = (\psi_0)^2 = const$

is a straight line parallel to the *x* axis:



The probability density is the same for all values of *x*

The particle has equal probabilities of being anywhere along the *x* axis: **all positions are equally likely expected**

4. The Heisenberg's uncertainty principle

- In the example of a free particle, we see that if its momentum is <u>completely specified</u>, then its position is <u>completely unspecified</u>
- When the momentum p is completely specified we write:

$$\Delta p = 0 \quad (\text{because: } \Delta p = p_1 - p_2 = 0)$$

and when the position x is completely unspecified we write:

$$\Delta x \to \infty$$

- In general, we always have: $\Delta x \cdot \Delta p \geq$ a constant

  This constant is known as:

(called *h-bar*) $\longleftarrow$ $\hbar = \dfrac{h}{2\pi}$

h is the Planck's constant

$$(h = 6.625 \times 10^{-34}\, J.s)$$

So we can write: $\boxed{\Delta x \cdot \Delta p \geq \hbar}$

That is the **Heisenberg's uncertainty principle**

" it is impossible to know simultaneously and with exactness both the position and the momentum of the fundamental particles"

N.B.: • We also have for the particle moving in three dimensions

$$\boxed{\Delta x \cdot \Delta p_x \geq \hbar} \quad \boxed{\Delta y \cdot \Delta p_y \geq \hbar} \quad \boxed{\Delta z \cdot \Delta p_z \geq \hbar}$$

• With the definition of the constant $\hbar$:

$$p = h / \lambda = hK / 2\pi \longrightarrow \boxed{p = \hbar K}$$

• Uncertainty for energy :

$$\boxed{\Delta \mathrm{E} \cdot \Delta \mathrm{t} \geq \hbar}$$

PROBLEM 3 An electron is moving along *x* axis with the speed of 2×106 m/s (known with a precision of 0.50%).
What is the minimum uncertainty with which we can simultaneously measure the position of the electron along the *x* axis? Given the mass of an electron 9.1×10-31 kg

SOLUTION

From the uncertainty principle: $\boxed{\Delta x \cdot \Delta p \geq \hbar}$

if we want to have the minimum uncertainty: $\Delta x \cdot \Delta p = \hbar$

We evaluate the momentum: $p = mv = (9.1\times10^{-31})\times(2.05\times10^{6})$

$$p = 9.35\times10^{-27}\, kg.m/s$$

The uncertainty of the momentum is:

$$\Delta p = 0.5\%\, p = 0.5/100\times1.87\times10^{-24} = 9.35\times10^{-27}\, kg.m/s$$

$$\Rightarrow \quad \Delta x = \frac{\hbar}{\Delta p} = \frac{6.635\times10^{-34}/2\pi}{9.35\times10^{-27}} = 1.13\times10^{-8}\, m \approx 11 nm$$

PROBLEM 4 In an experiment, an electron is determined to be within 0.1mm of a particular point. If we try to measure the electron's velocity, what will be the minimum uncertainty?

SOLUTION

$$\Delta v = \frac{\Delta p}{m} \geq \frac{\hbar}{m\Delta x}$$

$$\Delta v \geq \frac{6.63\times10^{-34}\,J.s}{9.1\times10^{-31}kg\times1.0\times10^{-4}m\times2\pi}$$

$$\Delta v \geq 1.2 m/s$$

<u>Observation:</u>

We can predict the velocity of the electron to within 1.2m/s. Locating the electron at one position affects our ability to know where it will be at later times

PROBLEM 5 A grain of sand with the mass of 1.00 mg appears to be at rest on a smooth surface. We locate its position to within 0.01mm. What velocity limit is implied by our measurement of its position?

SOLUTION

$$\Delta v = \frac{\Delta p}{m} \geq \frac{\hbar}{m \Delta x}$$

$$\Delta v \geq \frac{6.63 \times 10^{-34} \, J.s}{1 \times 10^{-6} kg \times 1.0 \times 10^{-5} m \times 2\pi}$$

$$\Delta v \geq 1.1 \times 10^{-23} m / s$$

<u>Observation:</u>

The uncertainty of velocity of the grain is so small that we do not observe it: The grain of sand may still be considered at rest, as our experience says it should

PROBLEM 6 An electron is confined within a region of width 1.0×10^{-10} m. (a) Estimate the minimum uncertainty in the x-component of the electron's momentum.
(b) If the electron has momentum with magnitude equal to the uncertainty found in part (a), what is its kinetic energy? Express the result in jou1es and in electron volts.

SOLUTION

(a)

$$(\Delta p_x)_{\min} = \frac{\hbar}{\Delta x} = \frac{1.055\times10^{-34}\ \mathrm{J\cdot s}}{1.0\times10^{-10}\ \mathrm{m}} = 1.1\times10^{-24}\ \mathrm{kg\cdot m/s}$$

(b)

$$K = \frac{p^2}{2m} = \frac{(1.1\times10^{-24}\ \mathrm{kg\cdot m/s})^2}{2(9.11\times10^{-31}\ \mathrm{kg})}$$

$$= 6.1\times10^{-19}\ \mathrm{J} = 3.8\ \mathrm{eV}$$

PROBLEM 7 A sodium atom is in one of the states labeled "Lowest excited levels". It remains in that state for an average time of 1.6×10^{-8} s before it makes a transition back to a ground state, emitting a photon with wavelength 589.0 nm and energy 2.105 eV. What is the uncertainty in energy of that excited state? What is the wavelength spread of the corresponding spectrum line?

SOLUTION

$$\Delta E = \frac{\hbar}{\Delta t} = \frac{1.055 \times 10^{-34}\ \mathrm{J\cdot s}}{1.6 \times 10^{-8}\ \mathrm{s}}$$

$$= 6.6 \times 10^{-27}\ \mathrm{J} = 4.1 \times 10^{-8}\ \mathrm{eV}$$

The fractional uncertainty of the photon energy is

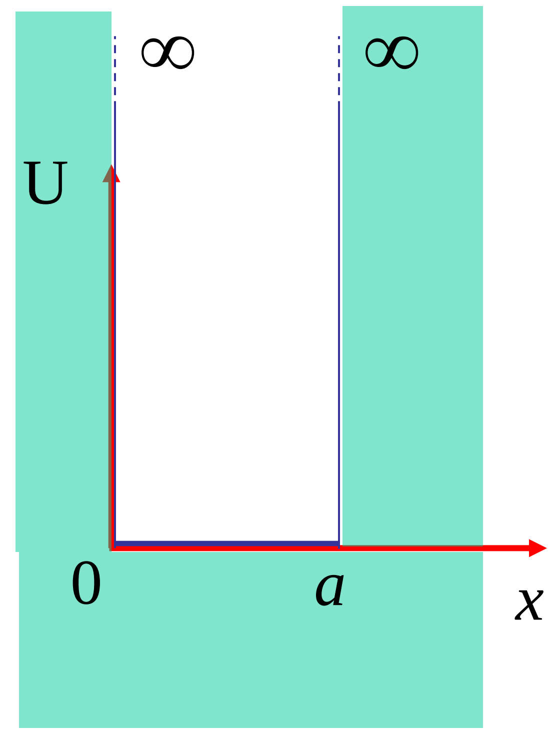
$$\frac{4.1 \times 10^{-8}\ \mathrm{eV}}{2.105\ \mathrm{eV}} = 1.95 \times 10^{-8}$$

$$\Delta\lambda = (1.95 \times 10^{-8})(589.0\ \mathrm{nm}) = 0.000011\ \mathrm{nm}$$

5. Particle in a square well

- Consider a particle confined to a region $0 \le x \le a$ where it can move freely, but subject to strong force at $x = 0$ and $x = a$

$$\begin{cases} U = 0 \quad when: \quad 0 \le x \le a \\ U \to \infty \; when: \quad x = 0 \quad or \quad x = a \end{cases}$$



Infinitely deep potential energy well

1. ***Solution of the Schrödinger's equation***

Schrödinger's equation for the particle in the box:

$$\boxed{\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0}$$

By putting: $K^2 = \dfrac{8\pi^2 m}{h^2} E$

$$\longrightarrow \quad \frac{d^2\psi}{dx^2} + K^2\psi = 0$$

$$\frac{d^2\psi}{dx^2} + K^2\psi = 0 \longrightarrow \psi(x) = Ae^{iKx} + Be^{-iKx}$$

What values can take the constants A, B, and the condition for K ?

- With the boundary condition: $\psi\,(x=0) = 0$

$$\psi(x) = Ae^{iKx} + Be^{-iKx} = Ae^{0} + Be^{0} = A + B = 0$$

$$\longrightarrow B = -A \longrightarrow \psi(x) = A(e^{iKx} - e^{-iKx})$$

- <u>Revision:</u> We have the relations

$$\cos x = \frac{e^{ix} + e^{-ix}}{2} \quad \text{and:} \quad \sin x = \frac{e^{ix} - e^{-ix}}{2i}$$

$$\psi(x) = 2iA\sin Kx \longrightarrow \boxed{\psi(x) = C\sin Kx}$$

- With the boundary condition: $\psi(x=a)=0$

$$\psi(x)=C\sin Ka=0 \longrightarrow Ka=n\pi \longrightarrow \boxed{K=n\pi/a}$$

The momentum of the particle is: $p=\hbar K=\hbar n\pi/a$

The possible values of energy: $E=\dfrac{p^2}{2m}=\left(\dfrac{\pi^2\hbar^2}{2ma^2}\right)n^2$

Bound states

Because n is an integer: $n = 1; 2; 3;\ldots$

the energy can only have the <u>discrete values</u>: $E_n = \left(\dfrac{\pi^2\hbar^2}{2ma^2}\right)n^2$

$$E_n = \left(\frac{\pi^2(h/2\pi)^2}{2ma^2}\right)n^2 = \frac{h^2}{8ma^2}n^2 \longrightarrow \boxed{E_n = \frac{h^2}{8ma^2}n^2}$$

We say that the <u>energy is quantized</u>

these values of energy are called <u>energy levels</u>

$n = 1 \longrightarrow$ ground state (E_1)

$n = 2 \longrightarrow$ first excited state (E_2)

$n = 3 \longrightarrow$ second excited state (E_3)

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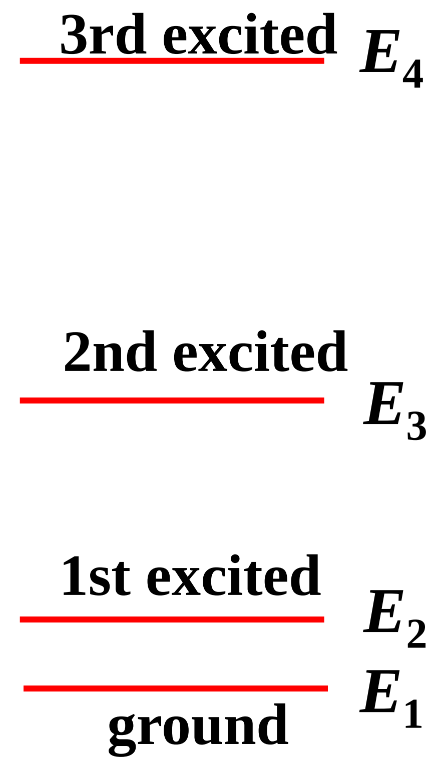
The integer n is called <u>the quantum number</u>



energy-level diagram

PROBLEM 8

An electron is confined to a one-dimensional, infinitely deep potential energy well of width a = 100pm.

1/ What is the least energy (in eV) the electron can have?

2/ Compute the energy level of the first excited state, of the second excited state. Draw the energy level diagram.

SOLUTION

1/ The least energy corresponds to the least quantum number: n = 1 for the ground state. Thus:

$$E_1 = \frac{h^2}{8ma^2} \times 1^2 = \frac{(6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (100 \times 10^{-12})^2} \times 1^2$$

$$E_1 = 6.03 \times 10^{-18} J = \frac{6.03 \times 10^{-18}}{1.6 \times 10^{-19}} \longrightarrow \boxed{E_1 = 37.7 eV}$$

2/ The energy level of the first excited state corresponds to $n = 2$:

$$E_2 = \frac{h^2}{8ma^2} \times 2^2 = 4E_1 \longrightarrow E_2 = 4 \times 37.7 eV \longrightarrow \boxed{E_2 = 150.8 eV}$$

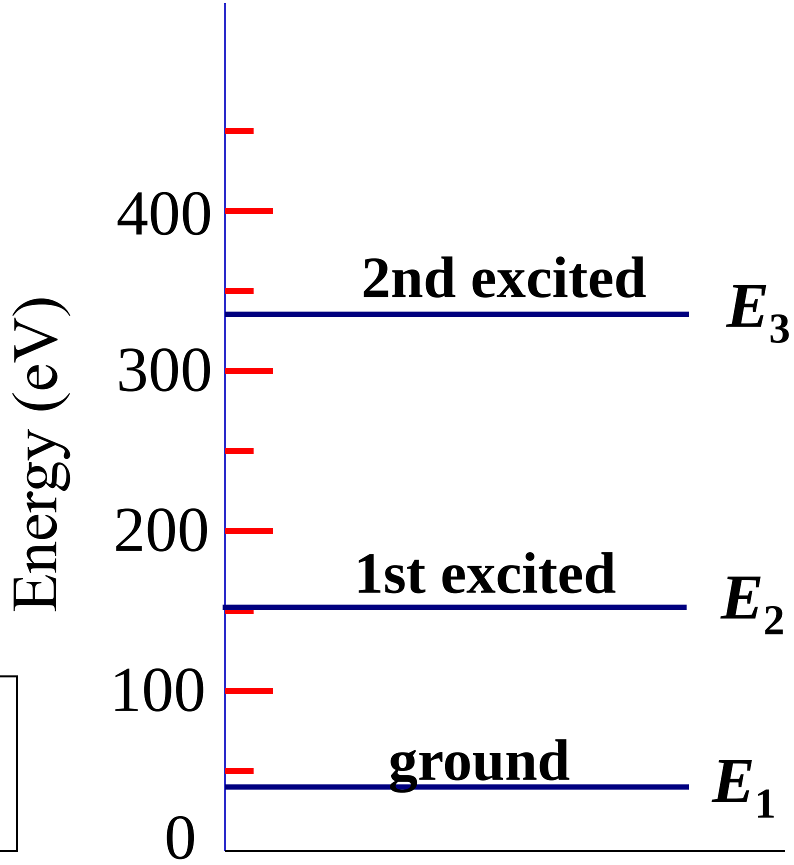
The energy level of the second excited state corresponds to $n = 3$:

$$E_3 = \frac{h^2}{8ma^2} \times 3^2$$

$$= 9E_1$$

$$= 9 \times 37.7 eV$$

$$\longrightarrow \boxed{E_3 = 339.3 eV}$$



Observation:

The levels are not equidistant

PROBLEM 9

The wave function of a particle confined to an infinitely deep potential energy well is $\psi(x) = C \sin Kx$

Determine the value of C, knowing that the particle must be somewhere **in all space**

SOLUTION

If the probability density is $|\psi(x)|^2$

The probability of finding the particle in width *dx* is $|\psi(x)|^2 dx$

The probability of finding the particle in all space is

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx$$

Because we are **sure to find the particle somewhere in all space**, the probability equals the unit:

Normalization condition: $$\boxed{\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1}$$

For a particle confined to an infinitely deep potential energy well:

$$\boxed{\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \int_0^a |C\sin(Kx)|^2 dx = C^2 \frac{1}{K}\int_0^{Ka} \sin^2 X dX}$$

With: $\cos 2X = 1 - 2\sin^2 X$

$$\int_0^{Ka} \sin^2 X dX = \frac{1}{2}\int_0^{Ka} [1-\cos(2X)]\, dX = \frac{1}{2}\int_0^{Ka} dX - \frac{1}{2}\int_0^{Ka} (\cos 2X) dX$$

$$\frac{1}{2}\int_0^{Ka} dX = \frac{Ka}{2}$$

$$\int_0^{Ka} (\cos 2X) dX = \frac{1}{2}[\sin 2X]_0^{Ka} = \frac{1}{2}\sin 2Ka = \frac{1}{2}\sin 2n\pi = 0$$

$$\boxed{\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = C^2 \frac{1}{K}\frac{Ka}{2} = C^2 \frac{a}{2}}$$

Normalization condition:

$$\boxed{\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1} \longrightarrow C = \sqrt{2/a}$$

$$\longrightarrow \boxed{\psi(x) = \sqrt{2/a}\sin Kx}$$

PROBLEM 10

The wave function of a particle confined to an infinitely deep potential energy well is $\psi(x) = \sqrt{2/a}\sin Kx$

The depth of the well is a = 100 pm

What is the probability density of finding the particle at the distance x = 50 pm for the value of the quantum number

1/ n = 1 ?

2/ n = 2 ?

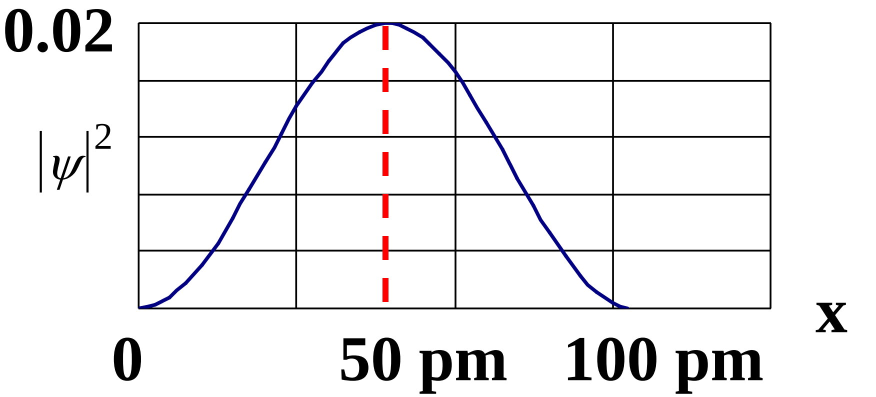
SOLUTION

We have $K = n\pi/a \longrightarrow \psi(x) = \sqrt{2/a}\sin\left(\frac{n\pi}{a}x\right)$

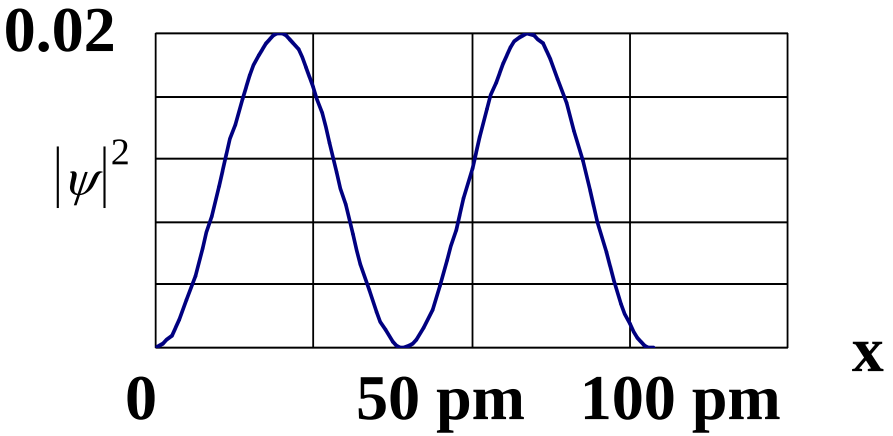
The probability density is $|\psi(x)|^2 = \frac{2}{a}\sin^2\left(\frac{n\pi}{a}x\right)$

SOLUTION

1/ For $n = 1$: $\left|\psi(x)\right|^2 = 0.02\sin^2\left(\frac{\pi}{100}x\right)$ (x: pm)



2/ For $n = 2$: $\left|\psi(x)\right|^2 = 0.02\sin^2\left(\frac{\pi}{50}x\right)$ (x: pm)

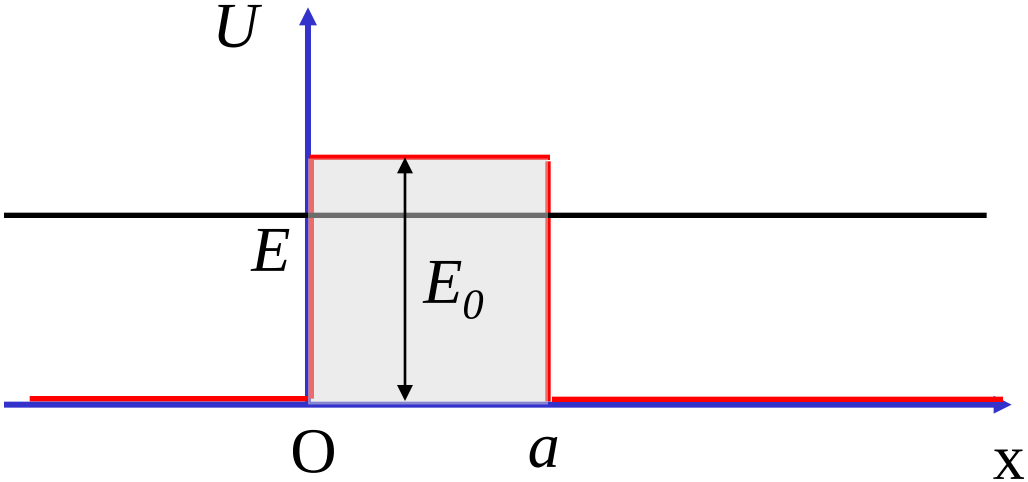


6. Tunneling Phenomena

a. The Square Barrier

The square barrier is represented by a potential energy $U(x)$

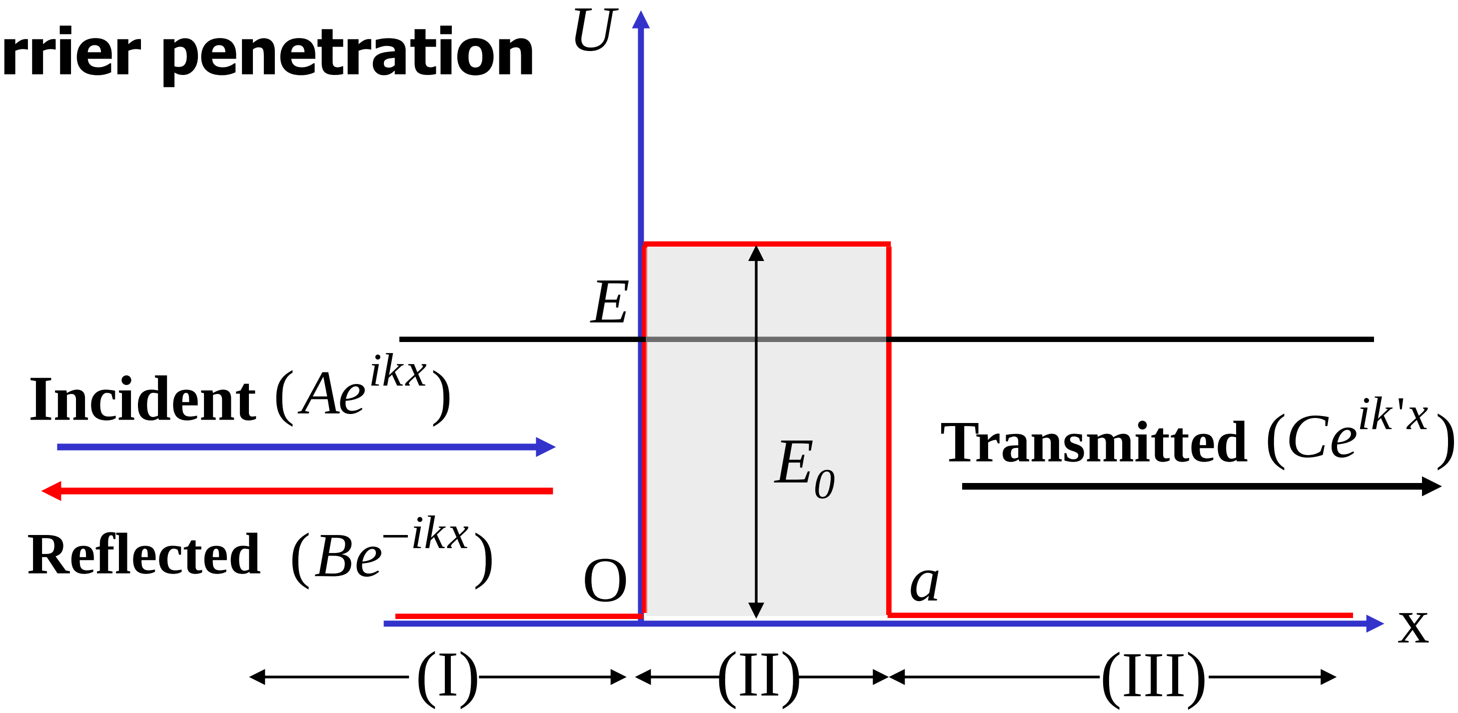
$$U = \begin{cases} E_0 = const & 0 \le x \le a \\ 0 & x \le 0\,;\, x \ge a \end{cases}$$



• <u>For case of classical particles:</u>

If a particle comes from the left with energy $E < E_0$, it will be reflected back at $x = 0$.

b. Barrier penetration



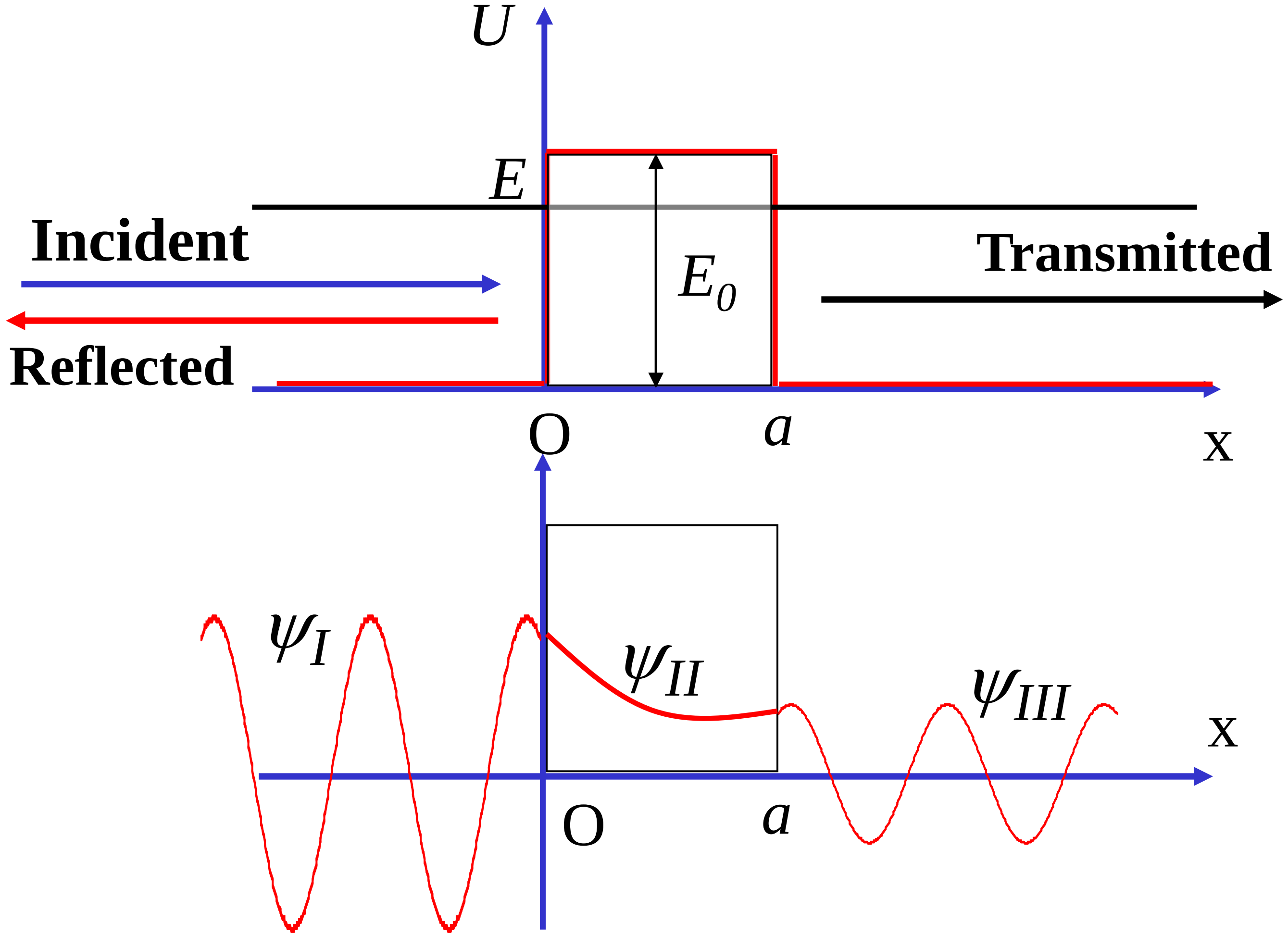
• <u>In quantum mechanics:</u>

The matter waves will have the solution for the region (I):

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx}$$

And the solution for the region (III): $\psi_{III}(x) = Ce^{ik'x}$

→ **A particle can go through the potential barrier even if its kinetic energy is less than the height of the barrier: <u>tunneling effect</u>**



The wave function ψ_I: free incident particles

The wave function ψ_{II}: decays exponentially in the forbidden region

The wave function ψ_{III}: transmitted particles

APPLICATIONS: Scanning Tunneling Microscopes

The scanning tunneling microscope (STM): To obtain highly detailed images of surfaces at resolutions comparable to the size of a *single atom* (approximately 0.2 nm).

For an optical microscope: The resolution ≥ 200 nm