Physics for Computer Science Students
Lecture 13

Quantum Mechanics

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Introduction

- What was the origin?
- And today?

Introduction

The need to construct the new model of physics has appeared at the turn of the XIX and XX centuries: the new facts were observed without the possibility of their physical interpretation. It was found e.g. that matter consists of elements smaller than atoms (see the experiments of Maria Skłodowska-Curie with radioactivity)

Introduction

Before 1900 a number of facts was discovered that were not explainable in the frames od Newton's mechanics.

It was known that Newton equations described exactly astronomical and local phenomena. The kinetic theory of gases has worked also very well. The electron discovered by J.J. Thomsona in 1897 has behaved also according to the Newton's dynamics. The experiments of Young in 1803 with diffraction of light have confirmed the wave nature of light. The Maxwell theory in 1864 has confirmed the connection between optical and electrical phenomena.

Introduction

The main problem was the discrepancy between the theoretical description and experimental data concerning the model of atom, Röntgen radiation and natural radioactivity. There were also the facts for which there were not theoretical explanations at all. They were, e.g.:

- spectrum of the radiation of the ideally black body;
- specific heat of solids at low temperatures;
- 5 degrees of freedom of the free two-atom particles at the room temperature only.

Introduction

The first step to clear the discrepancies spectrum of the radiation of the ideally black body was made by Max Planck in 1900. He proposed that the electromagnetic radiation can be emitted and absorbed in discrete portions only, called **quants**, every with the energy

$$E = h\,\nu\,.$$

where h – Planck constant. It was used later by A. Einstein to describe the photoelectric phenomenon.

Introduction

The **dual** nature of the electromagnetic radiation: sometimes like as a wave and sometimes like a flux of the quasiparticles, i.e. quants of energy.

It was found that some parameters of atomic systems take the discrete values, e.g.:

- Einstein and Debye constants in the theory of the specific heat of solids;
- Ritz classification of spectral lines;
- discrete values of energy losses in collisions of atoms and electrons in Franck-Hertz experiment;
- discrete values of the magnetic momentum components of atoms in the external magnetic field in Stern-Gerlach experiment.

Introduction

Table 1. Experiments and theoretical explanations

Diffraction (Young 1803, Lune 1912)	electromagnetic waves
Radiation of ideally black body (Planck 1900) Photoelectric phenomenon (Einstein 1904) Compton's effect (1923) Combination rule (Ritz-Rydberg 1908)	electromagnetic quants

Bohr's model of atom

Niels Bohr was the first who understood that only energy but also momentum has to take discrete values. He succeeded in obtaining the theoretical equation for the experimental Balmer formula for the lengthes of the hydrogen spectral lines (1913), but had to make assumptions contradictory with the classical physics.
It is easy to understand, because his approach was contradictory to the accepted knowledge about the conservation of energy and momentum laws. E.g., Otto Stern and Max von Laue said, that they stop to work in physics if the nonsenses of Bohr appear to be true.
Niels Bohr has made in his model the following assumptions:

Bohr's model of atom

1. electrons circulate on circulate orbits; there exist stationary orbits, i.e. on these orbits electrons do not radiate energy, i.e. their energy do not change;
2. during the transition from one orbit to another one, the energy is transmitted or absorbed according to the Planck formula

$$E = \hbar \, \nu \,, \tag{1}$$

where $\hbar = 6.63 \cdot 10^{-34}$J·s $= 4.14 \cdot 10^{-15}$ eV·s – Planck constant.

Arthur Compton experiment

Einstein observed in 1916, that if the wave has energy E, so it has also a momentum p, because it follows from

$$E = \hbar\,\nu\,,$$

that

$$p = \frac{E}{c} = \frac{\hbar\,\nu}{c} = \frac{\hbar}{\lambda}\,, \qquad (2)$$

where λ – length of the photon wave. This assumption was confirmed experimentally by Arthur Compton in 1923, but it was not explainable in frames of the classical physics.

Louis de Broglie postulate

In 1924 the French physician Louis de Broglie asked the question:

if the light ray is a wave, but energy is transferred in the form od quants, so why not the real particles can behave like waves?

The conclusion was: equation (2) can be used for all elementary particles, and

$$\lambda = \frac{\hbar}{p}\,, \tag{3}$$

where λ - length of the de Broiglie wave of the moving elementary particle.

Schrödinger equation

Erwin Schrödinger proposed in 1926 the equation describing the waves of matter:

$$i\hbar\frac{d\psi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi\,, \tag{4}$$

where m – mass of a particle, U – potential energy, ψ – complex wave function.

Schrödinger equation

Wave function

Interpretation of the wave function as given by quantum mechanics:

the product $\psi\ \psi^*$ is the probability density that a particle at a given instant there is in a given place of space in the infinitesimal volume dV

(ψ^* – complex conjugated function to ψ function).

Schrödinger equation

Wave function

It is assumed:

1. wave function ψ is normalized, because the condition has to be fulfilled
$$\int \psi \, \psi^* dV = 1 \,, \tag{5}$$
because the probability that the particle is present in all the space equals 1;
2. the wave function ψ and all of its derivatives $\dfrac{d\psi}{dx}$ and $\dfrac{d\psi}{dt}$ have to be finite, unique and continuous in all the space.

Solution of free Schrödinger equation

To solve the Schrödinger equation, the potential $U = U(x,t)$ has to be given. If it vanishes, i.e. $U = 0$, the particles move on the parallel trajectories with the constant velocity v. Solution, i.e. the wave function, has a form of a plane wave

$$\psi = A\ e^{-2\pi i\left(\nu t - \frac{x}{\lambda}\right)} \tag{6}$$

and Schrödinger equation

$$i\hbar\frac{d\psi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\,, \tag{7}$$

is called the wave equation.
As it is seen from equation (6), the wave function and the square of it at every point of space depend on time.

In certain situations, like electron on the atomic orbit, this temporal dependence does not appear. The probability density is constant in time and such the state is called

the stationary state .

Such states are very important in physics: every state can be represented as a combination of stationary states.

Stationary state

Let us consider a particle with the defined and constant energy. Its wave function can be given in a form

$$\psi(x,t) = A(x)\ exp\left(-\frac{iEt}{\hbar}\right)\,, \tag{8}$$

and

$$|\psi(x,t)|^2 = |\psi(x,t)\ \psi^*(x,t)| = A^2(x)\,, \tag{9}$$

is independent on time, so the probability density has the same property.

Free particle

Free particle – no forces and potential energy $U = 0$. The kinetic energy $E = p^2/2m$ is the only energy of that particle. Let us assume that the wave function has a form

$$\psi(x,t) = A\ cos(kx - \omega t) + B\ sin(kx - \omega t)\,, \tag{10}$$

where A and B – certain constants, $k = 2\pi/\lambda$ – wave function, $\omega = 2\pi\nu$ – frequency.
The wave function (10) can have the stationary form if $B = i\,A$, because

$$\begin{aligned}\psi(x,t) &= A\ cos(kx - \omega t) + i\ A\ sin(kx - \omega t) \\ &= A[cos(kx - \omega t) + i\ sin(kx - \omega t)] \\ &= Aexp[i(kx - \omega t)] = A\ exp(ikx)exp(-i\omega t)\,.\end{aligned} \tag{11}$$

Euler equations

$$e^{i\phi} = cos\phi + i\, sin\phi\,, \qquad e^{-i\phi} = cos\phi - i\, sin\phi\,.$$

Comparing equations (11) and (10), it is ease to see that our wave function $\psi(x) = A\, exp(ikx)$ describes the stationary state with the energy $E = \hbar\omega$ and fulfills the Schrödinger equation

$$i\hbar\frac{d\psi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi\,.$$

Electron in the potential well

Electron in the bounded state: potential $U = U(x) \neq 0$ and has a minimum. According to the Newton mechanics, electron there is in a prison.

Assumption: potential well has a form of a rectangle of the length L and a finite height U_0 (Fig. 1).

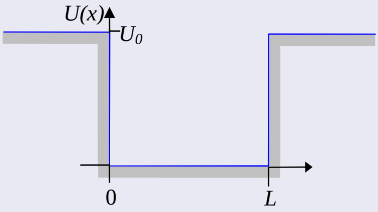

Fig. 1: Rectangular potential well

Two cases have to be considered:

1. $U(x) = U_0 = 0\,,$
2. $U(x) = U_0 \neq 0\,.$

1. Schrödinger equation takes a form:

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x)\,. \tag{12}$$

For $0 \leq x \leq L$:

$$\psi(x) = A\,cos\frac{\sqrt{2mE}}{\hbar}x + B\,sin\frac{\sqrt{2mE}}{\hbar}x\,, \tag{13}$$

where A and B certain constants.

2. For $x < 0$ and $x > L$ Schrödinger equation has a form:

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m(U_0 - E)}{\hbar^2}\psi(x)\,. \tag{14}$$

Expression $U_0 - E$ is positive $\hookrightarrow$ solutions are exponential functions

$$\psi(x) = C\,e^{\kappa x} + D\,e^{-\kappa x}\,, \tag{15}$$

where $\kappa = \dfrac{\sqrt{2m(U_0 - E)}}{\hbar}$, and C and D have different values to the left and to the right of the potential well.
The bounded states have the sinusoidal character, and outside the well – exponential.

The exponential functions should have forms allowing the normalization (16),

$$\int \psi\, \psi^* dV = 1\,, \tag{16}$$

so ψ outside the well:

1. if $x < 0$ then $D = 0$,
2. if $x > L$ then $C = 0$.

Finding of energy levels is very difficult and is usually made by using computer numerical methods. One fact is very important: the probability that the particle can be found outside the potential well is finite and > 0 (in classical mechanics it is impossible).

New purely quantum phenomenon – penetrating the potential barier. The shape given in Fig. 2). If the energy of a particle is greater then the height of the potential barier – the particle moves freely. In the case the energy of a particle is smaller then the height of the potential barier – there exists a finite probability that the particle overcome that obstacle. That phenomenon is called **tunneling**.

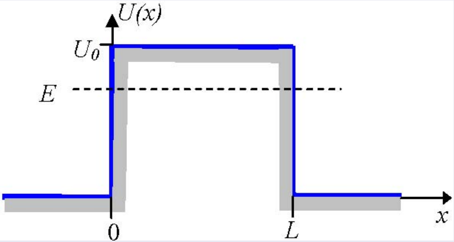

Fig. 2: Rectangular potential barrier

In Newton classical mechanics the particles always stays on one side of a barier.

Kinetic energy

$$K = E - U\,, \tag{17}$$

is smaller then zero, and it is imposable because

$$K = \frac{1}{2}\frac{mv^2}{2}\,, \tag{18}$$

what in our case means negative mass or imaginary velocity. The particle can overcome the barrier iff $E > U_0$.

Schrödinger equation for potential barrier from Fig. 2 $\hookrightarrow$ solutions have to be arranged as follows: be sinusoidal outside the barier and vanish exponentially inside the barier. It is a hard task!

If that probability is much smaller then 1, one has

$$P = G\, e^{-2\kappa L}\,, \tag{19}$$

where

$$G = 16\frac{E}{U_0}\left(1 - \frac{E}{U_0}\right)\,,$$

and

$$\kappa = \frac{\sqrt{2m(U_0 - E)}}{\hbar}\,.$$

Practical applications:

- tunnel diode
- scanning tunneling microscope (STM)
- atomic force microscope (AFM)

The End? :-(

The end of the lecture 13