

Experimental basis of quantum physics, the birth of quantum theory

At the end of 1800 years most of physicists thought, that the physics is a well worked out science, nearly finished. The Newtonian mechanics, Maxwell electrodynamics and thermodynamics are finished.

But by the end of the nineteenth century, and during the first quarter of the twentieth, some experimental evidence began to accumulate which indicated that the interaction of electromagnetic radiation with matter was not entirely in accordance with the laws of electrodynamics and thermodynamics.

1. Blackbody radiation

Experience show that the temperature of a hot and a cold objects equalize in vacuum as well. All objects in all temperature emit and absorb thermal radiation. This thermal radiation is electromagnetic radiation.

The radiant energy emitted by a surface, per unit time and per unit area, depends on the nature of the surface and on its temperature.

When a body is hotter than its surroundings, the rate of emission exceeds its rate of absorption. If a body is at lower temperature than its surroundings, the rate of absorption is larger than its rate of emission and its temperature rises. When a body is at the same temperature as its surroundings the two rates become equal. There is no net gain or loss of energy and no change in temperature, and they are in thermal equilibrium.

At low temperature the rate of radiation is small, and the radiant energy appears at small frequencies.

Increasing temperature the rate of radiation increases very rapidly, in proportion of the fourth power of the absolute temperature and the radiant energy appears at higher frequencies.

Introduce a new physical property the spectral emissivity: $e(f, T)$. It is the emitted energy by the object at a given T absolute temperature on a unit surface in unit time at a unit frequency interval around frequency f . The unit of the spectral emissivity:

$$[e] = \frac{\text{power}}{\text{surface} \cdot \text{frequency}} = \frac{W}{m^2 Hz}$$

Introduce the next physical property the spectral absorptivity: $a(f, T)$

It shows how much part is absorbed from radiation by the object at absolute temperature T at a unit frequency interval around frequency f . It is a dimensionless quantity, and $0 < a(f, T) < 1$.

The absolute blackbody is an idealization $a_{bb}(f, T) = 1$, this body absorbs all energy. The blackbody is a hypothetical object capable of absorbing all the electromagnetic radiation falling on it also called: full radiator.

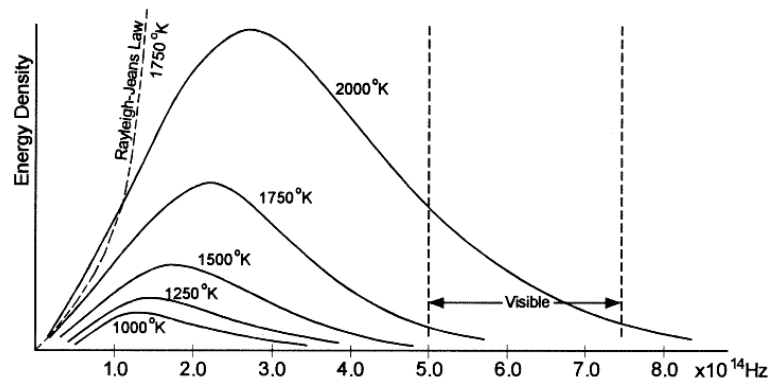
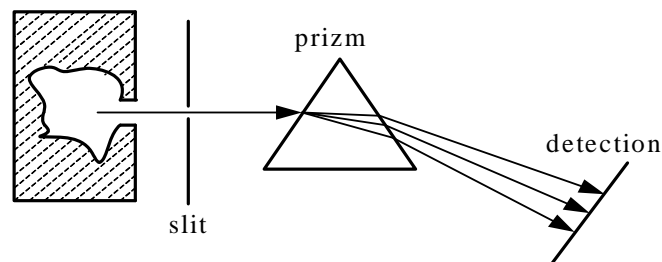
Kirchhoff's Radiation Law states that the spectral emissivity $e(f, T)$ is proportional with the spectral absorptivity $a(f, T)$, so their ratio is constant independent of the nature of the

radiating body. This ratio is just equal to the spectral emissivity of the blackbody $e_{bb}(f, T)$ (because its absorptivity is equal to 1) and depends on the radiation frequency f and on the absolute temperature T

$$\frac{e(f, T)}{a(f, T)} = \frac{e_{bb}(f, T)}{1} = e_{bb}(f, T)$$

An approximate realization of a black surface is a hole in the wall of a large enclosure. Any radiation entering the hole is reflected indefinitely or absorbed inside and is unlikely to re-emerge, making the hole a nearly perfect absorber.

A blackbody in thermal equilibrium (that is, at a constant temperature) emits electromagnetic radiation called black-body radiation. The spectral emissivity of a blackbody was measured, and the experimental setup and the result are shown on the next two figures



Wien's Displacement Law:

Wien's displacement law indicates how the maximum in an energy distribution is displaced within the radiation spectrum of a blackbody in case of a change in temperature.

$$\frac{T}{f_{\max}} = \text{constant}$$

The Stefan Boltzmann Law:

The total energy radiated from a blackbody is proportional to the fourth power of the absolute temperature of the body. $E = \sigma T^4$, where $E = \int_0^{\infty} e(f, T) df$, $\sigma = 5.67 \cdot 10^{-8} \frac{W}{m^2 K^4}$ is the Stefan Boltzmann constant.

It was impossible to explain the measured spectral emissivity distribution by the concepts of classical physics. In 1900 Max Planck wanted to derive theoretically a formula, and he had to suppose that the energy of the electromagnetic radiation is not continuous but quantized. He stated that electromagnetic energy could be emitted only in quantized form, in other words,

the energy could only be a multiple of an elementary unit $E = hf$, where h is Planck's constant $h = 6,626 \cdot 10^{-34}$ Js. Max Planck, in 1901, accurately described the radiation by assuming that electromagnetic radiation was emitted in discrete packets (or quanta). Planck's quantum hypothesis is a pioneering work, heralding advent of a new era of modern physics and quantum theory.

The Planck radiation law: $e(f, T) \sim K \frac{hf^3}{e^{kT} - 1}$. This equation is in good agreement with the measured spectral emissivity distribution, and the Wien's Displacement Law can be obtained by derivation, and the Stefan Boltzmann Law can be obtained by integration.

2. The behaviour of the molar heat capacity of solids at low temperature

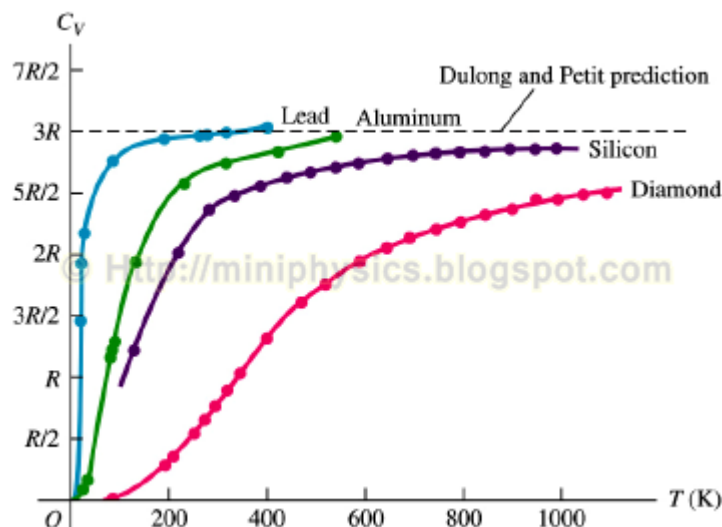
Determine first the energy of crystal lattice. Each atom in the lattice is an independent three dimension harmonic oscillator with six degrees of freedom f (an oscillator can be thought of as a spring connecting all the atoms in the solid lattice). The number of freedom of a linear oscillator is $f = 2$. For example its energy is: $E = \frac{1}{2}mv_x^2 + \frac{1}{2}Dx^2$, there is two quadratic term in the energy expression. The number of atoms is N . The equipartition theorem states that energy is shared equally amongst all energetically accessible quadratic degree of freedom. The average value for one degree of freedom is $\bar{\epsilon}_x = \frac{1}{2}kT$. The energy of the crystal

$E = N \cdot 6 \cdot \frac{1}{2}kT = 3NkT$. If heat is absorbed by the crystal as $V \sim \text{constant}$ $\Delta E = Q$, or

$Q = 3Nk\Delta T$. Introduce the heat capacity of the crystal $C = \frac{Q}{\Delta T} = 3Nk$. Now let's consider

one mole amount N_A the Avogadro constant. $C_{mole} = 3N_A k = 3R \approx 25 \frac{J}{mole \cdot K}$. This equation is called Dulong-Petit rule and states that the molar heat capacity is constant.

Later it was discovered experimentally that heat capacity decreased as temperature approached absolute zero. Applying the classical physics it was impossible to explain this result.

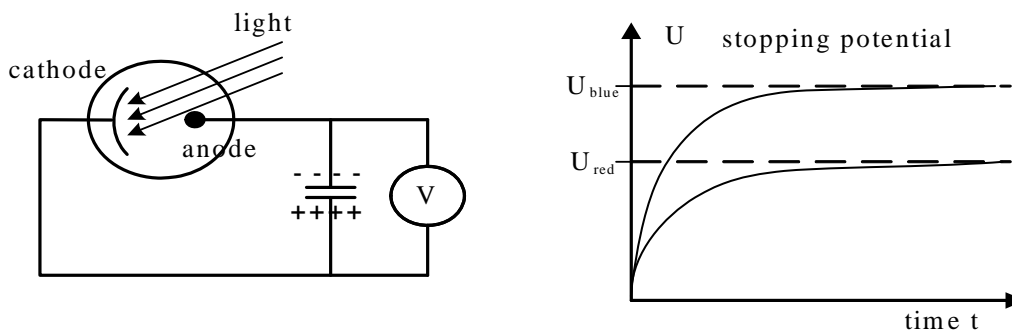


Einstein was who solved the problem with the help of the quantum hypothesis. He supposed that the Planck quantum hypothesis can be applied not only to the energy of the electromagnetic field, but for the energy of the crystal oscillator as well. By employing Planck's quantization assumption, Einstein's theory was in good agreement with observed experimental results.

3. Photoelectric effect

The experiences shows that zinc plate illuminated by ultraviolet light emit electrons. In case of alkali metals this effect can be generated by visible light as well. In the photocell two conducting electrodes are enclosed in an evacuated glass tube and the cathode covered with alkali metal is illuminated. (The tube is evacuated to a pressure of 0.01 Pa or less to minimize collisions between the electrons and gas molecules.)The emitted electrons travel across to the anode, producing a photocurrent in the external circuit and charging the capacitor. The charge separation will be stopped by a stopping potential and the photocurrent disappear. Measuring this stopping potential U_{stop} we can determine the maximum kinetic energy of the emitted

electrons. The electrons are emitted at the cathode by a maximal kinetic energy $\frac{1}{2}mv_{max}^2$, and slow down to zero at he anode.



$$\frac{1}{2}mv_{max}^2 = eU_{stop}$$

Experimental observations of photoelectric emission:

1. For a given metal, there exists a certain minimum frequency f_0 of incident radiation below which no photoelectrons are emitted. This frequency is called the threshold frequency.
2. Above the threshold frequency, the maximum kinetic energy of the emitted photoelectron depends on the frequency of the incident light and on the material, but is independent of the intensity of the incident light.
3. The rate at which photoelectrons are ejected is directly proportional to the intensity of the incident light.
4. The time lag between the incidence of radiation and the emission of a photoelectron is very small, less than 10^{-7} second.

The theory of the photoelectric effect must explain the experimental observations of the emission of electrons from an illuminated metal surface. But these experimental observations can't be explained by the wave properties of light. In 1905, Albert Einstein solved this problem by describing light as composed of discrete quanta, now called photons, rather than continuous waves.

In case of interaction between electromagnetic radiation, and the free electrons of a metal, the electromagnetic radiation shows particle properties rather than wave properties. The electrons can receive energy from electromagnetic field only in discrete portions (quanta that were called photons): an amount of energy $E = hf$, or $E = n \cdot hf$ where f is the frequency of the light, and h is Planck's constant.

So the famous Einstein photoelectric equation: $hf = A + \frac{1}{2}mv_{\max}^2$, where hf is the energy of the photon the particle of the electromagnetic radiation, and A is the so called work function characteristic for the metal. This is the minimum work (i.e. energy) needed to remove an electron from a solid to a point in the vacuum immediately outside the solid surface. Its value can be determined by the threshold frequency f_0 . $hf_0 = A$

Conclusion: The light and generally the electromagnetic radiation transfer its energy to the material in discrete portions (quanta). The magnitude of this quanta is $E = hf$.

4. A Compton-effect (1922)

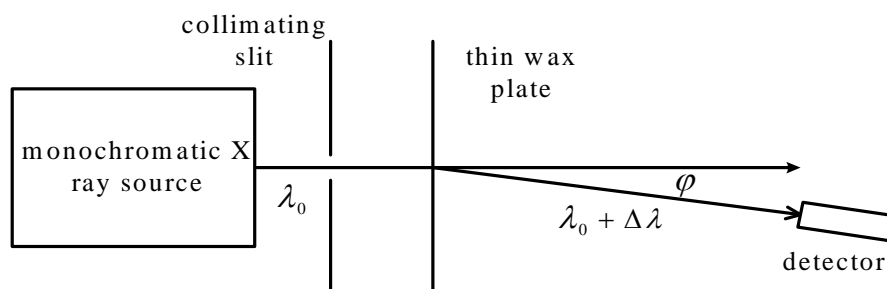
In Compton experiment 1922 high frequency and thus small wavelength of beam of x rays was directed onto a target made of wax

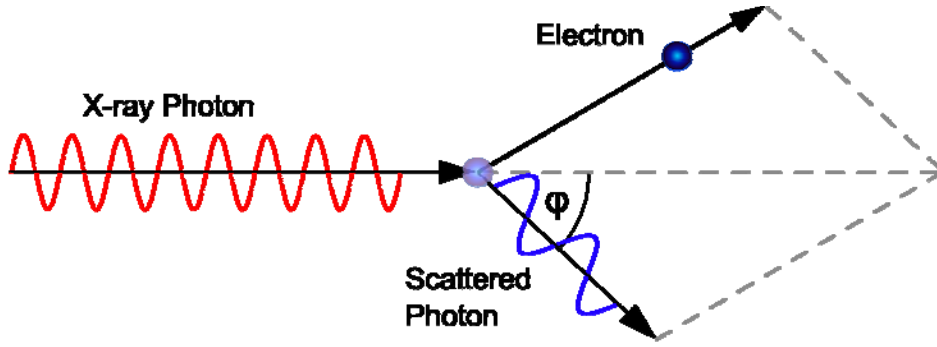
Compton measured the wavelengths and intensities of the x rays that were scattered in various directions from the target

it was discovered that some of the scattered radiation has smaller frequency (longer wavelength) than the incident radiation and that the change in wavelength depends on the angle through which the radiation is scattered

The wave model was not able to describe the experimental observations; the scattered x rays and incident x rays have the same frequency and same wavelength. In this effect the electromagnetic radiation shows particle properties again as it is quantized.

We can describe the Compton-scattering as the relativistic collision between the the incident x ray photon and a loosely bound electron of wax target that is initially at rest, both the energy and the momentum remains constant.





Energy conservation: $hf_0 + m_0c^2 = hf + mc^2$

$$h(f_0 - f) = m_0c^2(\gamma - 1)$$

$$h\left(\frac{c}{\lambda_0} - \frac{c}{\lambda}\right) = m_0c^2(\gamma - 1)$$

$\frac{h}{m_0c}\left(\frac{1}{\lambda_0} - \frac{1}{\lambda}\right) = (\gamma - 1)$, introduce $\Lambda = \frac{h}{m_0c}$ called the Compton wavelength of the electron

$$\Lambda\left(\frac{1}{\lambda_0} - \frac{1}{\lambda}\right) + 1 = \gamma$$

The Einstein proposed light quanta (photons) have energy $E = hf$ and linear momentum as

well. The momentum of the photon: $p_f = m_f c = \frac{E}{c^2} c = \frac{hf}{c} = \frac{h}{\lambda}$

The momentum conservation (cosine law): $(m_0\gamma\beta c)^2 = \left(\frac{h}{\lambda_0}\right)^2 + \left(\frac{h}{\lambda}\right)^2 - 2h^2 \frac{1}{\lambda_0} \frac{1}{\lambda} \cos\varphi$

$$\gamma^2\beta^2 = \left(\frac{h}{m_0c}\right)^2 \left(\frac{1}{\lambda_0^2} + \frac{1}{\lambda^2} - \frac{2}{\lambda\lambda_0} \cos\varphi\right)$$

$$\gamma^2\beta^2 = \Lambda^2 \left(\frac{1}{\lambda_0^2} + \frac{1}{\lambda^2} - \frac{2}{\lambda\lambda_0} \cos\varphi\right)$$

It is known identity: $\gamma^2\beta^2 = \gamma^2 - 1$

$$\Lambda^2 \left(\frac{1}{\lambda_0^2} + \frac{1}{\lambda^2} - \frac{2}{\lambda\lambda_0} \cos\varphi\right) = \Lambda^2 \left(\frac{1}{\lambda_0^2} + \frac{1}{\lambda^2} - \frac{2}{\lambda\lambda_0}\right) + 1 + 2\Lambda \left(\frac{1}{\lambda_0} - \frac{1}{\lambda}\right) - 1$$

$$\Lambda^2 \frac{2}{\lambda\lambda_0} (1 - \cos\varphi) = 2\Lambda \left(\frac{1}{\lambda_0} - \frac{1}{\lambda}\right)$$

$$\Lambda \frac{1}{\lambda\lambda_0} (1 - \cos\varphi) = \frac{\lambda - \lambda_0}{\lambda\lambda_0}$$

$$\Lambda(1 - \cos\varphi) = \lambda - \lambda_0$$

$$\Delta\lambda = \Lambda(1 - \cos\varphi)$$

$\Delta\lambda$ is called the Compton shift, and the value of the Compton shift varies with the angle at which the scattered X-rays are detected and is greater for a greater angle. The theory and the results of the experiment are in good agreement.

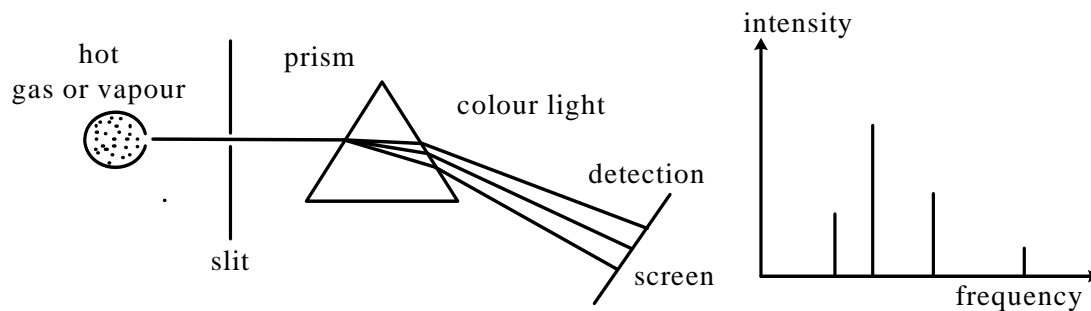
We can conclude light can be a wave or particle. This is called wave particle duality. Together with the photoelectric effect, this became one of the most important pieces of evidence for the need of quantization.

5. Line spectra

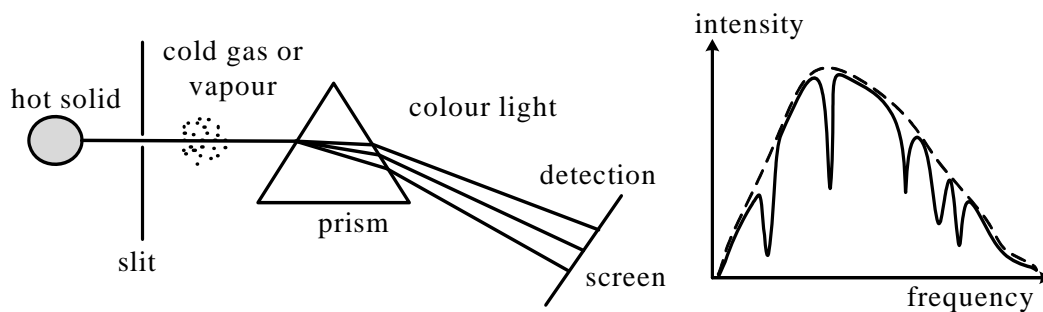
The quantum hypothesis also plays an important role in the understanding of atomic spectra.

The spectrum emitted by a hot solid such as the filament of a light bulb, is continuous, all wavelengths is present.

But if the source is a heated gas or vapour, the spectrum includes some colours in the form of isolated lines. This is called emission line spectrum, and the lines are called spectral lines. The wavelengths or frequencies of the lines are characteristic of the element emitting the light.



If we pass continuous-spectrum light through a cold gas or vapour, the so called absorption line spectrum can be obtained. Dispersed the transmitted light a series of dark lines appear in the spectrum.

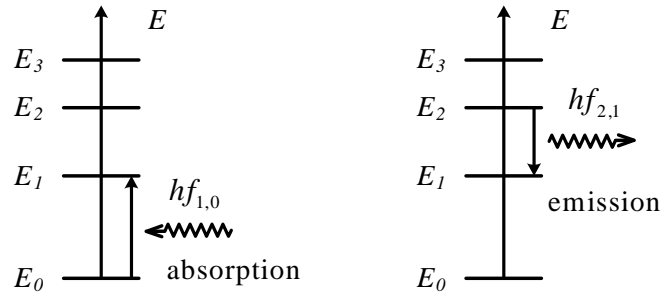


It is a very important fact that a given kind of atom absorbs the same lines when it is cool as it emits when heated. The explanation of the emission and absorption spectra is that the energy of the lonely atom or molecule could be only discrete value. Bohr explained the atomic spectra in 1913.

Bohr's postulates

1. Electrons in an atom exist in stationary states and they have discrete energies E_1, E_2, E_3, \dots . The electrons orbit the nucleus without emitting electromagnetic radiation.

2. Transmission between stationary states results emission or absorption of electromagnetic radiation. The emitted or absorbed frequency is given by the next equation: $E_i - E_k = hf_{i,k}$, called Bohr frequency condition.

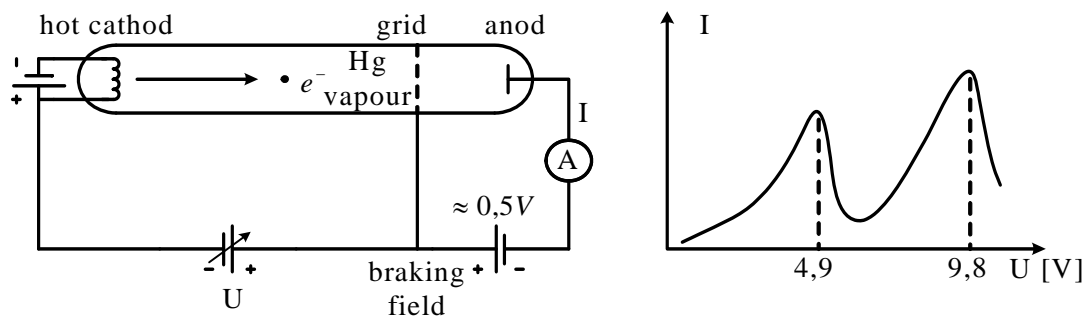


For example the absorbed frequency: $f_{1,0} = \frac{E_1 - E_0}{h}$, and the emitted frequency

$$f_{2,1} = \frac{E_2 - E_1}{h}.$$

The Bohr postulates were experimentally confirmed by Franck and Hertz in 1913.

Vacuum tube filled with low pressure mercury vapour contains a cathode, a grid and an anode. The electrons emitted by the cathode are accelerated towards the anode, but there is a small retarding potential 0.5 V as well.



First the electrons are accelerated and collide with mercury atoms but the collision is elastic.

At 4.9 V acceleration potential, the anode current drops sharply, it means that and the electrons lose their energy due to the inelastic collision with mercury atoms. So it was supposed that the mercury atoms have an excited energy level 4.9 eV above the ground level.

At 9.8 V potential the electrons are able to excite the mercury atoms twice.

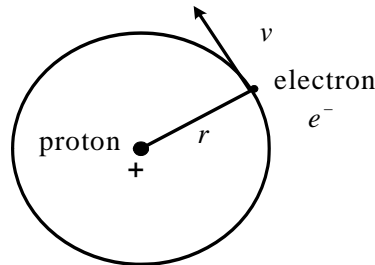
When the electrons in mercury atoms fall down to the lower energy level they emit the next frequency electromagnetic radiation: $f = \frac{\Delta E}{h} = \frac{4.9 \cdot 1.6 \cdot 10^{-19}}{6.623 \cdot 10^{-34}} = 1.183 \cdot 10^{15} \text{ Hz}$, and this was found in the experiment.

The Bohr model of hydrogen

Bohr supposed that only those orbital radii are allowed, for which the angular momentum is quantised by the next equation called Bohr quantum condition:

$$L_{e^-} = n \cdot \hbar, \quad n = 1, 2, 3, \dots \quad \hbar = \frac{h}{2\pi}$$

In case of circular path the angular momentum: $m v r = n \hbar$.



The negatively charged electron of the hydrogen atom is forced to a circular motion by the attractive electrostatic Coulomb force of the positively charged atomic nucleus at rest. The equation of motion:

$$k \frac{e^2}{r^2} = m \frac{v^2}{r}, \text{ so } k e^2 = m v r \cdot v, \text{ and } k e^2 = \hbar n v.$$

The velocity of the electron: $v = \frac{k e^2}{\hbar n}$.

The energy of the electron is the sum of the kinetic and potential energy:

$$E = T + V = \frac{1}{2} m v^2 - k \frac{e^2}{r} = \frac{1}{2} m v^2 - m v^2 = -\frac{1}{2} m v^2$$

In the previous transformation we applied the next formula: $k \frac{e^2}{r} = m v^2$.

The energy of the electron is quantized by n natural number; this is the meaning of the subscript:

$$E_n = -\frac{1}{2} m \cdot \frac{k^2 e^4}{\hbar^2 n^2} = -\frac{m k^2 e^4}{2 \hbar^2} \cdot \frac{1}{n^2}$$

The discrete energy values are:

$$E_n = -E^* \cdot \frac{1}{n^2}, \text{ where the constants is } E^* = \frac{m k^2 e^4}{2 \hbar^2} = 2,18 \cdot 10^{-18} J = 2,18 aJ$$

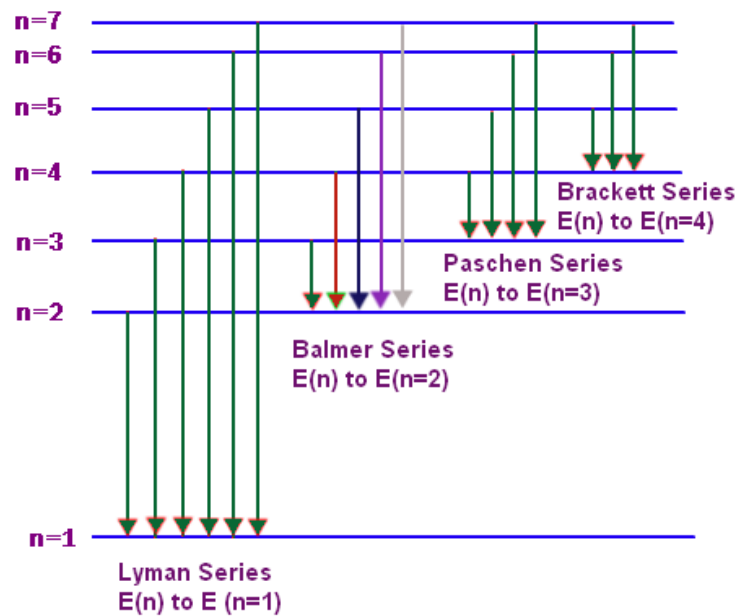
The emitted or absorbed frequency in case of transmission between two stationary states is given by the next equation:

$$f_{nm} = \frac{E_n - E_m}{h} = -\frac{E^*}{h} \left(\frac{1}{n^2} - \frac{1}{m^2} \right) = \frac{E^*}{h} \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$

From the experiments: $f_{nm} = R^* \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$, and the predicted and measured Rydberg constant R^* was in good agreement.

The Bohr model was successful to other one-electron atoms, such as singly ionized helium He^+ doubly ionized lithium Li^{++} and so on. Such atoms are called hydrogenlike atoms.

The measured series



Lyman-series: $m = 1, n > 1, f_{n1} = R^* \left(1 - \frac{1}{n^2} \right)$, ultraviolet region

Balmer-series: $m = 2, n > 2, f_{n2} = R^* \left(\frac{1}{4} - \frac{1}{n^2} \right)$, visible region

Paschen-series: $m = 3, n > 3, f_{n3} = R^* \left(\frac{1}{9} - \frac{1}{n^2} \right)$, infrared region

The biggest problem with the Bohr model is that it does not work for multi-electron atoms, and in the model the atom seems to be a disk, but in real it is a sphere.

Wave particle duality of particles, de-Broglie hypothesis

We have already seen the double nature of electromagnetic radiation or light. We concluded light can be a wave or particle. This was called wave particle duality.

In 1924 de-Broglie suggested the same duality in case of particles like protons or electrons. His question was: why can't we think of a moving electron—or any other particle—as a matter wave that transfers energy and momentum?

If a particle is a wave, it should have a wavelength and a frequency. De Broglie postulated that a free particle with rest mass m , moving with nonrelativistic velocity v has a momentum $p = mv$ should have a wavelength related to its momentum in the same way as for a photon.

The de Broglie wavelength and frequency of a particle is then: $\lambda = \frac{h}{p}$, and $f = \frac{E}{h}$,

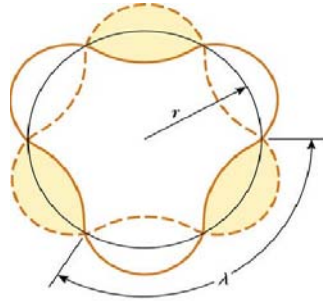
$h = 6,626 \cdot 10^{-34} Js$ the Planck constant.

With the de-Broglie hypothesis the Bohr's quantum condition sounds plausible:

$$m v r = n \hbar, \quad \text{so} \quad p r = n \frac{h}{2\pi}, \quad \text{and} \quad 2\pi r = n \frac{h}{p},$$

$$. 2\pi r = n \lambda$$

Only those orbital radii are allowed, that the circumference of the orbit is an integer multiple of the de-Broglie wavelength. So the existence of a standing wave around the nucleus is necessary for the electron.

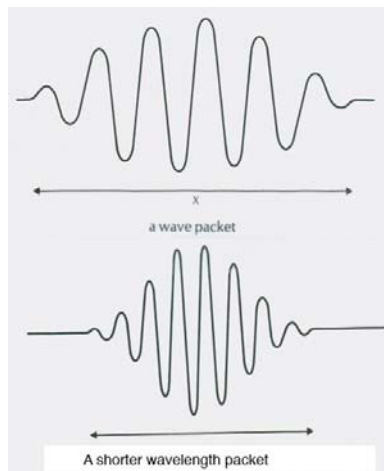


In case of a pure sine wave there is a contradiction, the phase velocity of the wave:

$$u = f \cdot \lambda = \frac{E}{h} \cdot \frac{h}{p} = \frac{m c^2}{m v} = \frac{c^2}{v} > c,$$

The phase velocity is greater than the speed of light.

Instead of a pure sine wave, a wave packet can be applied to describe the electron. The wave packet is the superposition of many pure sine waves with suitable amplitudes:



Considering a wave packet the contradiction is solved.

Calculate the speed of an electron accelerated at U potential difference, apply the work energy theorem:

$$eU = \frac{1}{2} m v^2, \quad \text{so} \quad v = \sqrt{\frac{2eU}{m}}, \quad e \text{ is the charge and } m \text{ is the mass of the electron.}$$

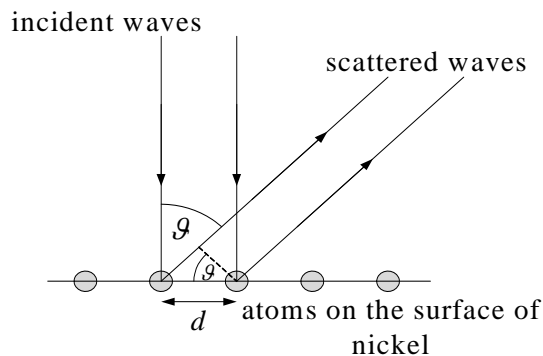
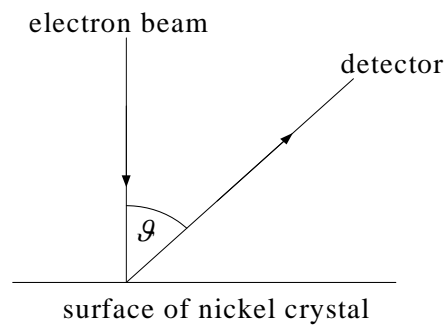
The momentum and the de-Broglie wavelength:

$$p = m v = m \sqrt{\frac{2eU}{m}} = \sqrt{2eU m},$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2eUm}}$$

Calculate the numerical value for 150V potential difference: $\lambda \approx 10^{-10} m$.

The existence of matter waves was first verified experimentally in 1927, by Davisson and Germer. They bombarded the surface of a nickel crystal and detected the diffracted electrons.

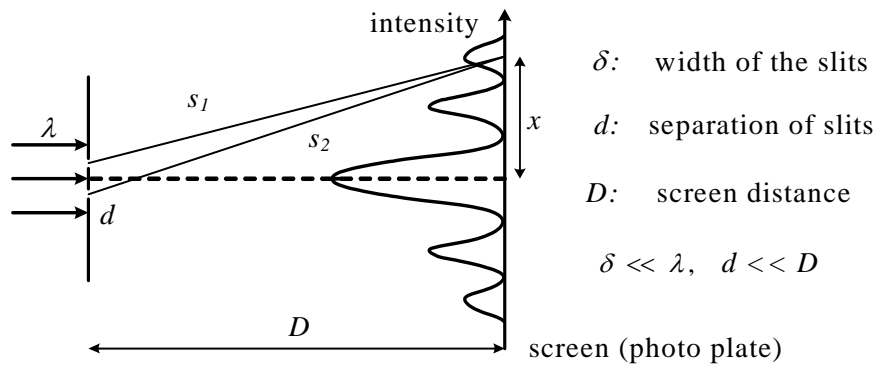


They found a periodical variation of the reflected electron beam intensity due to interference, and the obtained wavelength was in good agreement with the de-Broglie hypothesis. The condition of maximal intensity in case of interference is the path difference is $d \sin \theta = n \cdot \lambda$, if $n=1$ $d \sin \theta = \lambda$.

In case of macroscopic objects the momentum is too large and the de-Broglie wavelength is very small. The effects of such tiny wavelengths are so small that it is impossible to detect.

Two-slit interference of electrons

The two slits light interference experiment is well known and made by Young in 1802. This experiment was repeated by Jönsson in 1961 with electrons. Consider an electron beam directed to a plate with two slits. The electrons are accelerated to the same speed. Instead of a white screen a photographic film was applied. After exposition an interference pattern appeared on the plate. The explanation:



Calculate the path distance between the two paths.

$$s_1^2 = D^2 + \left(x - \frac{d}{2}\right)^2,$$

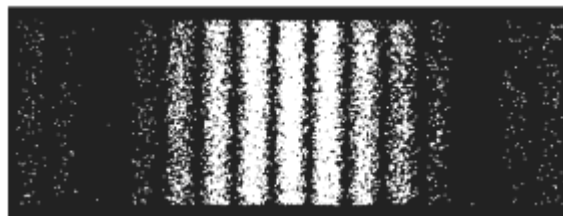
$$s_2^2 = D^2 + \left(x + \frac{d}{2}\right)^2,$$

$$(s_2 + s_1) \cdot (s_2 - s_1) = 2xd,$$

$$(s_2 + s_1) \approx 2D, \text{ and } (s_2 - s_1) = \Delta s, \text{ so } \Delta s = \frac{xd}{D}$$

for a maximum intensity fringe, we saw that Δs must be either zero or an integer number of wavelengths: $\Delta s = k \cdot \lambda$, where $k = 0, \pm 1, \pm 2, \dots$, it means $k \cdot \lambda = \frac{x_k d}{D}$, $x_k = k \frac{d}{D} \lambda$.

From the measured interference pattern the distances of the maximum intensity fringes can be obtained and the wavelength can be calculated. The measured wavelength was in a good agreement with the de-Broglie hypothesis.



It was the most beautiful verification of the de-Broglie hypothesis. We can say that particles in some experiment behave like waves. The wave-particle duality proposes that every elementary particle exhibits the properties of not only particles, but also waves, and it has a central concept of quantum mechanics.

In 1924 de-Broglie suggested to describe the discrete atomic states of the electron as wave properties and Schrödinger wrote his famous equation for the atomic electron wave.

The Heisenberg uncertainty principle

As we have already seen, instead of a pure sine wave, a wave packet can be applied to describe the electron. The wave packet is the superposition of many pure sine waves with suitable amplitudes. If a wave packet extends over a region Δx , the values of the wave numbers of the interfering waves which compose the wave packet fall within a range Δk , and according to the theory of Fourier analysis:

$$\Delta x \cdot \Delta k \sim 1.$$

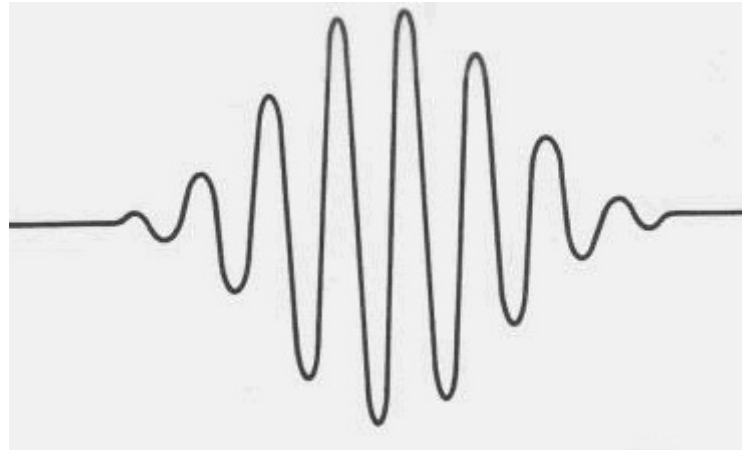
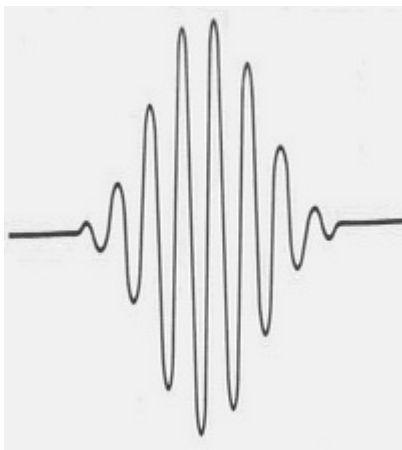
The wave number is $k = \frac{2\pi}{\lambda}$, and $\lambda = \frac{h}{p}$, so $k = \frac{2\pi}{h} p$. Considering the above equation:

$$\Delta k = \frac{2\pi}{h} \Delta p, \quad \Delta x \frac{2\pi}{h} \Delta p \sim 1,$$

$$\Delta x \Delta p \sim \frac{h}{2\pi}.$$

Defining a new constant designated by \hbar and called h-bar

$$\Delta x \Delta p \sim \hbar.$$



That is this relation implies that the larger Δx is the smaller Δp is, and conversely. In other words, information about the localization of a particle in space is obtained at the expense of knowledge about its momentum. We cannot accurately determine both the position and momentum of a particle simultaneously so that $\Delta x = 0$, and $\Delta p = 0$ at the same time.

The exact formulas of the Heisenberg uncertainty principle are:

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

$$\Delta y \Delta p_y \geq \frac{\hbar}{2}$$

$$\Delta z \Delta p_z \geq \frac{\hbar}{2}$$

$$\Delta E \Delta t \geq \frac{\hbar}{2}.$$

It states that, in general, it is impossible to simultaneously determine both the position and the corresponding momentum of a particle with arbitrarily great precision, as classical physics would predict. There is an uncertainty relation between time and energy as well.

A particle of well known momentum $\Delta p = 0$ is represented by a wave of constant amplitude extending over all space $\Delta x \sim \infty$, so that our knowledge of the position is nothing. If the particle is well localized $\Delta x = 0$, the knowledge of the momentum is nothing $\Delta p \sim \infty$.

What is the meaning of the symbol Δ ?

Measure the momentum of a particle described by a wave packet, and denote the measured values by p_i then the average value of the momentum is $\bar{p} = \frac{1}{n} \sum_{i=1}^n p_i$. The square of the

deviation is defined as $(\Delta p)^2 = \frac{1}{n} \sum_{i=1}^n (\bar{p} - p_i)^2$, and the deviation is $\Delta p = \sqrt{\frac{1}{n} \sum_{i=1}^n (\bar{p} - p_i)^2}$.

In case of position measurement the average is $\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$, and the deviation is

$$\Delta x = \sqrt{\frac{1}{n} \sum_{i=1}^n (\bar{x} - x_i)^2}.$$

The consequences of the Heisenberg uncertainty principle.

1. The path of a macroscopic mass point and a particle

Consider a mass point $m = 10^{-9} \text{ kg}$, and the deviation or uncertainty of its position

$$\Delta x \approx 10^{-5} \text{ m}. \quad \Delta x \Delta p_x = \frac{\hbar}{2}, \quad \Delta x \cdot m \Delta v_x = \frac{\hbar}{2}, \quad \text{and} \quad \Delta v_x = \frac{h}{4\pi \Delta x \cdot m} \approx 5 \cdot 10^{-21} \frac{\text{m}}{\text{s}}.$$

This quantity is so small that it is impossible to measure. In case of a macroscopic mass point we can speak about its trajectory, we know simultaneously where the mass point is and what its velocity is.

Consider now a particle for example an electron in an atom: $m = 9.1 \cdot 10^{-31} \text{ kg}$, and the

deviation or uncertainty of its position $\Delta x \approx 10^{-10} \text{ m}$. $\Delta x \Delta p_x = \frac{\hbar}{2}$, $\Delta x \cdot m \Delta v_x = \frac{\hbar}{2}$, and

$$\Delta v_x = \frac{h}{4\pi \Delta x \cdot m} \approx 5 \cdot 10^5 \frac{\text{m}}{\text{s}}.$$

In case of a particle the uncertainty of the velocity is so great that we cannot speak about its trajectory. For particles of atomic dimensions the concept of trajectory has no meaning.

2. The zero-point energy

Start again with the Heisenberg uncertainty relation: $\Delta x \Delta p_x = \frac{\hbar}{2}$, so $\Delta x \cdot m \Delta v_x \geq \frac{\hbar}{2}$, and

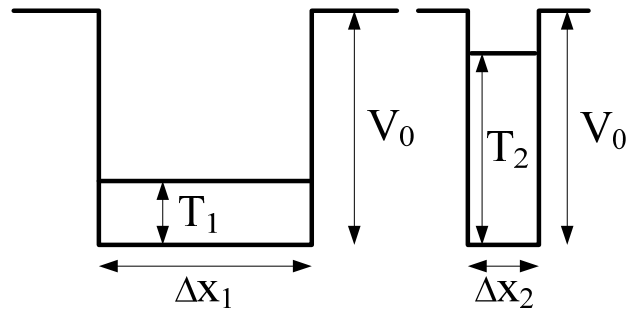
$$\Delta v_x \geq \frac{\hbar}{2 \Delta x \cdot m}.$$

The order of the deviation is about the maximal difference from the mean value, so $\Delta v_x \leq \bar{v}_x$. Then the kinetic energy in one dimension:

$$T = \frac{1}{2} m v_x^2 = \frac{1}{2} m \Delta v_x^2 \geq \frac{1}{2} m \frac{\hbar^2}{4 m^2 \Delta x^2} = \frac{\hbar^2}{8 m \Delta x^2}, \quad \text{that is } T \geq \frac{\hbar^2}{8 m \Delta x^2}.$$

This energy is referred to as zero-point energy. From Heisenberg uncertainty relation it is an inevitable conclusion that if a particle is restricted to a space Δx , even at absolute zero temperature must have a certain minimum energy.

If this minimum kinetic energy is less than the depth of the potential valley then the state is called bound state.



If $T_{\min} = \frac{\hbar^2}{8m\Delta x^2} > V_0$ there is no bound state. We can say that there is no bound state if the potential valley is not enough deep, or the particle is restricted to a very small place. This is the cause that it is impossible for an electron in a nucleus to be in bound state.