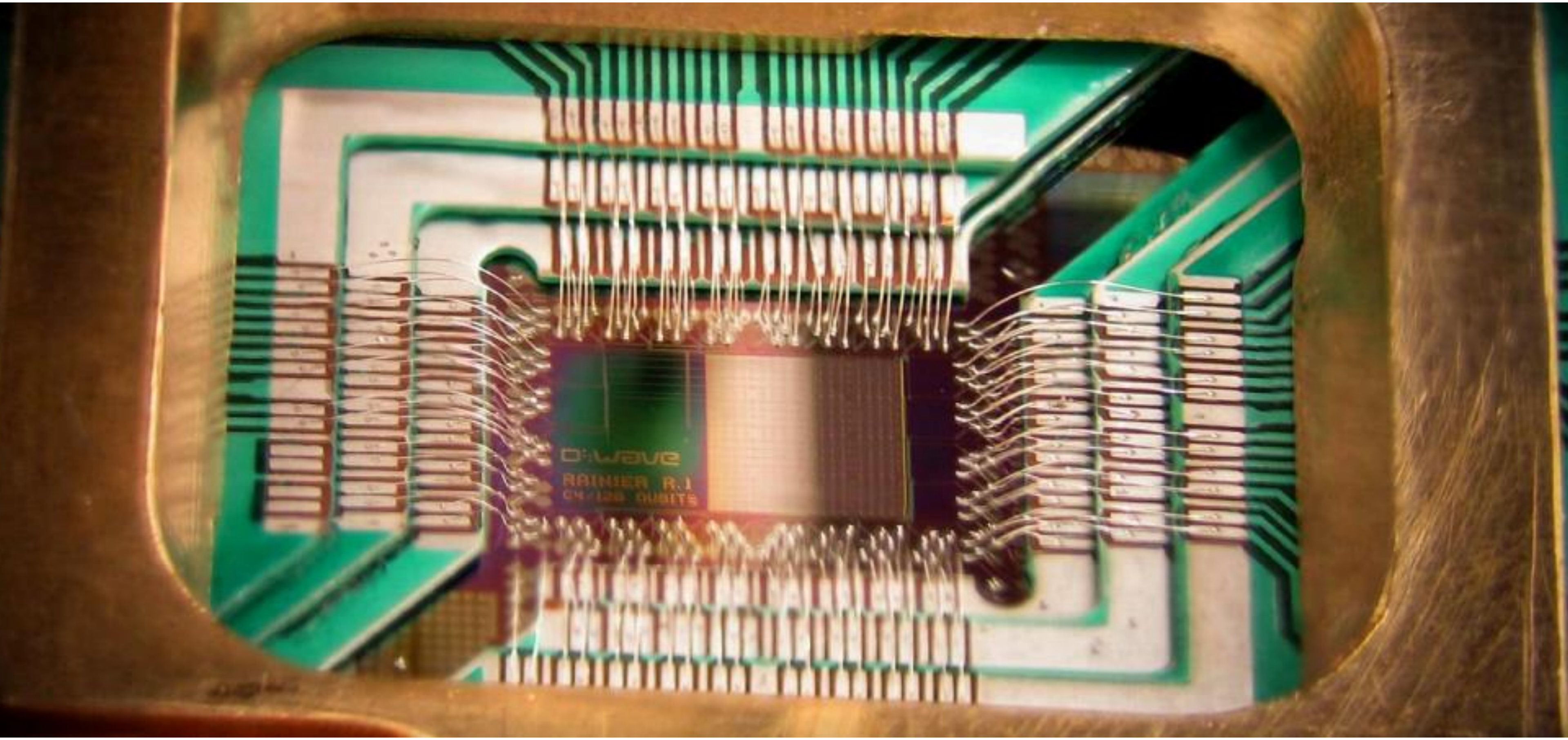
Chapter 27
Early Quantum Theory and Models of the Atom



A D-wave qubit processor: The brain of a quantum computer that encodes information in quantum bits to perform complex calculations.

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- Blackbody Radiation; Planck's Quantum Hypothesis
- Photon Theory of Light and the Photoelectric Effect
- Energy, Mass, and Momentum of a Photon
- Compton Effect
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27-1 Bonding in Molecules

Molecule: two or more atoms strongly held together to function as a unit

This attachment is called a chemical bond

Two types of bond:

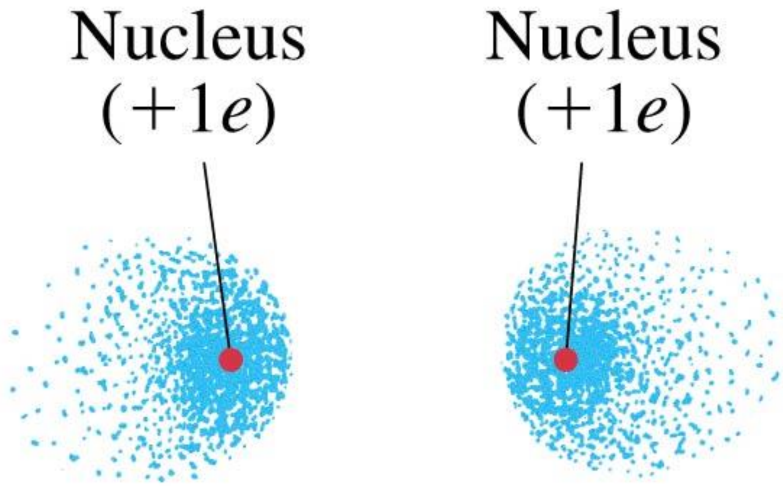
1. Covalent

2. Ionic

27-1 Bonding in Molecules

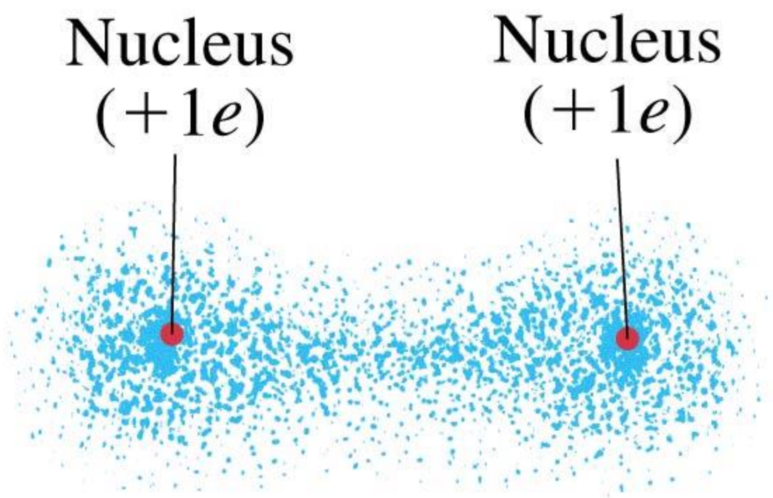
Hydrogen molecule, H_2, is bound covalently.

If the atoms have their spins in the same direction, so $S = 1$ for the molecule, the atoms will not bond due to the exclusion principle.



27-1 Bonding in Molecules

The molecule will only form if $S = 0$. The two electrons are shared by both atoms:

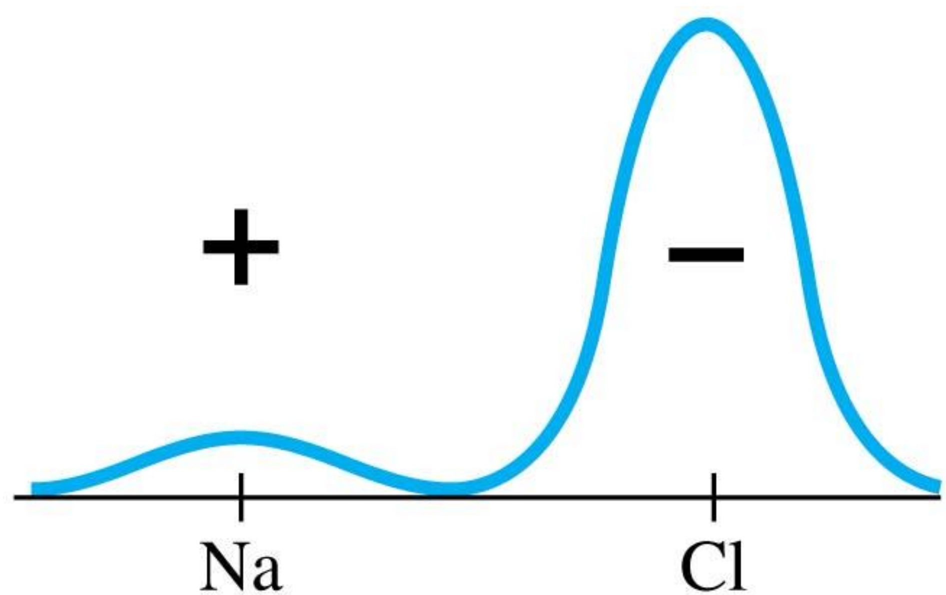


The energy needed to separate the atoms is called the binding energy.

27-1 Bonding in Molecules

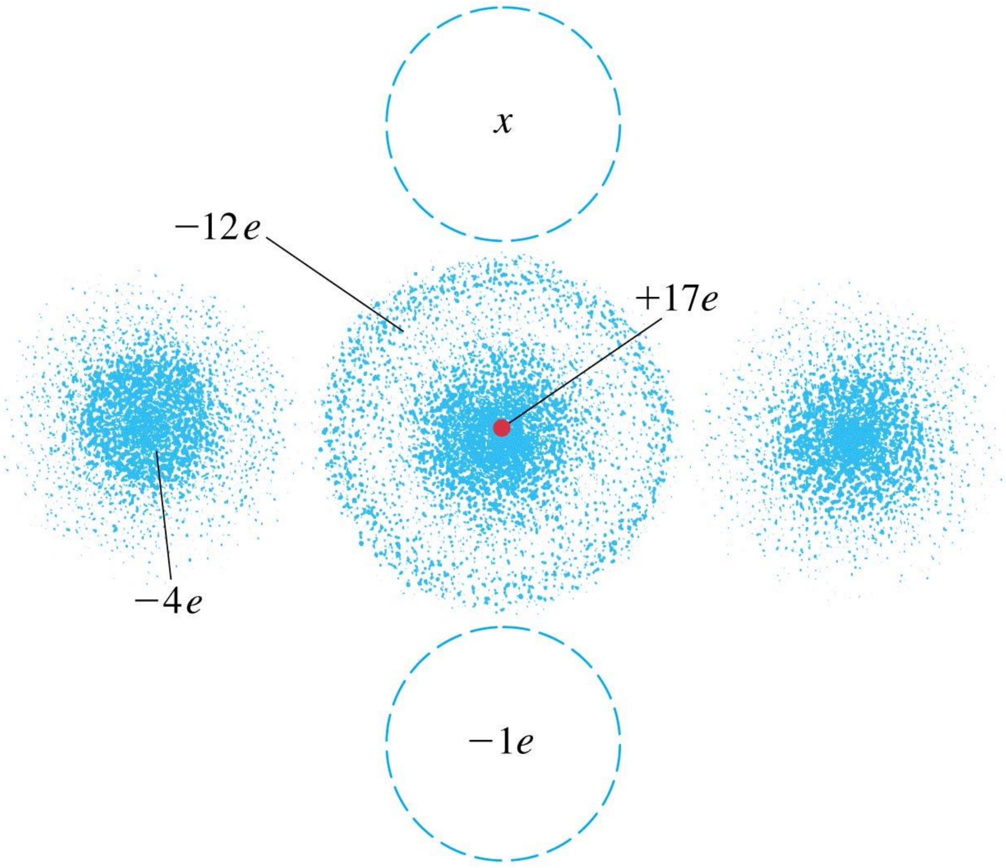
An ionic bond is created by the attraction of ions.

For example, the outermost electron in the sodium atom spends most of its time around the chlorine atom in NaCl.



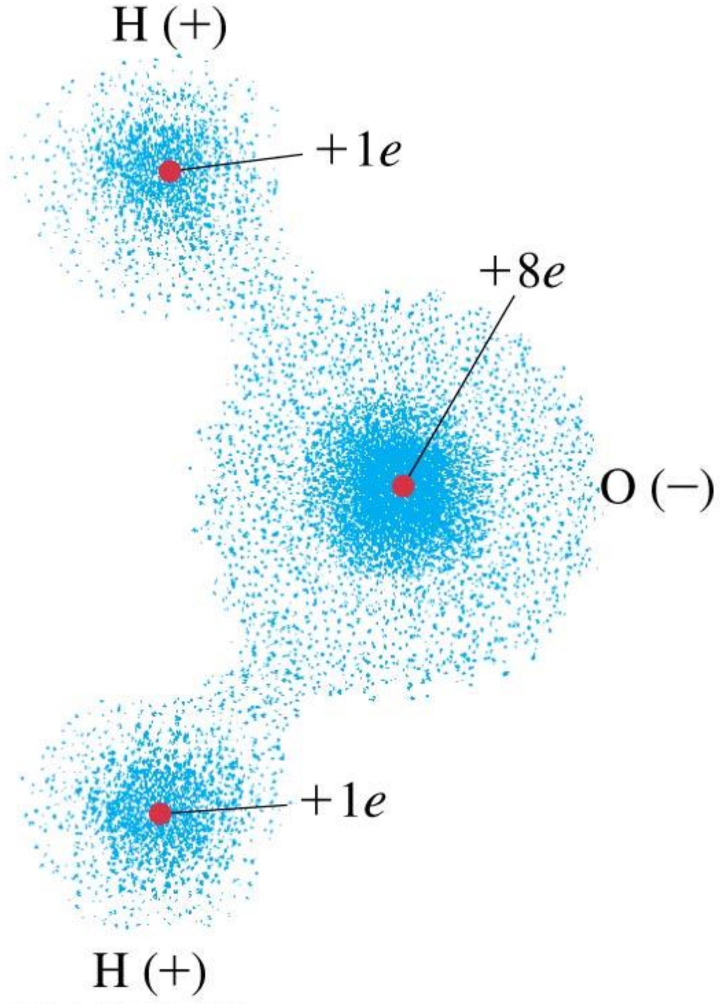
27-1 Bonding in Molecules

The reason this happens is that sodium has a single electron outside a closed shell, and it is not tightly bound. Conversely, the chlorine atom has an empty space; there is only one electron where two can be accommodated.



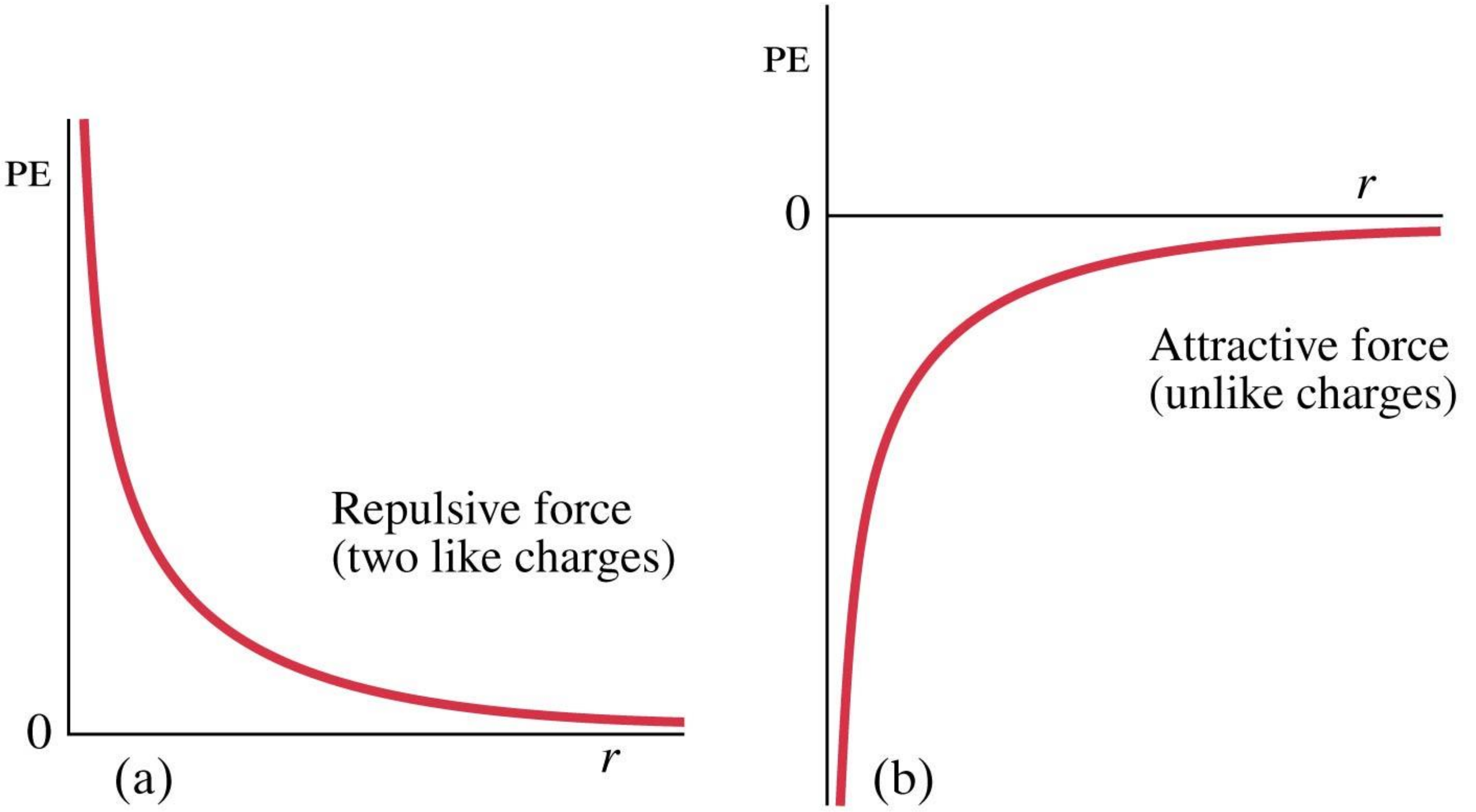
27-1 Bonding in Molecules

Pure covalent bonds are found in molecules consisting of only one type of atom. Otherwise, electrons are likely to spend more time around one type of atom than another, giving a partial ionic character. Water is one such molecule.



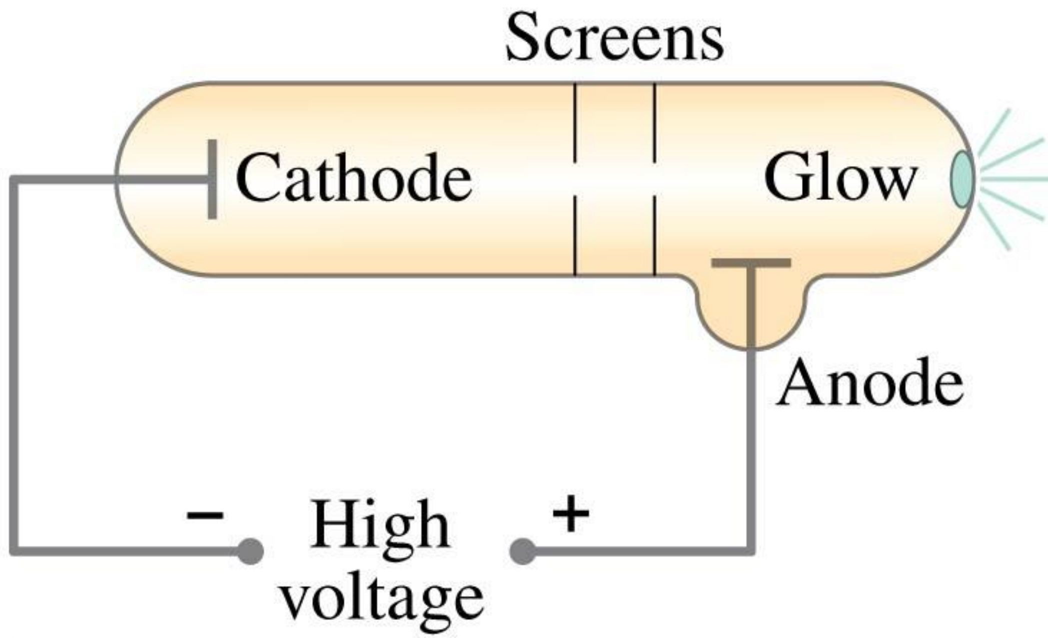
27-2 Potential-Energy Diagrams for Molecules

Potential energy of two point charges:



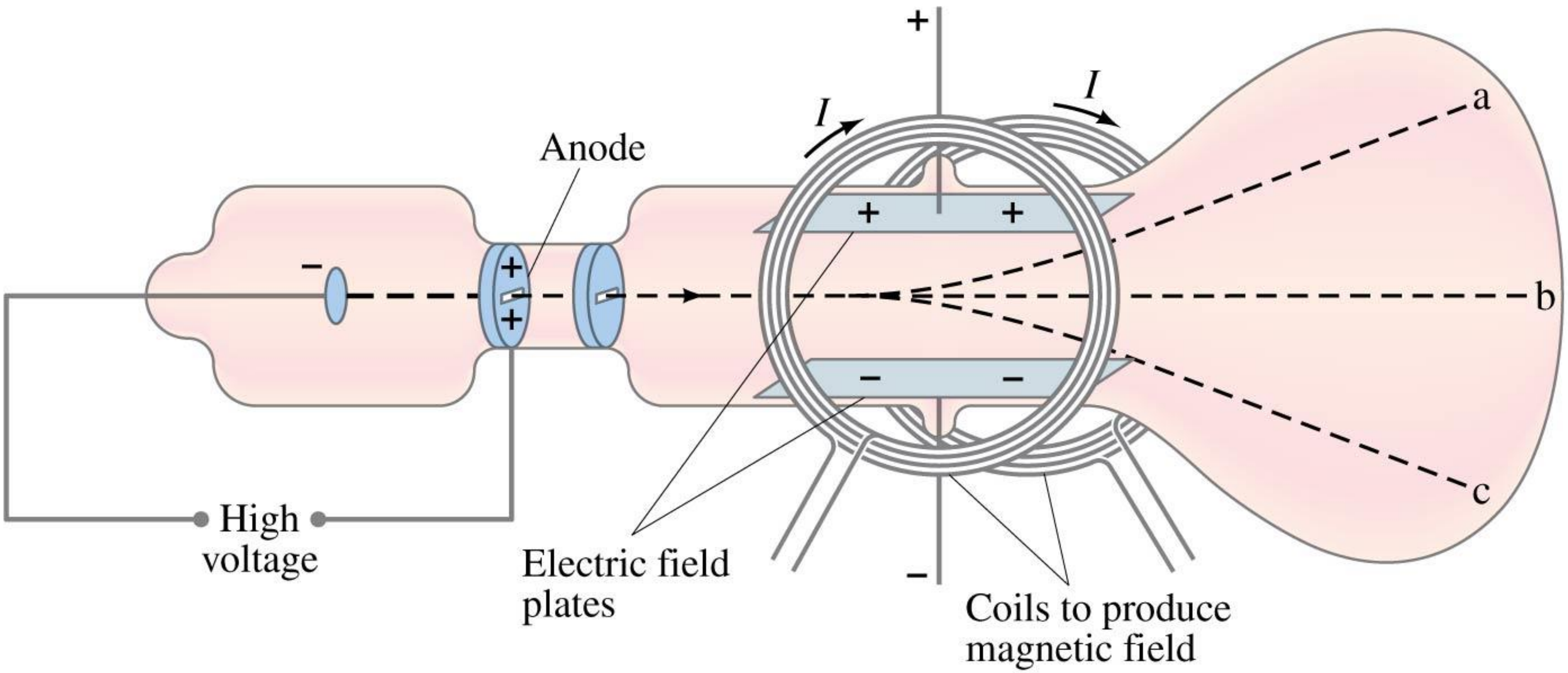
27-1 Discovery and Properties of the Electron

In the late 19th century, discharge tubes were made that emitted “cathode rays.”



27-1 Discovery and Properties of the Electron

It was found that these rays could be deflected by electric or magnetic fields.



27-1 Discovery and Properties of the Electron

By accelerating the rays through a known potential and then measuring the radius of their path in a known magnetic field, the charge to mass ratio could be measured:

$$\frac{e}{m} = \frac{E}{B^2 r}. \quad (27\text{-}1)$$

The result is $e/m = 1.76 \times 10^{11}$ C/kg.

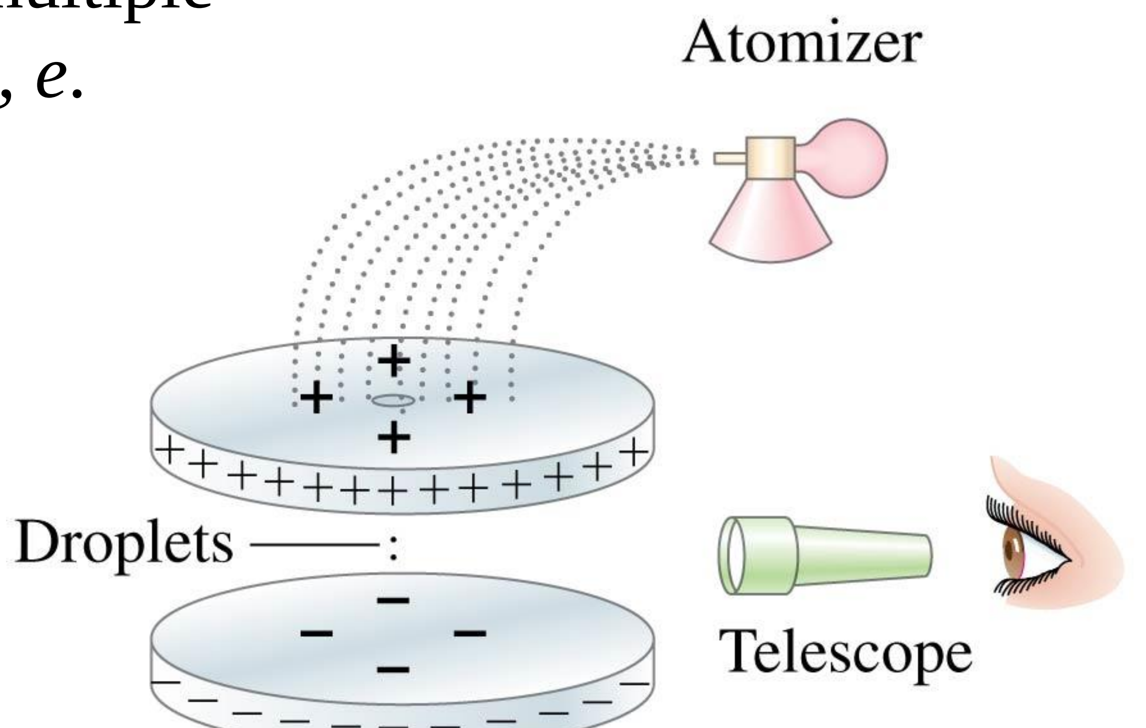
27-1 Discovery and Properties of the Electron

Cathode rays were soon called electrons.

Millikan devised an experiment to measure the charge on the electron by measuring the electric field needed to suspend an oil droplet of known mass between parallel plates.

27-1 Discovery and Properties of the Electron

The mass and charge of each droplet were measured; careful analysis of the data showed that the charge was always an integral multiple of a smallest charge, *e*.



27-1 Discovery and Properties of the Electron

The currently accepted value of *e* is:

$$e = 1.602 \times 10^{-19}\ \mathrm{C}$$

Knowing *e* allows the electron mass to be calculated:

$$m_{\mathrm{e}} = 9.11 \times 10^{-31}\ \mathrm{kg}$$

27-2 Blackbody Radiation; Planck's Quantum Hypothesis

All objects emit radiation whose total intensity is proportional to the fourth power of their temperature. This is called thermal radiation; a blackbody is an object that emits thermal radiation only.

The spectrum of blackbody radiation has been measured; it is found that the frequency of peak intensity increases linearly with temperature.

28-3 Radioactivity

Towards the end of the 19th century, minerals were found that would darken a photographic plate even in the absence of light.

This phenomenon is now called radioactivity.

Marie and Pierre Curie isolated two new elements that were highly radioactive; they are now called polonium and radium.

28-3 Radioactivity

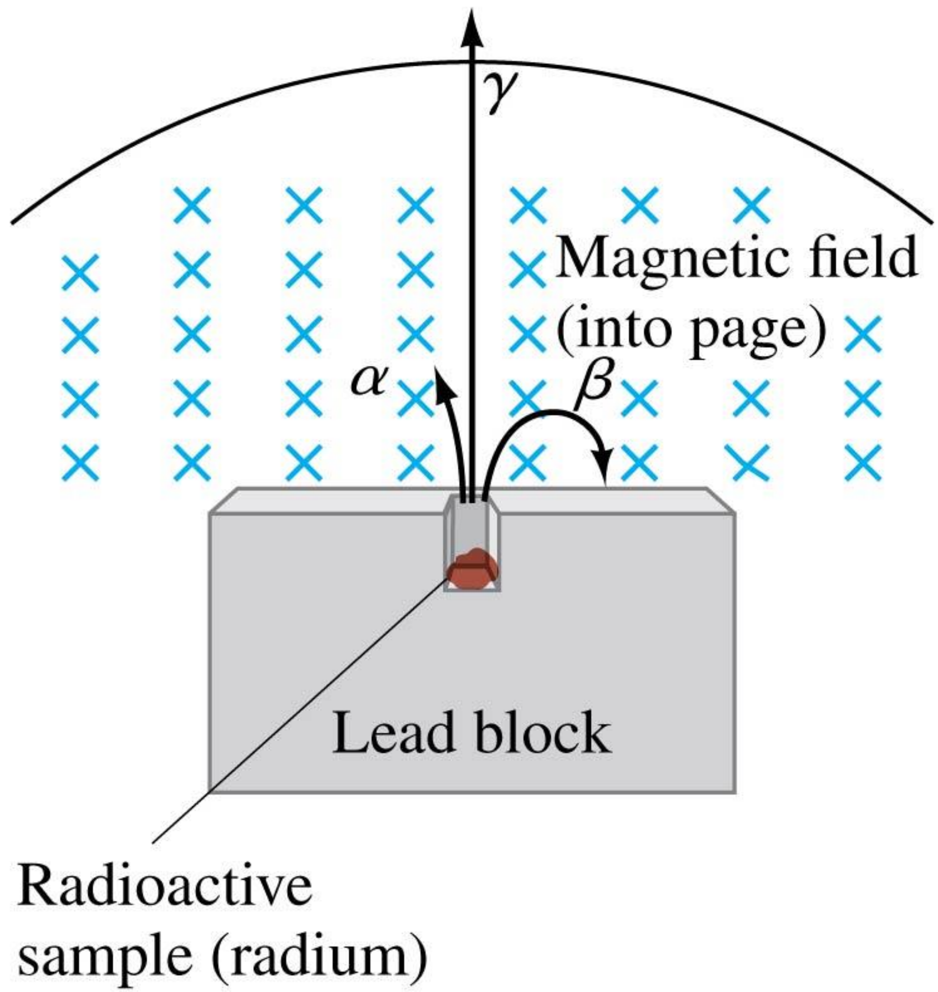
Radioactive rays were observed to be of three types:

1. Alpha rays, which could barely penetrate a piece of paper
2. Beta rays, which could penetrate 3 mm of aluminum
3. Gamma rays, which could penetrate several centimeters of lead

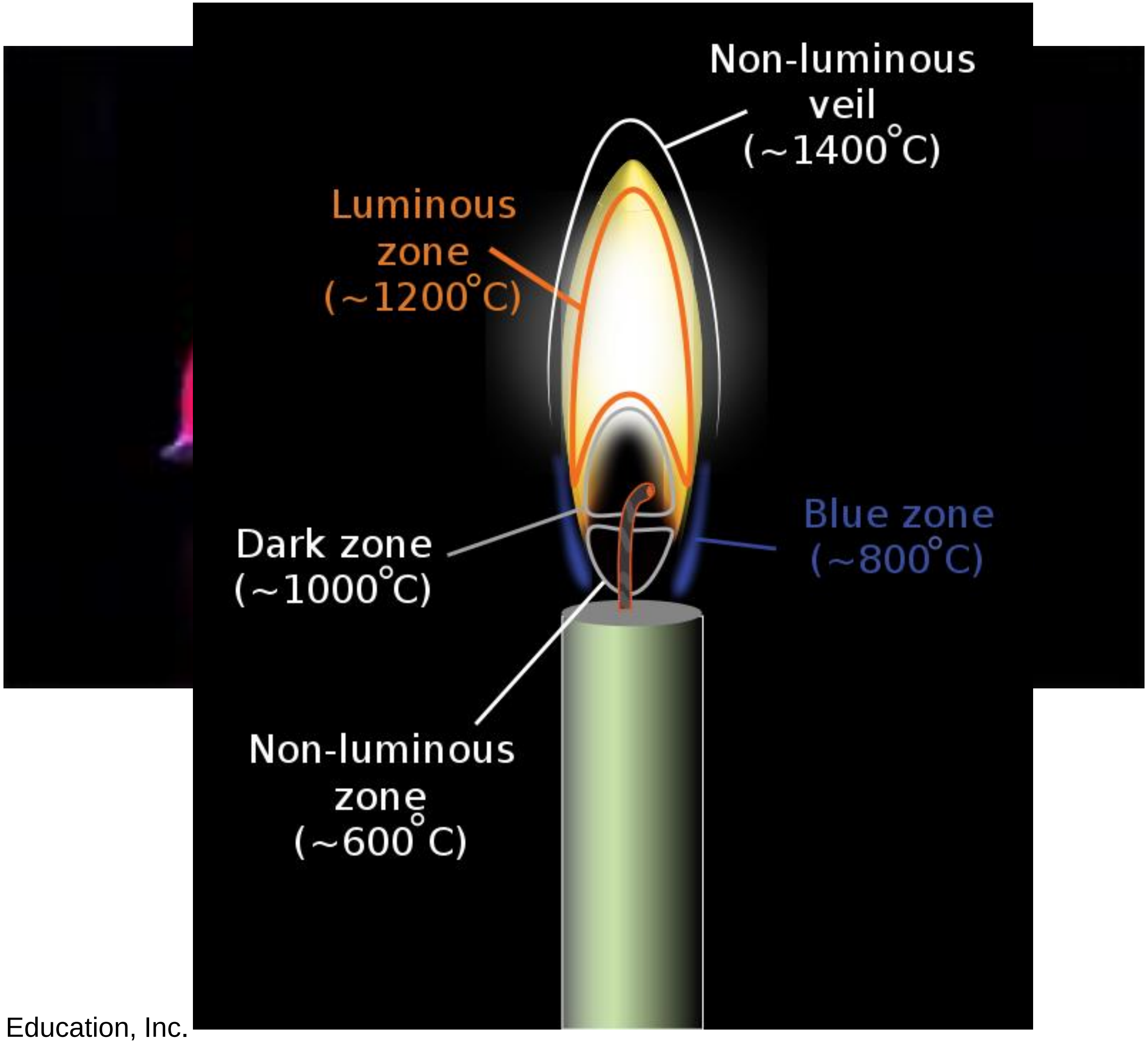
We now know that alpha rays are helium nuclei, beta rays are electrons, and gamma rays are electromagnetic radiation.

28-3 Radioactivity

Alpha and beta rays are bent in opposite directions in a magnetic field, while gamma rays are not bent at all.

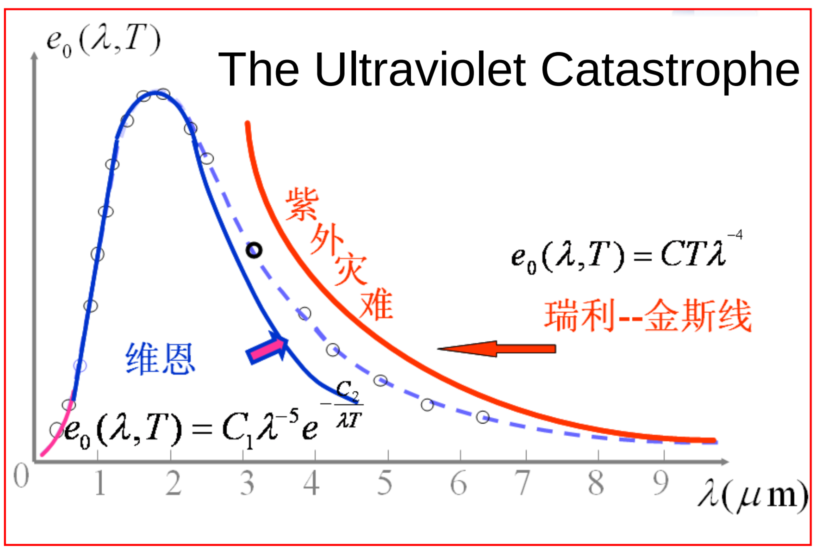


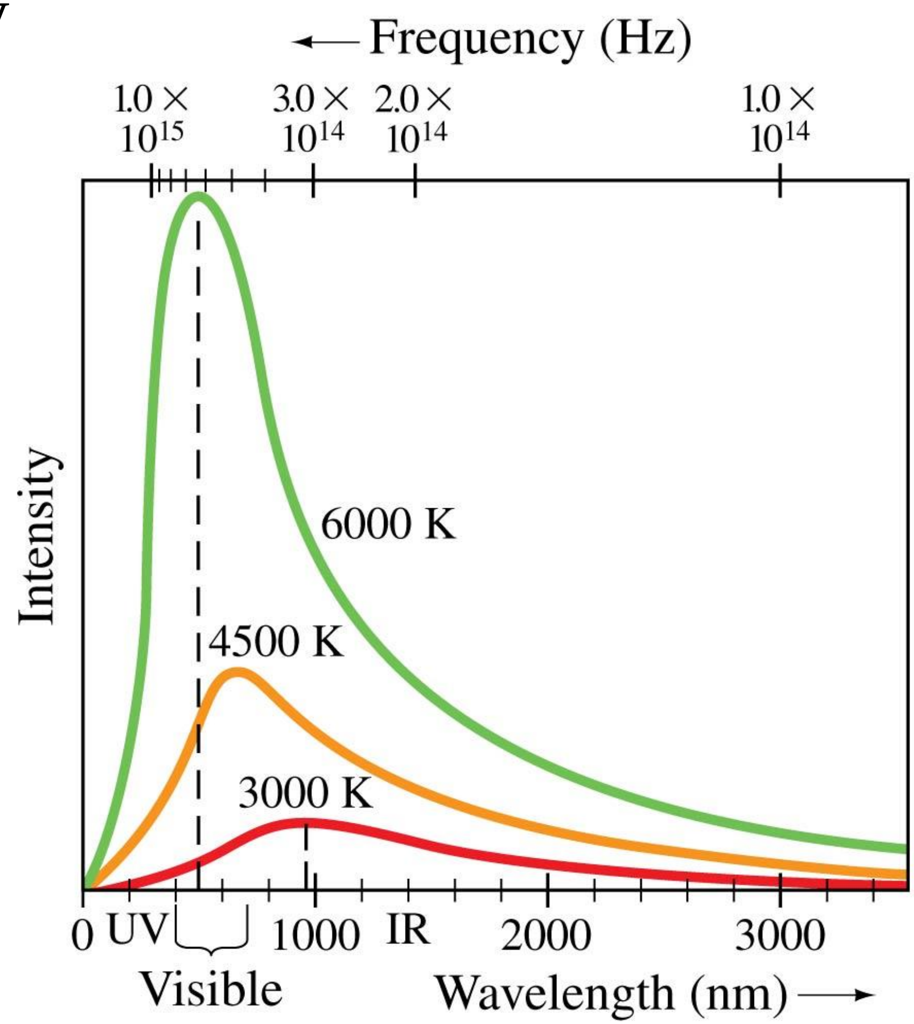
The color of flame



27-2 Blackbody Radiation; Planck's Quantum Hypothesis

This figure shows blackbody radiation curves for three different temperatures. Note that frequency increases to the left.





27-2 Blackbody Radiation; Planck's Quantum Hypothesis

Monochromatic radiation power(单色辐射本领） $e_0(\lambda, T)$

1. Rayleigh Jeans formula： $e_0(\lambda, T) = CT\lambda^{-4}$

Starting point: Law of equipartition of energy

将能量按自由度均分原理用到电磁辐射上长波与实验曲线吻合，短波相差很大

—— 紫外灾难。

2. Wien formula： $e_0(\lambda, T) = C_1\lambda^{-5}e^{-\frac{C_2}{\lambda T}}$

Starting point： Boltzmann velocity distribution

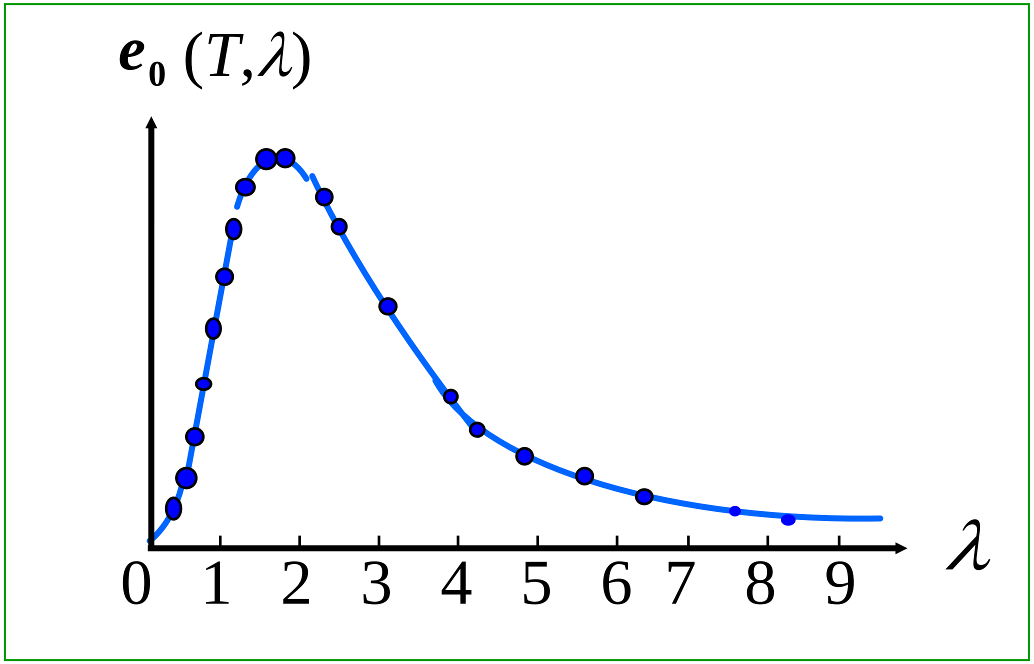
将类似分子速率分布的规律用到电磁辐射上短波与实验曲线接近，长波相差很大。

3、 Planck's Quantum Hypothesis

1. Empirical formula

Data fitting method:

$$e_0(\lambda, T) = 2\pi hc^2\lambda^{-5}\left(e^{\frac{hc}{k\lambda T}} - 1\right)^{-1}$$



27-2 Blackbody Radiation; Planck's Quantum Hypothesis

This spectrum could not be reproduced using 19^{th}-century physics.

The solution was proposed by Max Planck in 1900:

The energy of atomic oscillations within atoms cannot have an arbitrary value; it is related to the frequency:
$E = hf = h/T$

The constant h is now called Planck's constant.

27-2 Blackbody Radiation; Planck's Quantum Hypothesis

Planck found the value of his constant by fitting blackbody curves:

$$h = 6.626 \times 10^{-34}\ \mathrm{J{\cdot}s}$$

Planck's proposal was that the energy of an oscillation had to be an integral multiple of hf. This is called the **quantization of energy**.

It overturns the classical principle that all natural processes are continuous

27-6 Photon Interactions; Pair Production

Photons passing through matter can undergo the following interactions:

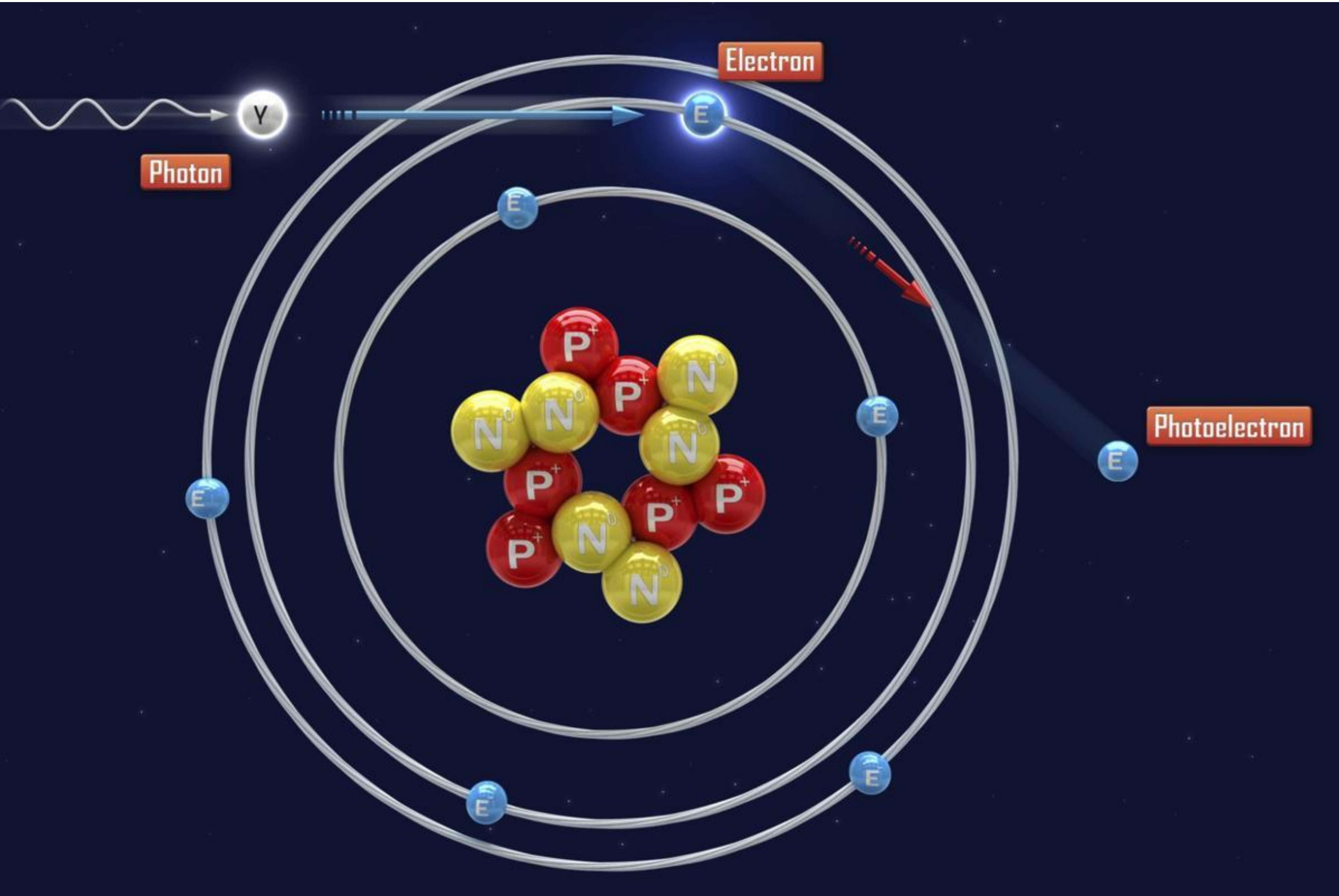
1. Photon may be totally absorbed by electron, but not have enough energy to eject it; the electron moves into an excited state

2. Photoelectric effect: photon is completely absorbed, electron is ejected

3. The photon can scatter from an atom and lose some energy

4. The photon can produce an electron-positron pair.

Photon Theory of Light and the Photoelectric Effect

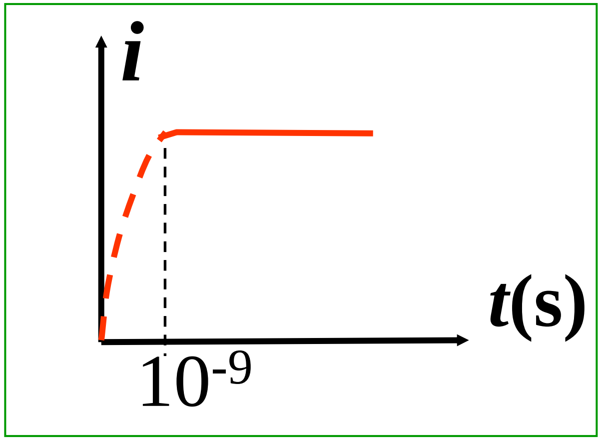


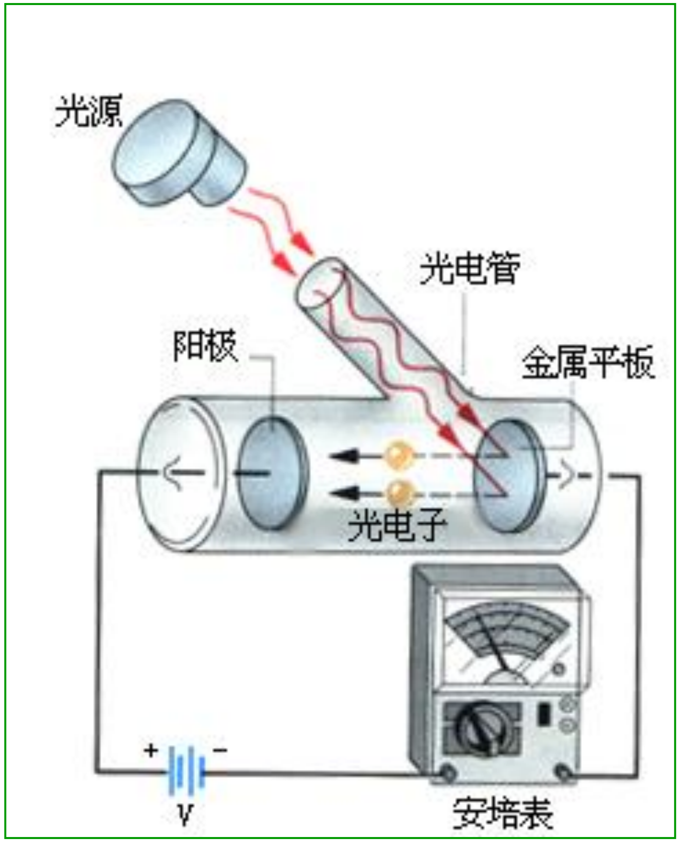
4. The Photoelectric Effect

When light strikes a metal conductor, it is possible for electrons in the metal to escape from the surface. This phenomenon is called the photoelectric effect

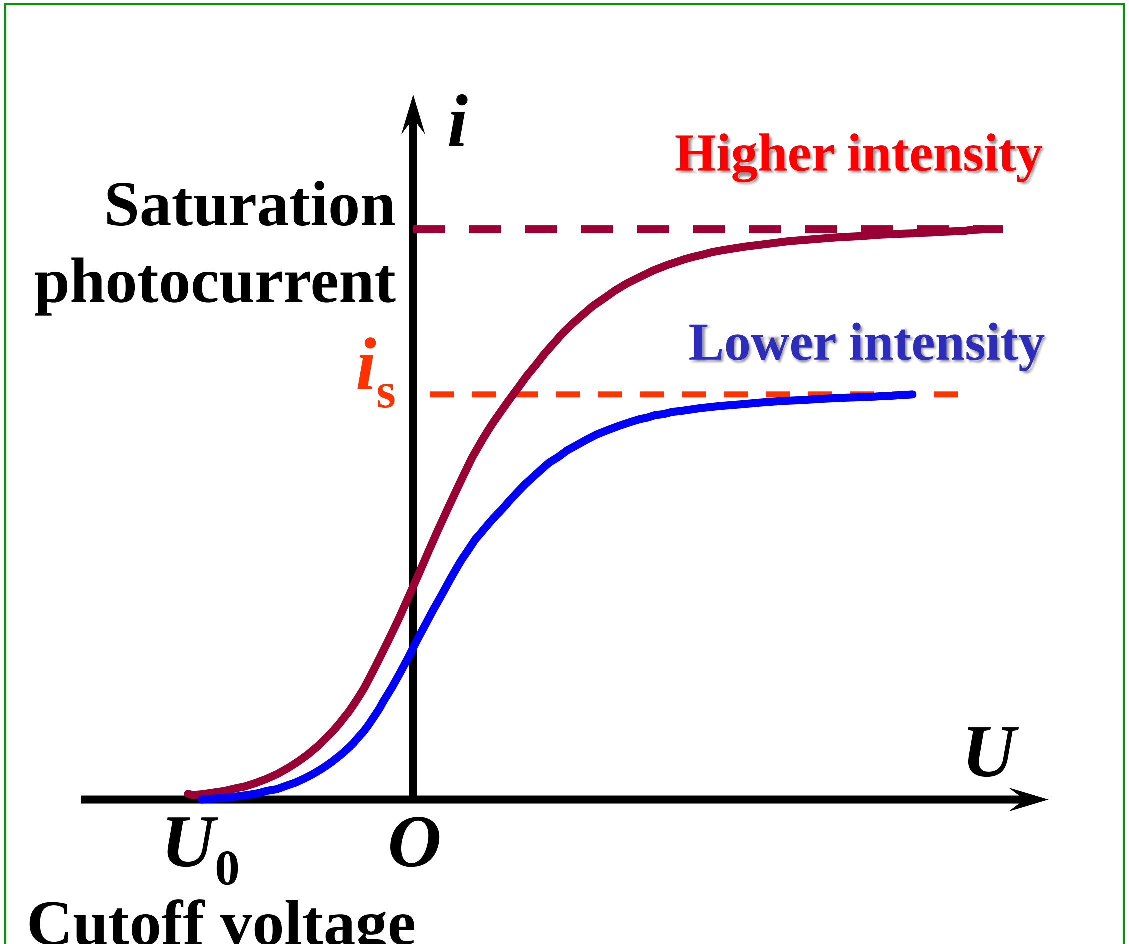
1. Experimental results

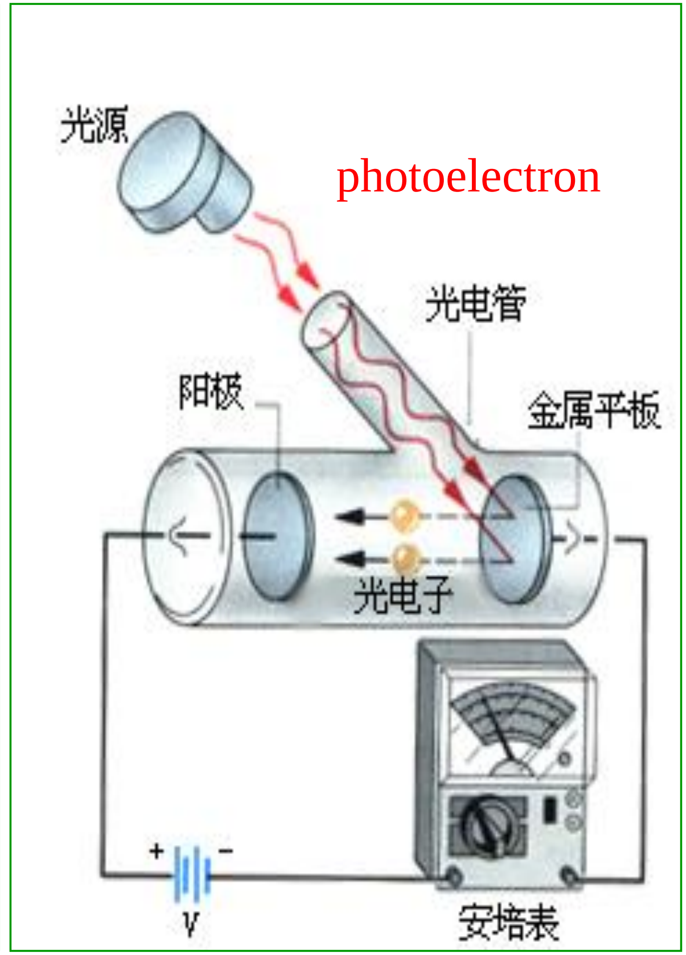
(1) The photoelectric effect is instantaneous



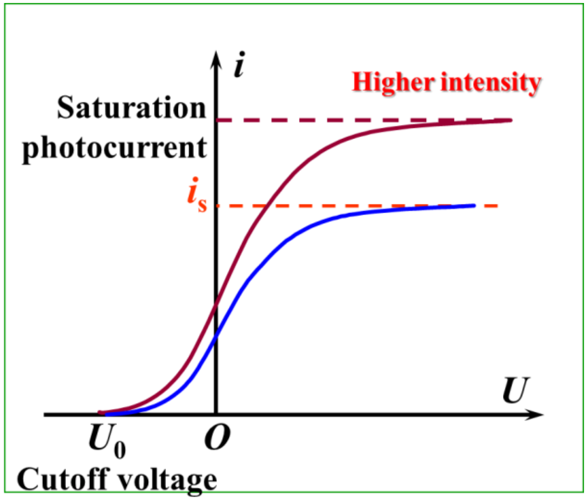


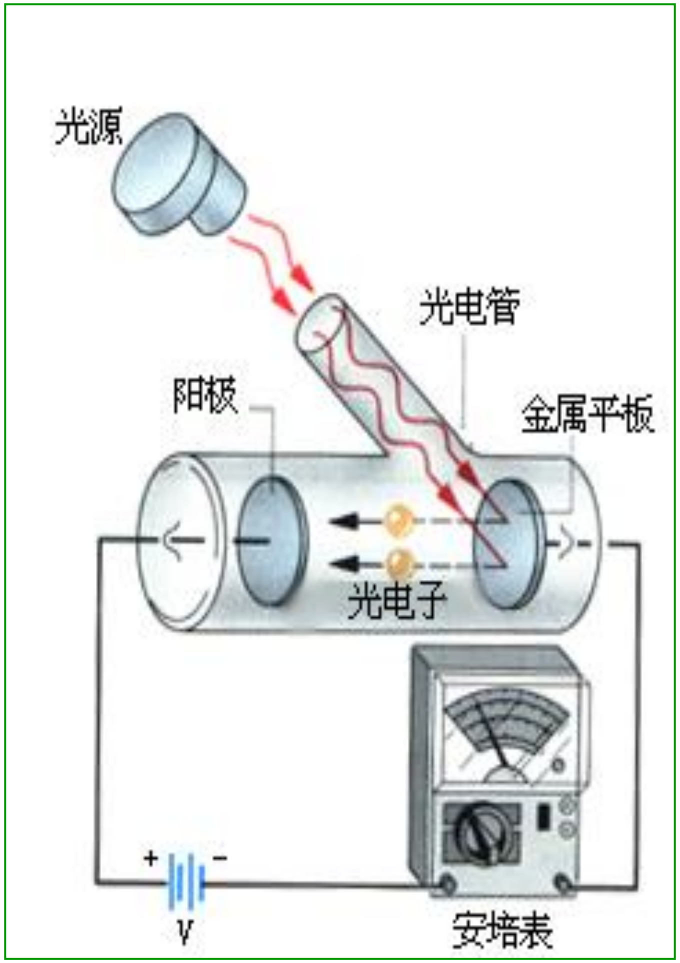
(2) The saturation photocurrent is proportional to the intensity of incident light





(2) The saturation photocurrent is proportional to the intensity of incident light





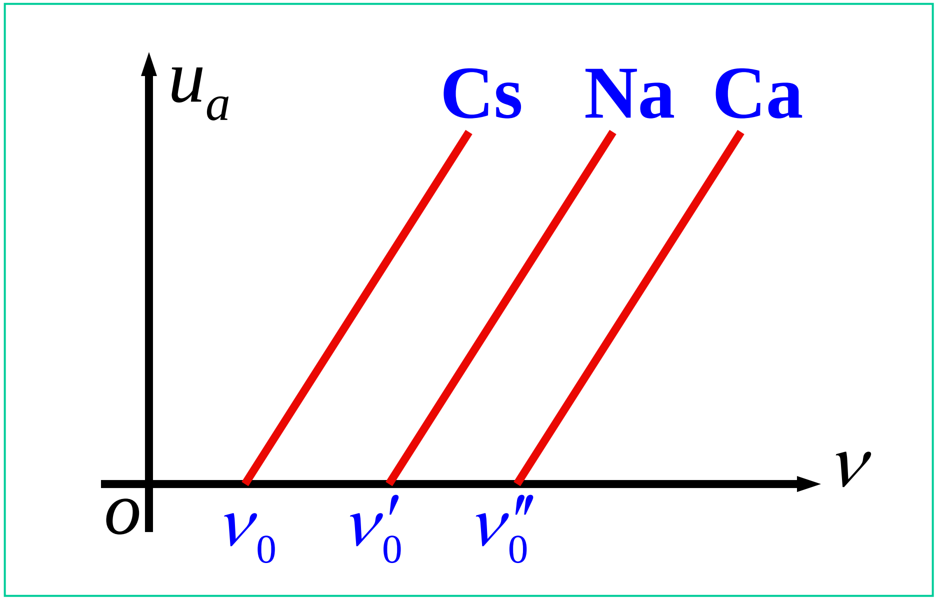
The existence of cutoff voltage indicates that the photoelectron has initial kinetic energy,

$$eU_a = \frac{1}{2} m v_{\mathrm{m}}^2$$

(3) The relationship between the initial kinetic energy of the photoelectron and the frequency of incident light

The experimental results show that there is a linear relation between cutoff voltage and incident light frequency：

$$eU_a = \frac{1}{2} m v_{\mathrm{m}}^2$$



(4) For any metal, there is a cutoff frequency ν_0

$$E = hf,$$

27-3 Photon Theory of Light and the Photoelectric Effect

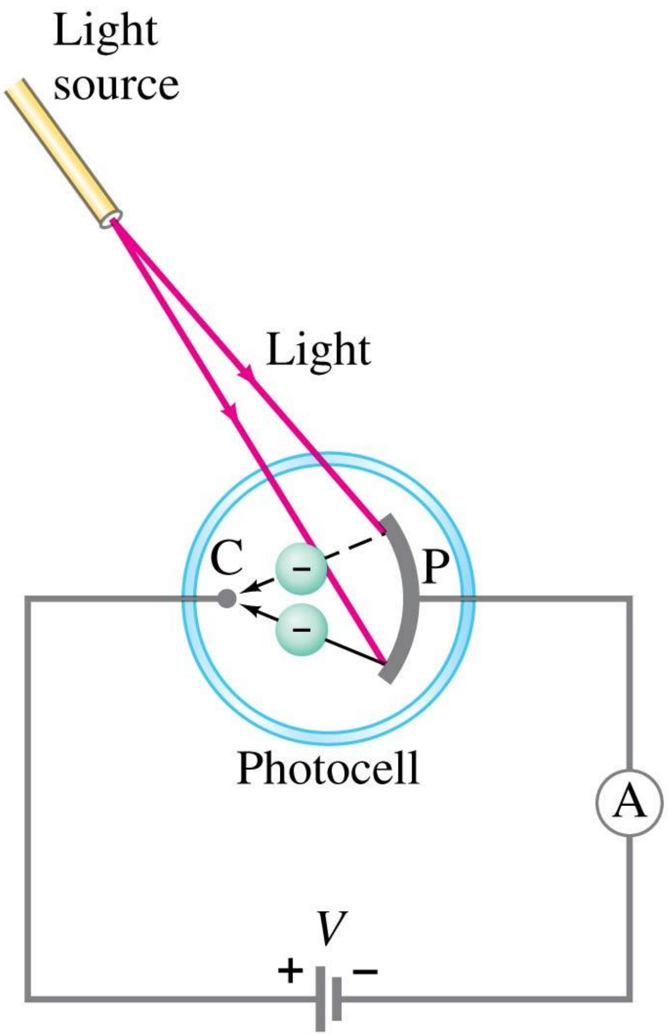
Einstein suggested that, given the success of Planck's theory, light must exist as a set of small energy packets:

$$\boxed{E = hf,} \quad (27\text{-}4)$$

These tiny packets, or particles, are called photons.

27-3 Photon Theory of Light and the Photoelectric Effect

The photoelectric effect:
If light strikes a metal, electrons are emitted. The effect does not occur if the frequency of the light is too low; the kinetic energy of the electrons increases with frequency.



27-3 Photon Theory of Light and the Photoelectric Effect

If light is a wave, theory predicts for the photoelectric effect:

1. Number of electrons and their energy should increase with intensity
2. Frequency should not matter

27-3 Photon Theory of Light and the Photoelectric Effect

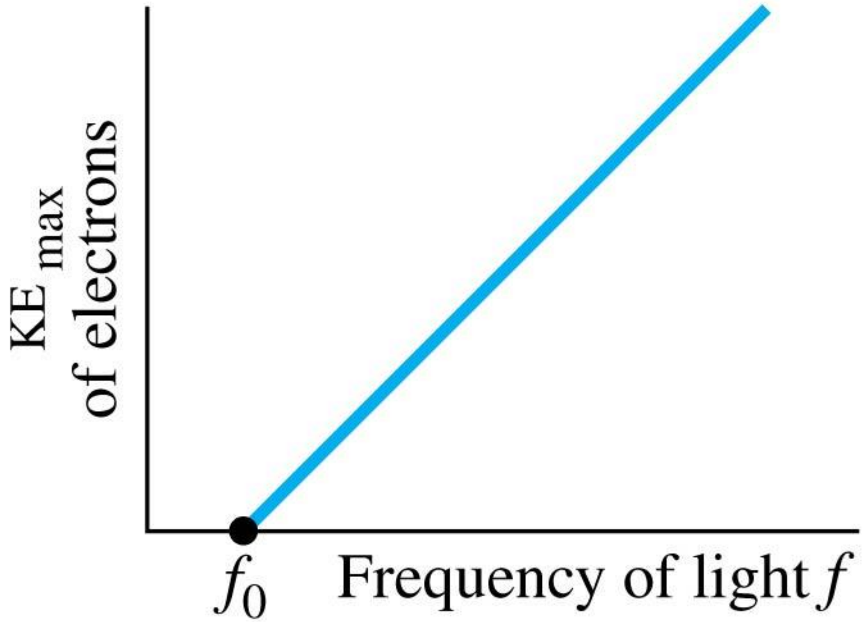
If light is particles (photons), theory predicts for the photoelectric effect:

- Increasing intensity increases number of electrons but not energy
- Above a minimum energy required to break atomic bond, kinetic energy will increase linearly with frequency
- There is a **cutoff frequency** below which no electrons will be emitted, regardless of intensity

27-3 Photon Theory of Light and the Photoelectric Effect

The particle theory assumes that an electron absorbs a single photon.

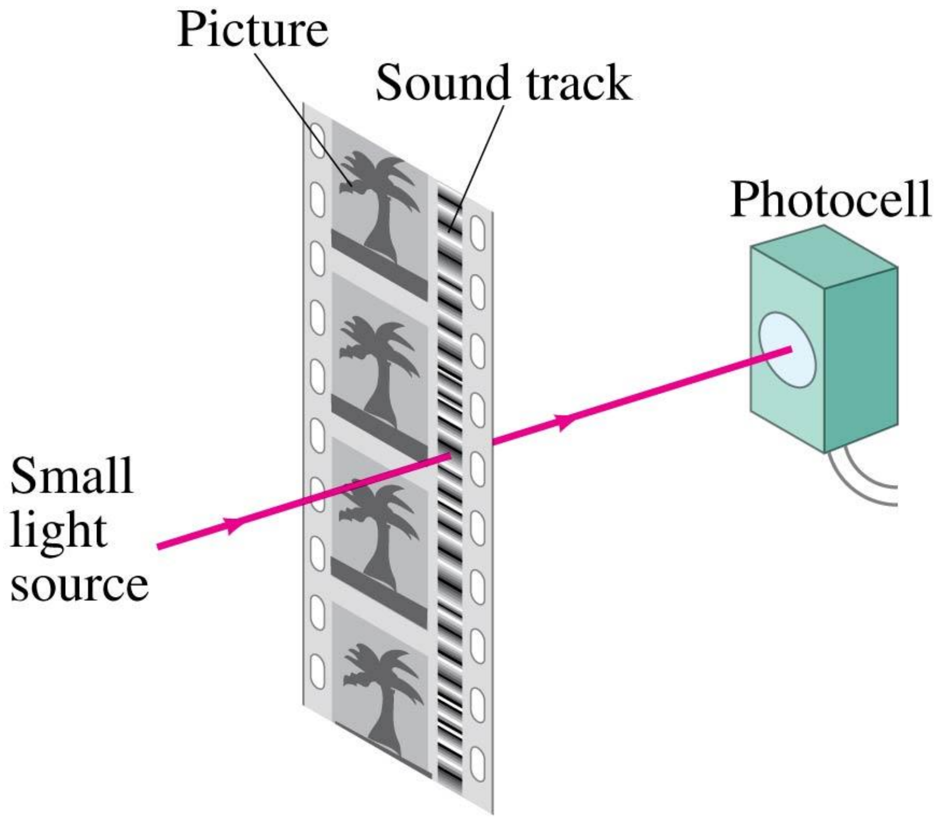
Plotting the kinetic energy vs. frequency:



This shows clear agreement with the photon theory, and not with wave theory.

27-3 Photon Theory of Light and the Photoelectric Effect

The photoelectric effect is how “electric eye” detectors work. It is also used for movie film soundtracks.



27-4 Energy, Mass, and Momentum of a Photon

Photons must travel at the speed of light. Looking at the relativistic equation for momentum, it is clear that this can only happen if its rest mass is zero.

We already know that the energy is *hf*; we can put this in the relativistic energy-momentum relation and find the momentum:

$$p = \frac{E}{c} = \frac{hf}{c} = \frac{h}{\lambda}. \quad (27\text{-}6)$$

27-6 Photon Interactions; Pair Production

Photons passing through matter can undergo the following interactions:

1. Photon may be totally absorbed by electron, but not have enough energy to eject it; the electron moves into an excited state
2. Photoelectric effect: photon is completely absorbed, electron is ejected
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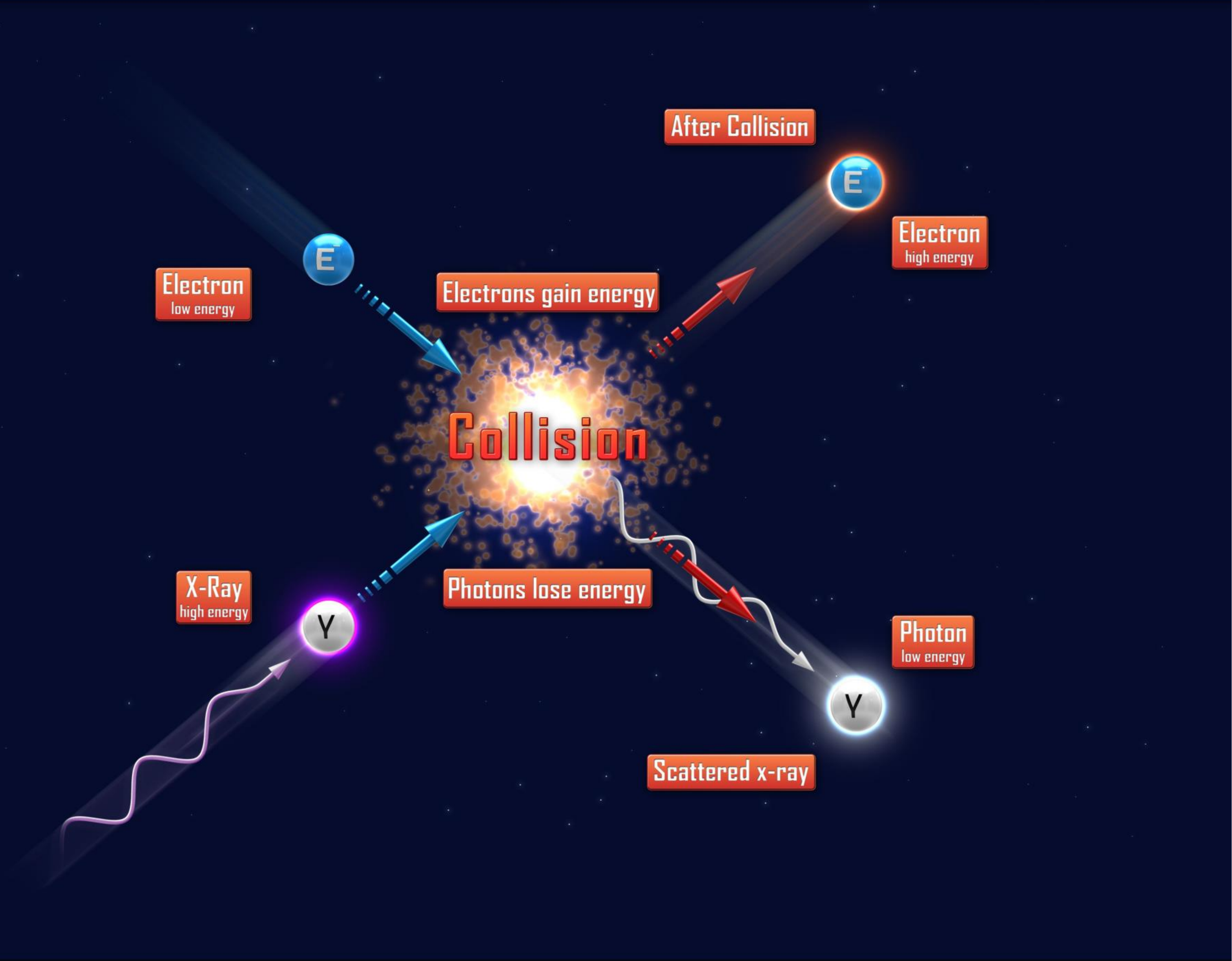
Compton Scattering (Compton Effect)



Compton Effect:

①散射光 $\begin{cases} \text{原波长}\lambda_0\text{成分 — 瑞利散射} \\ \lambda > \lambda_0\text{成分 — 康普顿散射} \end{cases}$

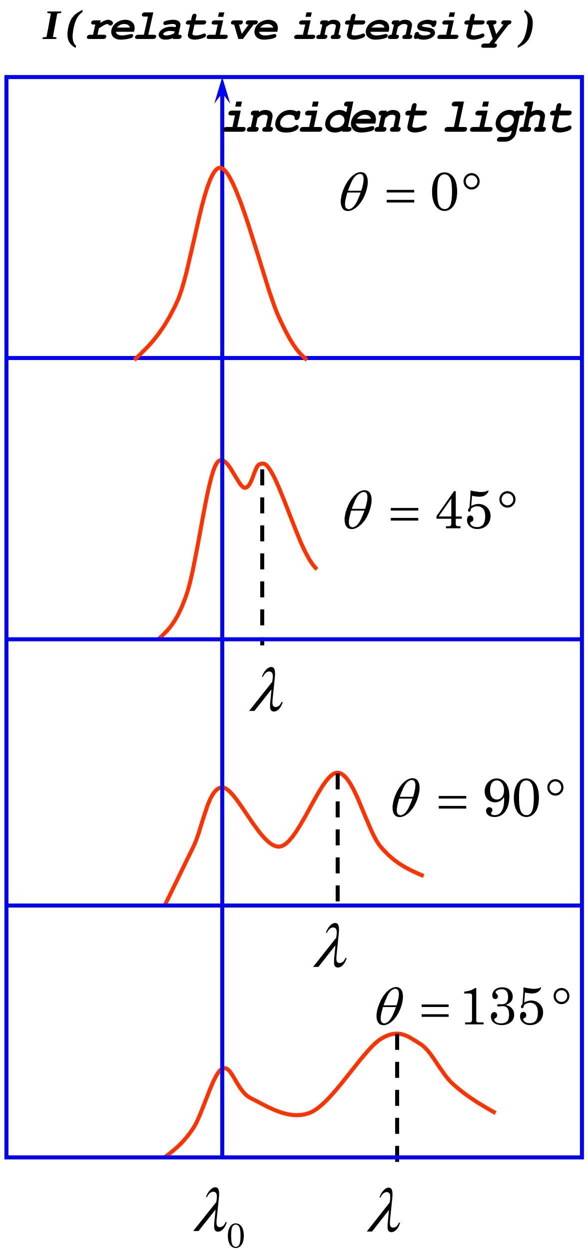
②波长改变量 $\Delta\lambda$ $\begin{cases} \text{与}\lambda_0\text{和散射物质无关} \\ \text{只与散射方向 }\varphi\text{有关} \end{cases}$

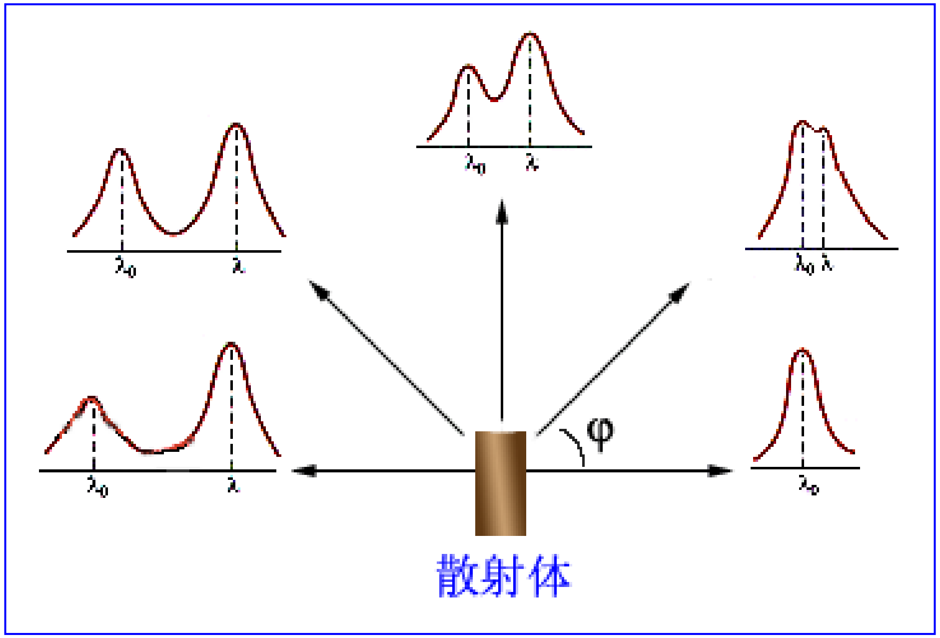
$\varphi\uparrow$: $\Delta\lambda\uparrow$; $I_{\lambda_0}\downarrow, I_\lambda\uparrow$

③原子量越小的物质，康普顿效应越显著

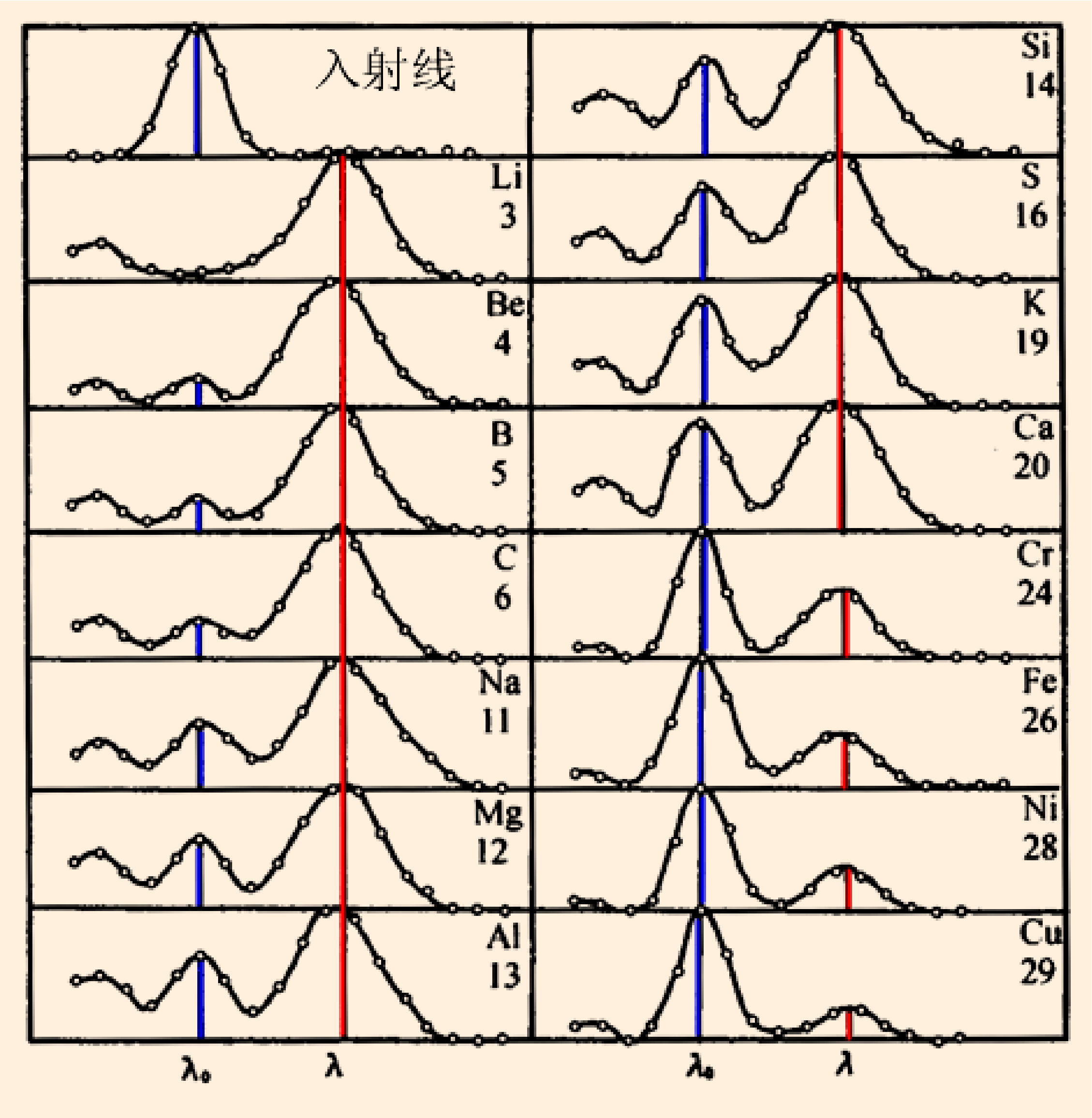
φ一定，$\Delta\lambda$一定，轻元素散射 $\dfrac{I_\lambda}{I_{\lambda_0}}$较大

Compton scattering and scattering Angle

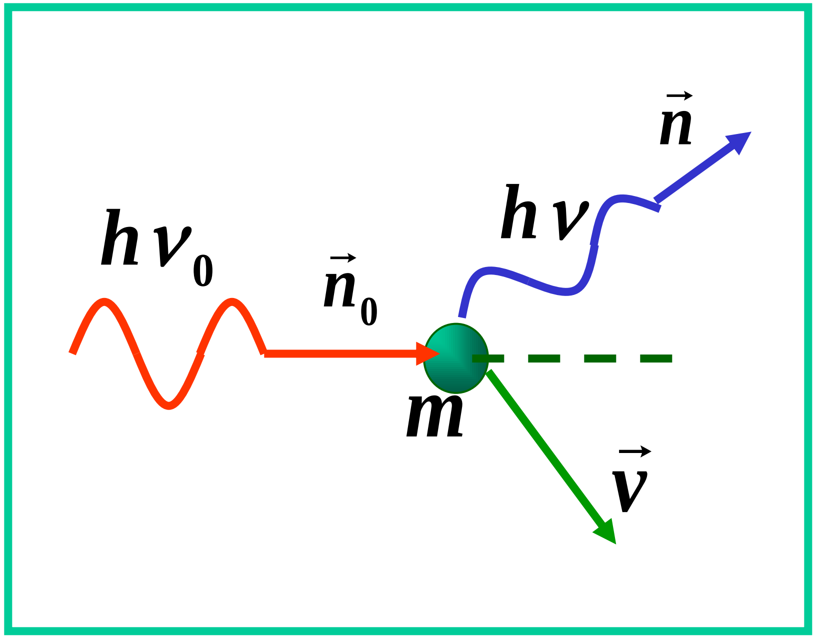


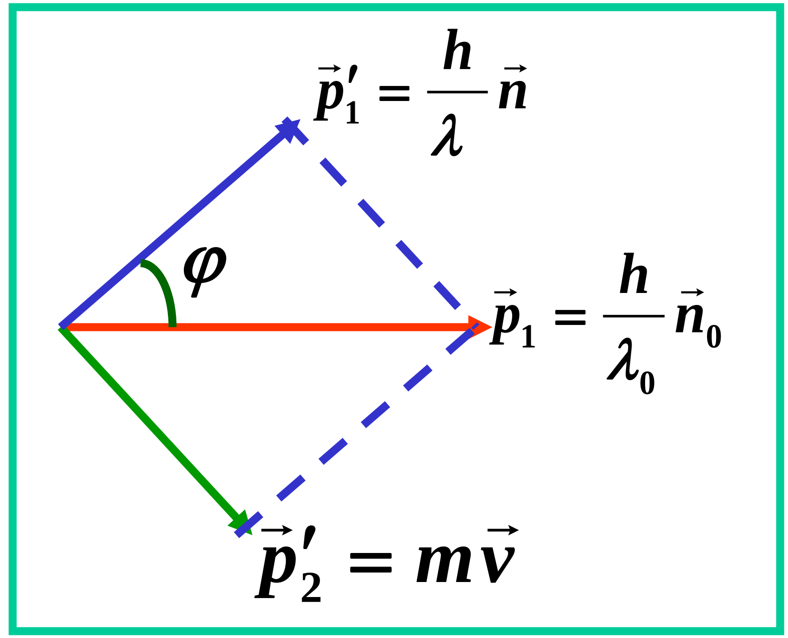


At the same scattering Angle, $I_{\lambda} / I_{\lambda_0}$ varying with different materials



Atomic number





	before	after
photon	$E_1 = h\nu_0 = \frac{hc}{\lambda_0}$ $\quad \vec{p}_1 = \frac{h}{\lambda_0}\vec{n}_0$	$E_1' = \frac{hc}{\lambda}$ $\quad \vec{p}_1' = \frac{h}{\lambda}\vec{n}$
electron	$E_2 = m_0 c^2$ $\quad \vec{p}_2 = 0$	$E_2' = mc^2$ $\quad \vec{p}_2' = m\vec{v}$

27-5 Compton Effect

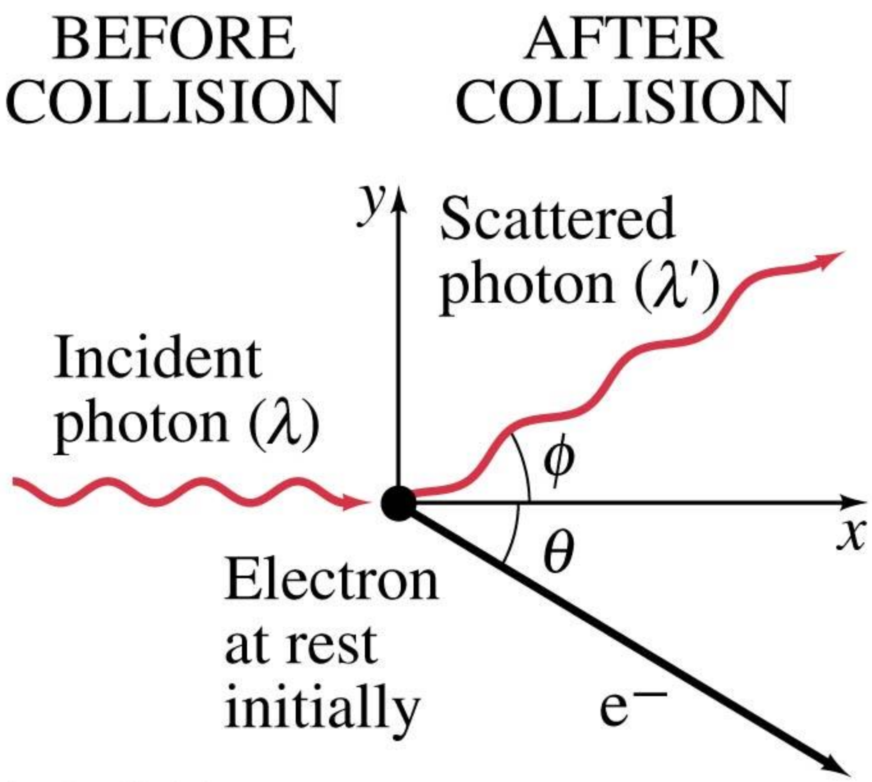
Compton did experiments in which he scattered X-rays from different materials. He found that the scattered X-rays had a slightly longer wavelength than the incident ones, and that the wavelength depended on the scattering angle:

$$\lambda' = \lambda + \frac{h}{m_e c}(1 - \cos\phi), \quad (27\text{-}7)$$

$$\lambda - \lambda_0 = \frac{h}{m_0 c}(1 - \cos\varphi) = \frac{2h}{m_0 c}\sin^2\frac{\varphi}{2}$$

27-5 Compton Effect

This is another effect that is correctly predicted by the photon model and not by the wave model.



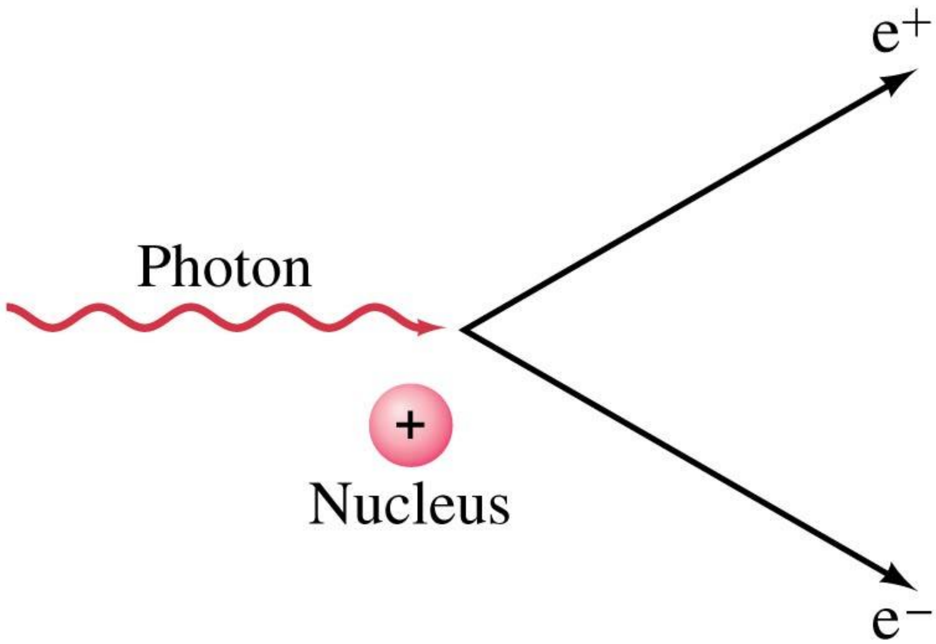
27-6 Photon Interactions; Pair Production

Photons passing through matter can undergo the following interactions:

1. Photoelectric effect: photon is completely absorbed, electron is ejected
2. Photon may be totally absorbed by electron, but not have enough energy to eject it; the electron moves into an excited state
3. The photon can scatter from an atom and lose some energy
4. The photon can produce an electron-positron pair.

27-6 Photon Interactions; Pair Production

In pair production, energy, electric charge, and momentum must all be conserved.



Energy will be conserved through the mass and kinetic energy of the electron and positron; their opposite charges conserve charge; and the interaction must take place in the electromagnetic field of a nucleus, which can contribute momentum.

27-7 Wave-Particle Duality; the Principle of Complementarity

We have phenomena such as diffraction and interference that show that light is a wave, and phenomena such as the photoelectric effect and the Compton effect that show that it is a particle.

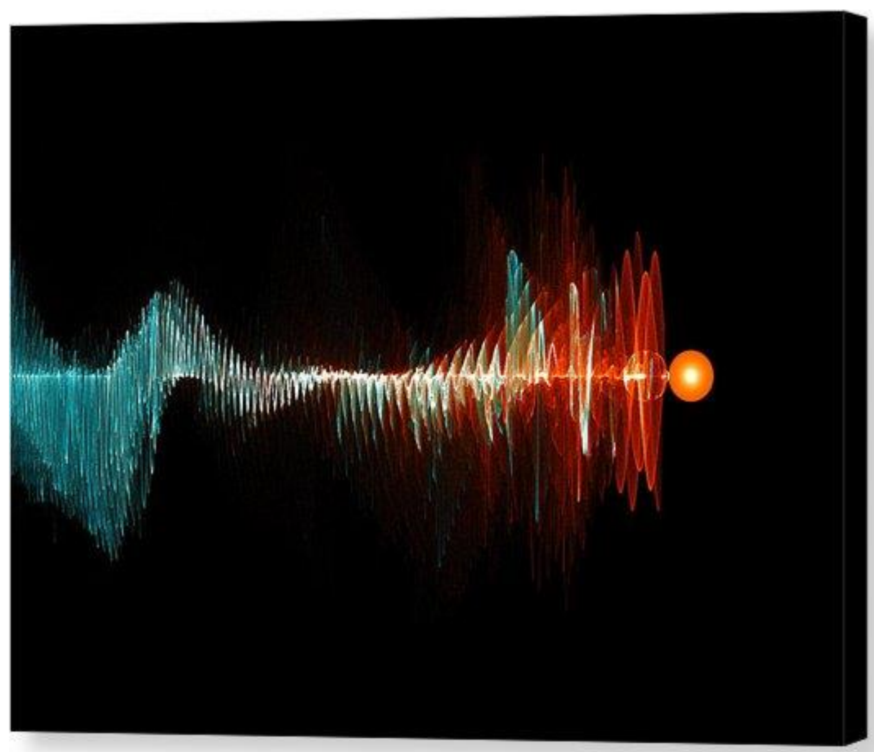
Which is it?

This question has no answer; we must accept the dual wave-particle nature of light.

27-7 Wave-Particle Duality; the Principle of Complementarity

The principle of complementarity states that both the wave and particle aspects of light are fundamental to its nature.

Indeed, waves and particles are just our interpretations of how light behaves.



27-8 Wave Nature of Matter

Just as light sometimes behaves as a particle, matter sometimes behaves like a wave.

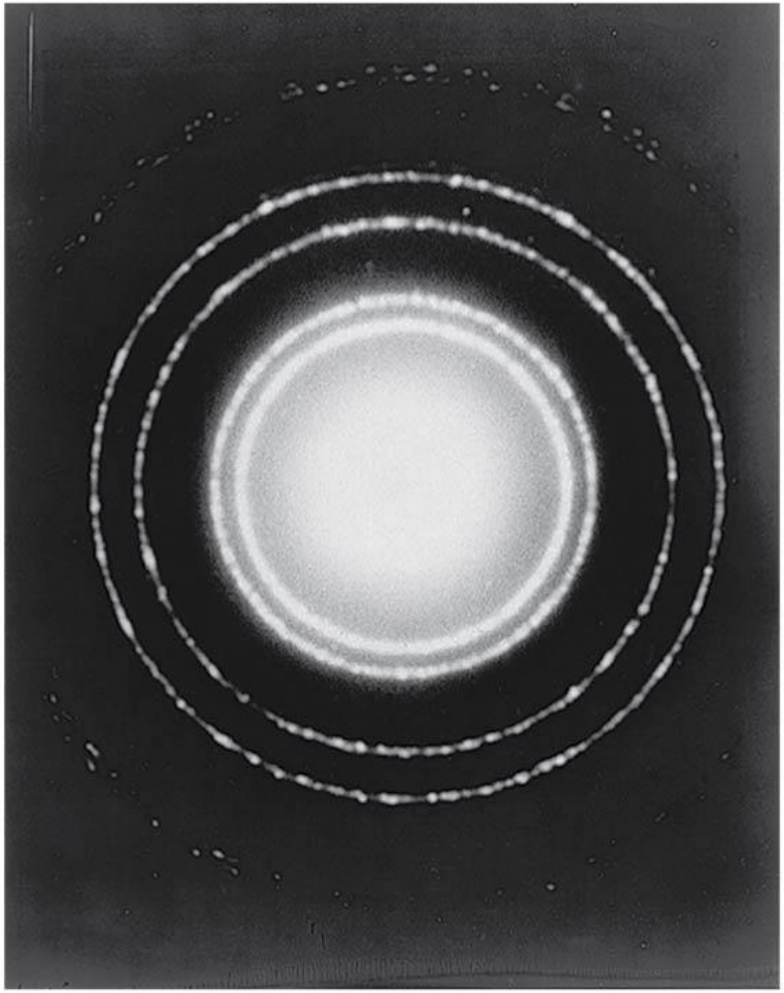
The wavelength of a particle of matter is:

$$\lambda = \frac{h}{p}, \qquad (27\text{-}8)$$

This wavelength is extraordinarily small for most objects. The wave nature of matter becomes more important for very light particles such as the electron.

27-8 Wave Nature of Matter

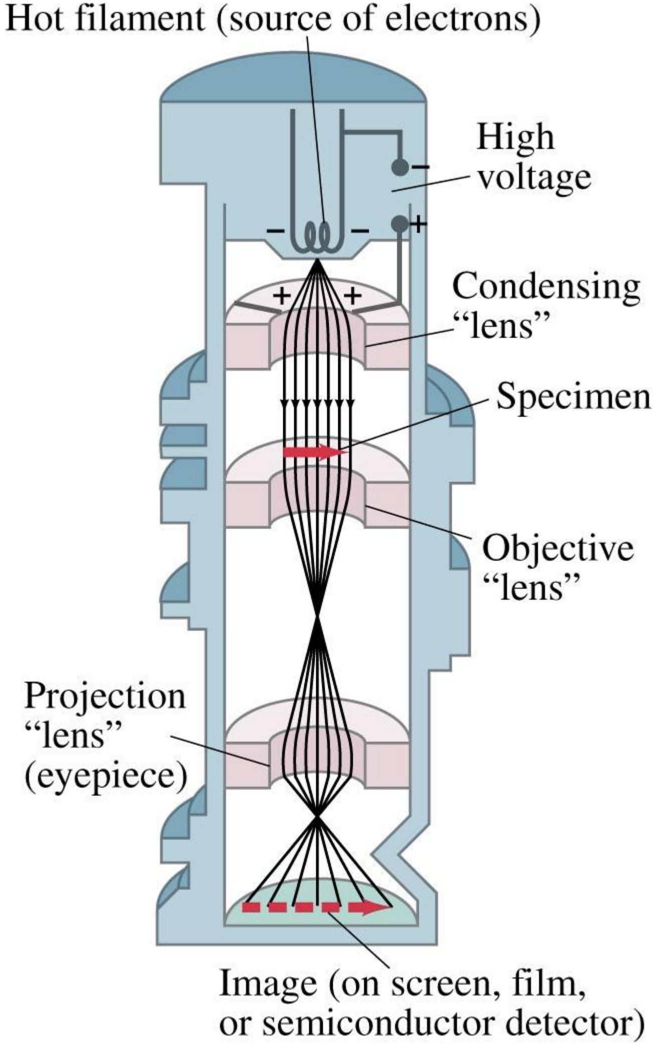
Electron wavelengths can easily be on the order of 10^{-10} m; electrons can be diffracted by crystals just as X-rays can.



27-9 Electron Microscopes

The wavelength of electrons will vary with energy, but is still quite short. This makes electrons useful for imaging, remember that the smallest object that can be resolved is about one wavelength. Electrons used in electron microscopes have wavelengths of about 0.004 nm.

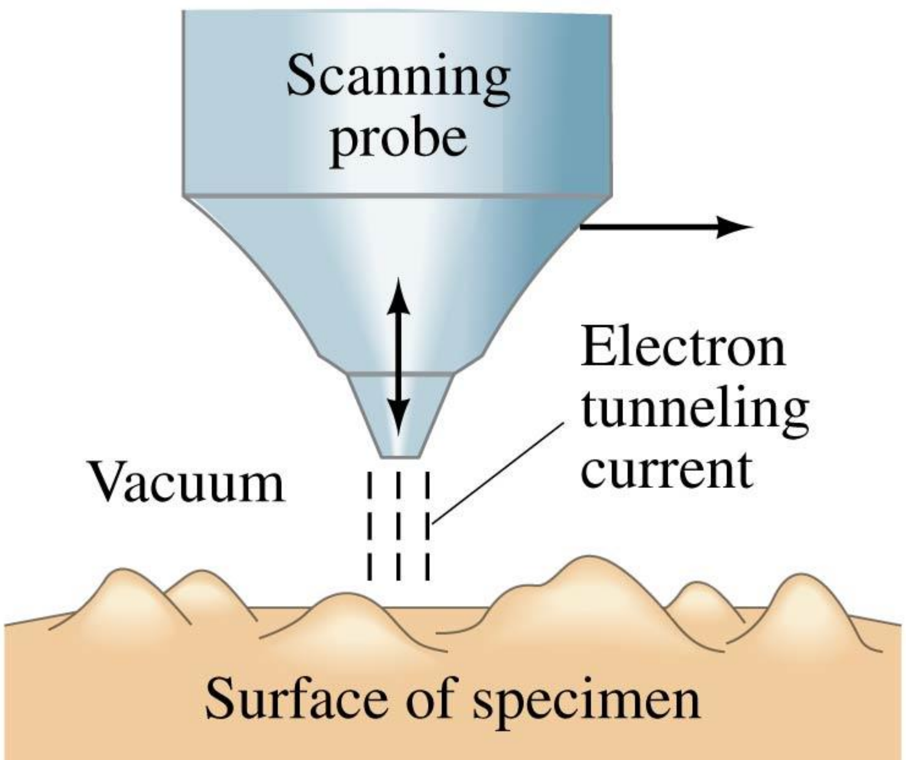
27-9 Electron Microscopes



Transmission electron microscope—the electrons are focused by magnetic coils

27-9 Electron Microscopes

Scanning tunneling microscope—up and down motion of the probe keeps the current constant.



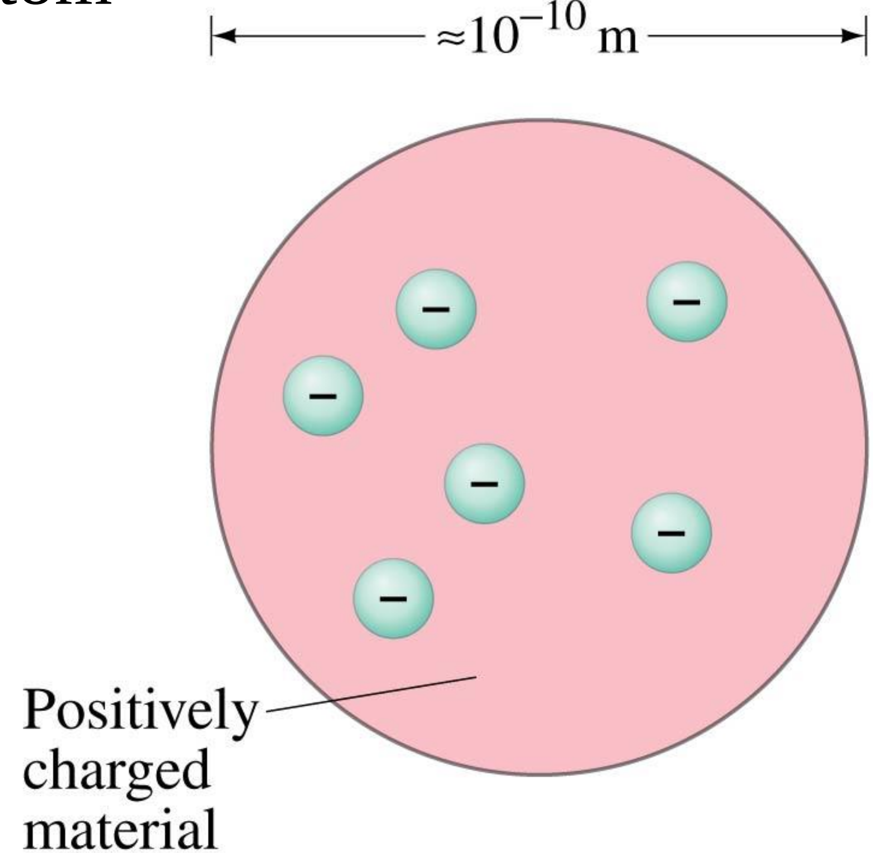
Plotting that motion produces an image of the surface.

27-10 Early Models of the Atom

It was known in the late 19th century that atoms were electrically neutral, but that they could become charged, implying that there were positive and negative charges and that some of them could be removed.

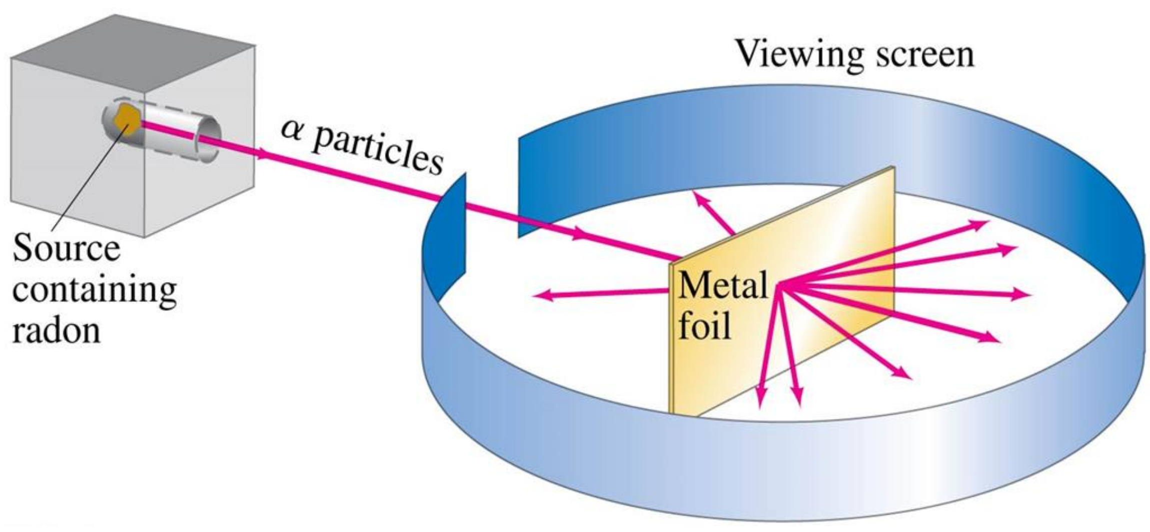
27-10 Early Models of the Atom

One popular atomic model was the "plum-pudding" model. This model had the atom consisting of a bulk positive charge, with negative electrons buried throughout.



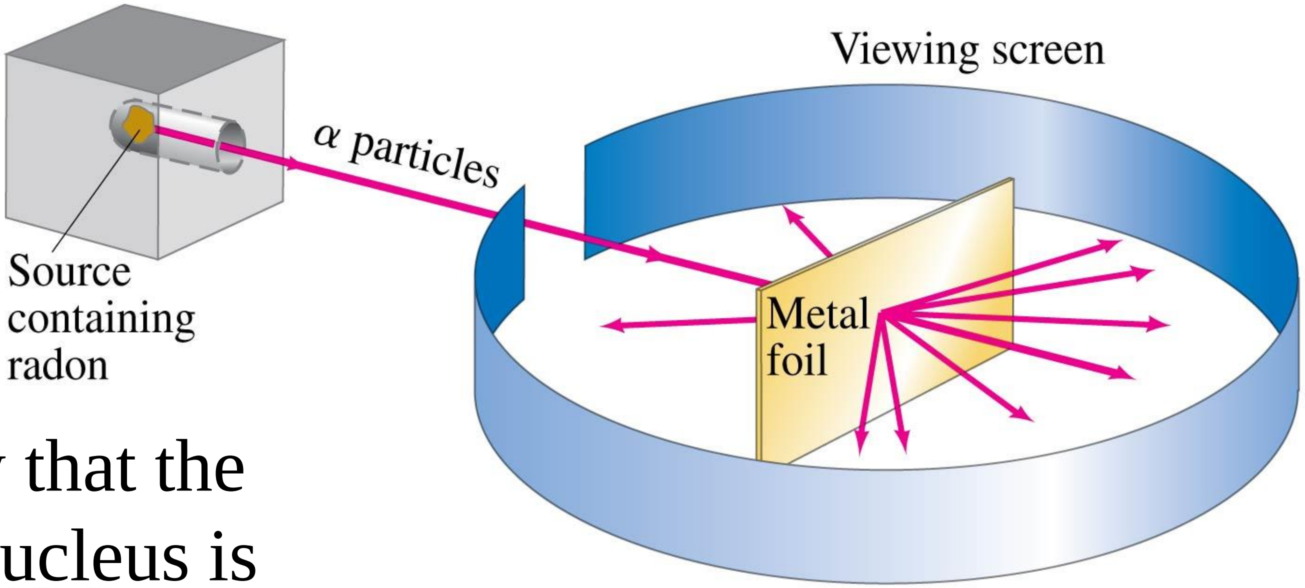
27-10 Early Models of the Atom

Around 1911, Rutherford did an experiment which showed that the positively charged nucleus must be extremely small compared to the rest of the atom. He scattered alpha particles—helium nuclei—from a metal foil and observed the scattering angle. He found that some of the angles were far larger than the plum-pudding model would allow.



27-10 Early Models of the Atom

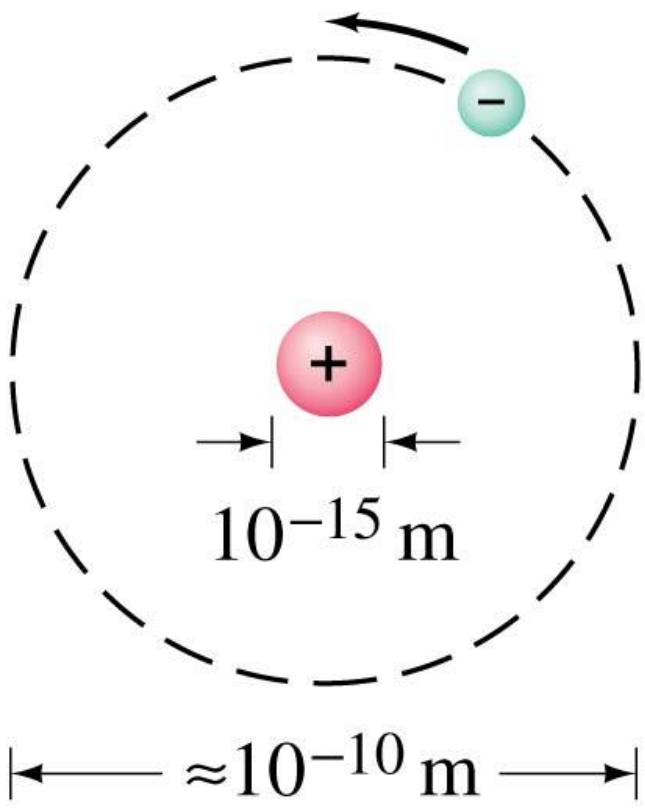
The only way to account for the large angles was to assume that all the positive charge was contained within a tiny volume.



Now we know that the radius of the nucleus is 1/10000 that of the atom.

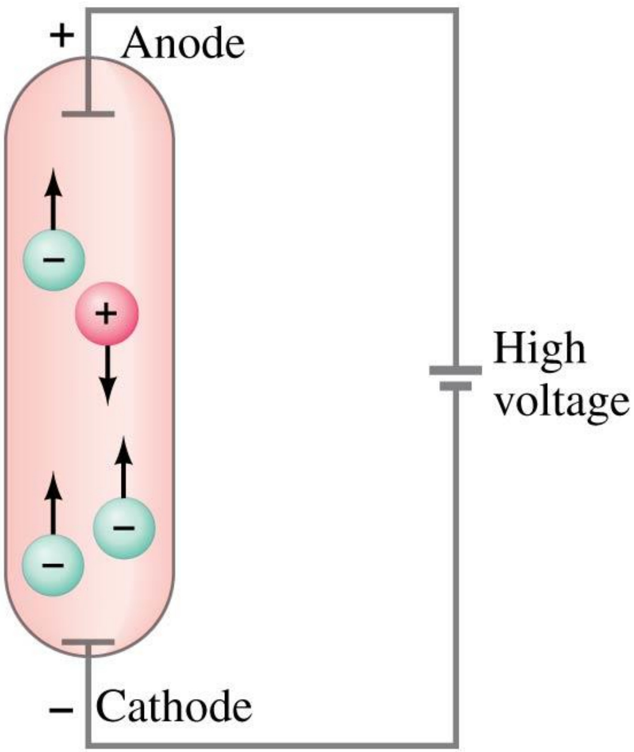
27-10 Early Models of the Atom

Therefore, Rutherford's model of the atom is mostly empty space:

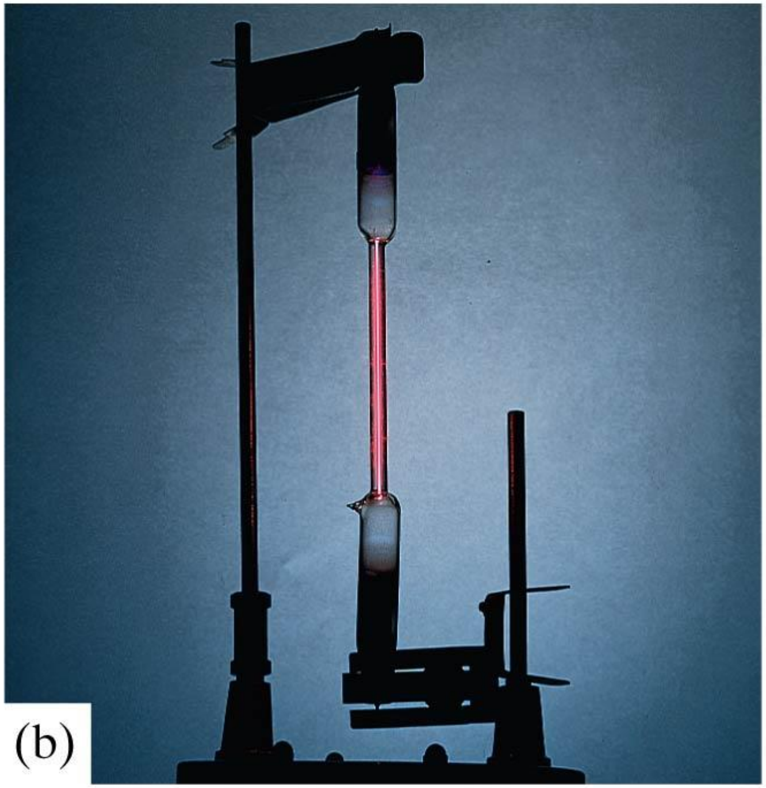


27-11 Atomic Spectra: Key to the Structure of the Atom

A very thin gas heated in a discharge tube emits light only at characteristic frequencies.



(a)



(b)

27-11 Atomic Spectra: Key to the Structure of the Atom

An atomic spectrum is a line spectrum—only certain frequencies appear. If white light passes through such a gas, it absorbs at those same frequencies.


(a)


(b)


(c)

27-11 Atomic Spectra: Key to the Structure of the Atom

The wavelengths of photons emitted from hydrogen have a regular pattern:

$$\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right), \qquad n = 3, 4, \cdots. \quad (27\text{-}9)$$

This is called the Balmer series. *R* is the Rydberg constant:

$$R = 1.0974 \times 10^7 \text{ m}^{-1}$$

27-11 Atomic Spectra: Key to the Structure of the Atom

Other series include the Lyman series:

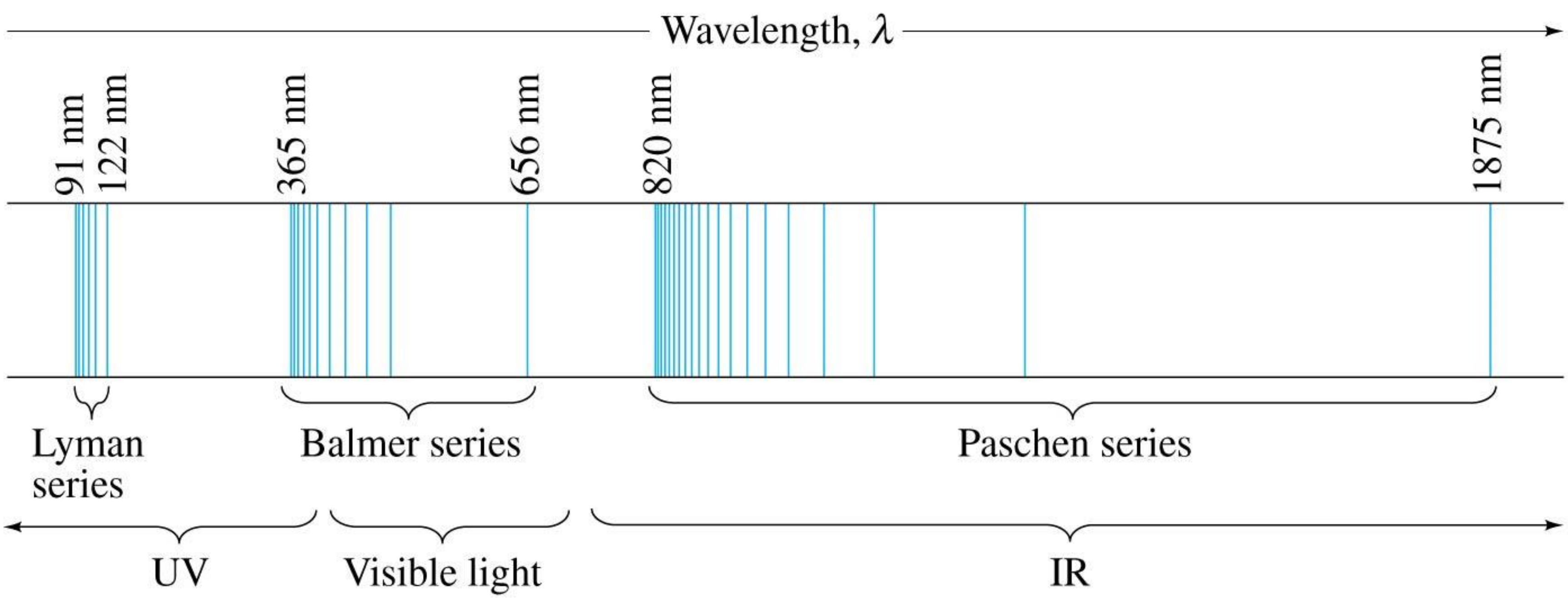
$$\frac{1}{\lambda} = R\left(\frac{1}{1^2} - \frac{1}{n^2}\right), \qquad n = 2, 3, \cdots .$$

And the Paschen series:

$$\frac{1}{\lambda} = R\left(\frac{1}{3^2} - \frac{1}{n^2}\right), \qquad n = 4, 5, \cdots .$$

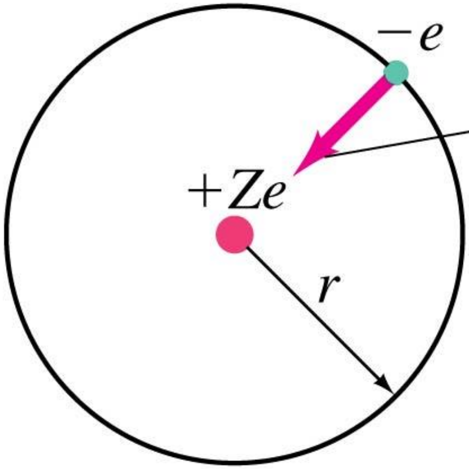
27-11 Atomic Spectra: Key to the Structure of the Atom

A portion of the complete spectrum of hydrogen is shown here. The lines cannot be explained by the Rutherford theory.



27-12 The Bohr Atom

An electron is held in orbit by the Coulomb force:



$$F = \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r^2} = m\frac{v^2}{r}$$

Radius $\boldsymbol{r = \dfrac{Ze^2}{4\pi\varepsilon_0 m v^2}}$

Frequency $\boldsymbol{f = \dfrac{v}{2\pi r} = \dfrac{1}{2\pi r}\times\sqrt{\dfrac{Ze^2}{4\pi\varepsilon_0 m r}}}$

Energy $\boldsymbol{E = \dfrac{1}{2}mv^2 - \dfrac{Ze}{4\pi\varepsilon_0 r^2} = -\dfrac{Ze}{8\pi\varepsilon_0 r}}$

$$\begin{cases} r\uparrow \quad E\uparrow \\ E < 0 \end{cases}$$

3. The basic hypothesis of Bohr’s theory

1) The stationary state hypothesis (定态假设)- an atom is in a stable state (stationary state for short) and has a certain amount of energy when the electron can move in a certain circular orbit without radiating electromagnetic waves.

2) Quantization condition(定态条件)

Only those orbits in which the electron's angular momentum L is equal to an integral multiple of h / 2 are stable when the electron moves around the nucleus at a velocity v on a circumference of radius r:

$$L = mvr = n\hbar \qquad n = 1,2,3,\ldots$$

主量子数

Principal quantum number

3) Frequency hypothesis

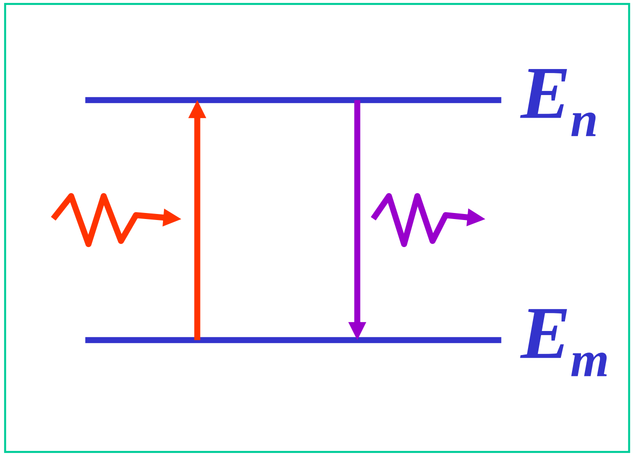
When an an atom transitions from a stationary state E_2 to a certain state E_1, it radiates electromagnetic waves, the frequency of which is determined by the following equation:

$$h\nu = E_2 - E_1$$

跃迁(transition):

原子体系在两个定态之间发生跃迁时，要发射或吸收光子，其频率由两定态的能量差决定：

$$h\nu_{nm} = E_n - E_m$$



27-12 The Bohr Atom

Bohr found that the angular momentum was quantized:

$$L = mvr_n = n\frac{h}{2\pi}, \qquad n = 1, 2, 3, \cdots, \quad (27\text{-}11)$$

1) Circular orbit quantization

$$\left.\begin{aligned} F &= \frac{Z}{4\pi\varepsilon_0}\frac{e^2}{r^2} = m\frac{v^2}{r} \\ L &= mvr = n\hbar \end{aligned}\right\} \quad \boxed{r = a_1\frac{n^2}{Z}} \qquad n = 1,2,3,\ldots$$

氢原子 $Z = 1$ $\qquad r = a_1 n^2 \quad n = 1,2,3,\ldots$

$$\boxed{a_1 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 0.529\times10^{-10}\ \mathrm{m}}$$

玻尔轨道

Bohr orbit

27-12 The Bohr Atom

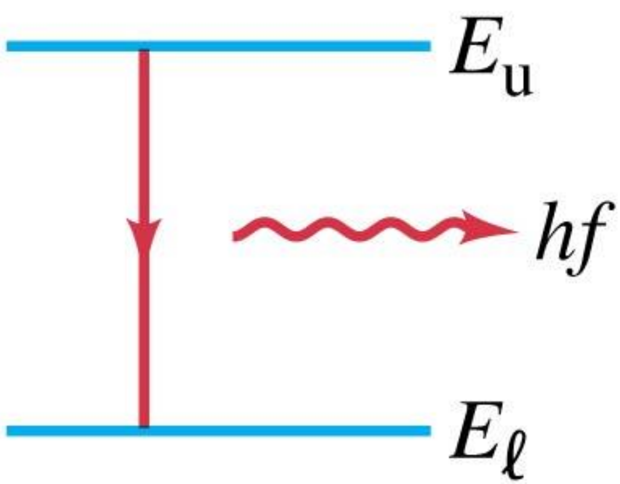
Bohr proposed that the possible energy states for atomic electrons were quantized—only certain values were possible. Then the spectrum could be explained as transitions from one level to another.

$$E_n = E_k + E_p$$

动能 $E_k = \frac{1}{2} m_e v_n^2$

势能 $E_p = -\frac{Ze^2}{4\pi\varepsilon_0 r_n}$

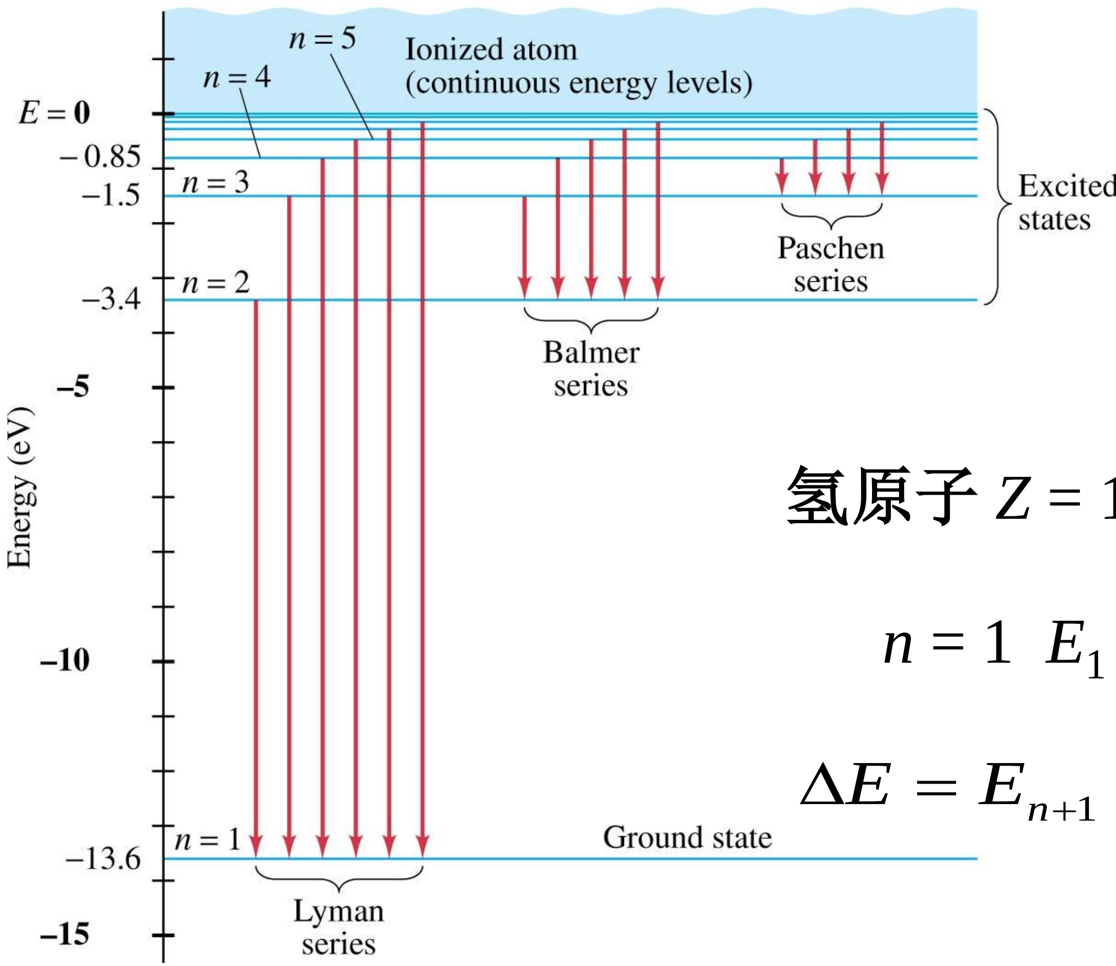
$$r_n = n^2\left(\frac{\varepsilon_0 h^2}{\pi m_e e^2}\right)$$



$$E_n = -\frac{Ze}{8\pi\varepsilon_0 r} = -\frac{Z^2 me^4}{2(4\pi\varepsilon_0)^2}\cdot\frac{1}{n^2\hbar^2} \qquad n = 1,2,3,\ldots$$

27-12 The Bohr Atom

$$E_n = -\frac{Ze}{8\pi\varepsilon_0 r} = -\frac{Z^2 me^4}{2(4\pi\varepsilon_0)^2}\cdot\frac{1}{n^2\hbar^2} \qquad n = 1,2,3,\ldots$$



The lowest energy level is called the ground state; the others are excited states.

氢原子 $Z = 1$ $$E_n = -\frac{13.6}{n^2}\,\text{eV}$$

$n = 1$ $E_1 = -13.6\text{eV}$ 基态

$$\Delta E = E_{n+1} - E_n = 13.6\frac{2n+1}{n^2(n+1)^2}eV$$

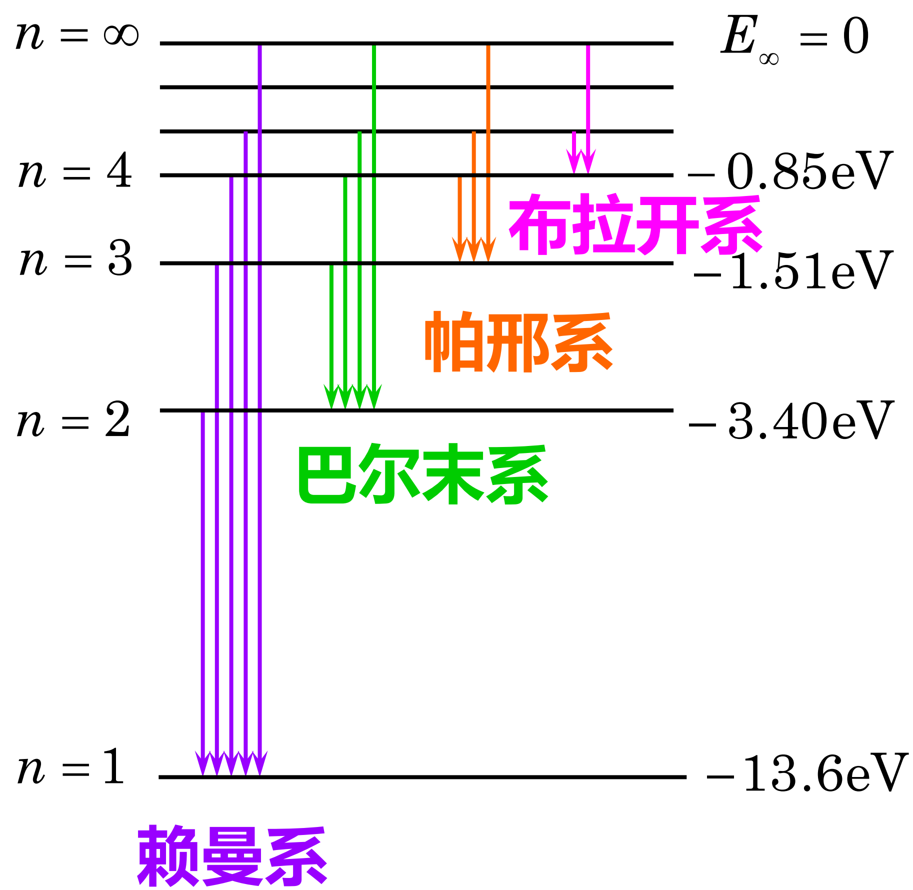
$$n\uparrow \rightarrow \Delta E\downarrow$$

3) Discrete spectrum line of the hydrogen atom

$$E_2 = \frac{E_1}{2^2} = -3.4\text{eV}$$

$$E_3 = \frac{E_1}{3^2} = -1.51\text{eV}$$

$$E_4 = \frac{E_1}{4^2} = -0.85\text{eV}$$



氢原子的电离能

当 $n \to \infty$

原子被电离----自由态，

电子不受原子核束缚。

$$E = 13.6\,eV$$

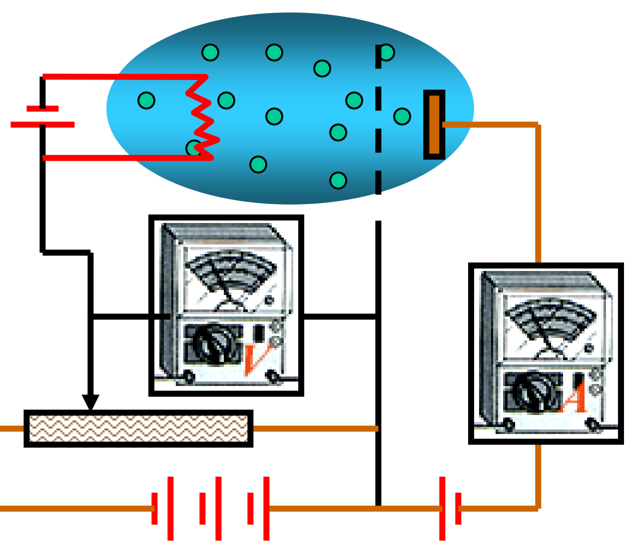
5. 玻尔理论的成功与缺陷

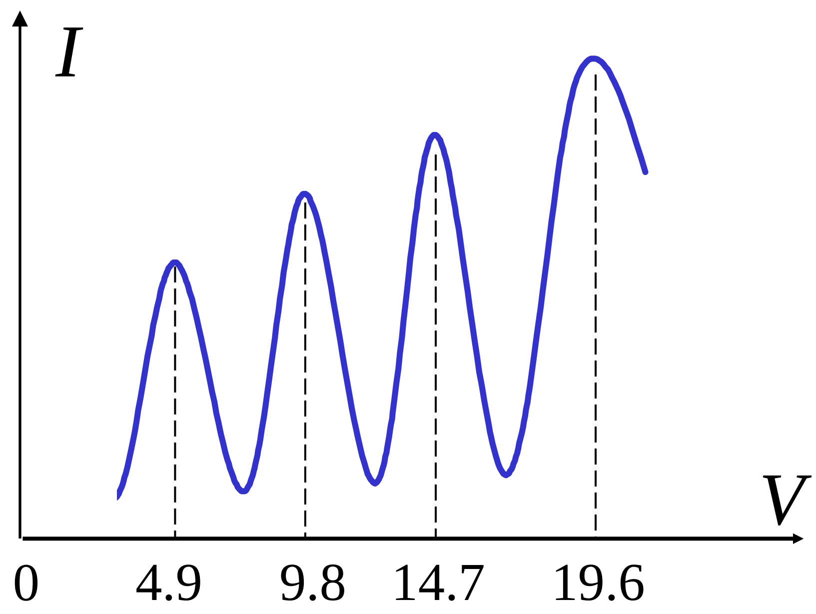
成功　1. 提出的定态、轨道、能量量子化、辐射跃迁等概念成为量子力学的先驱

2. 成功地解释了氢原子及类氢原子光谱现象

3. 再次验证了h 判据

玻尔定态能级验证实验：夫兰克 — 赫兹实验

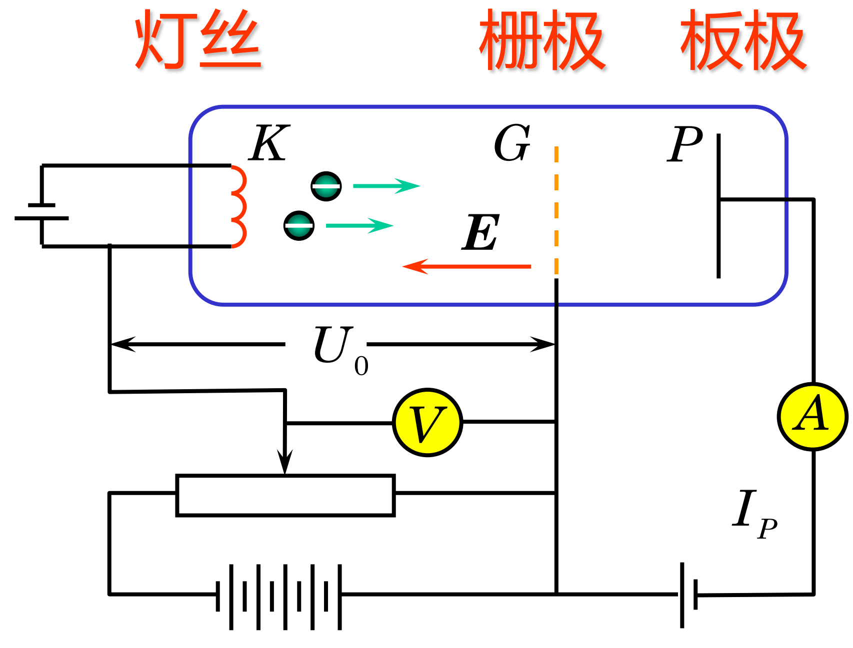


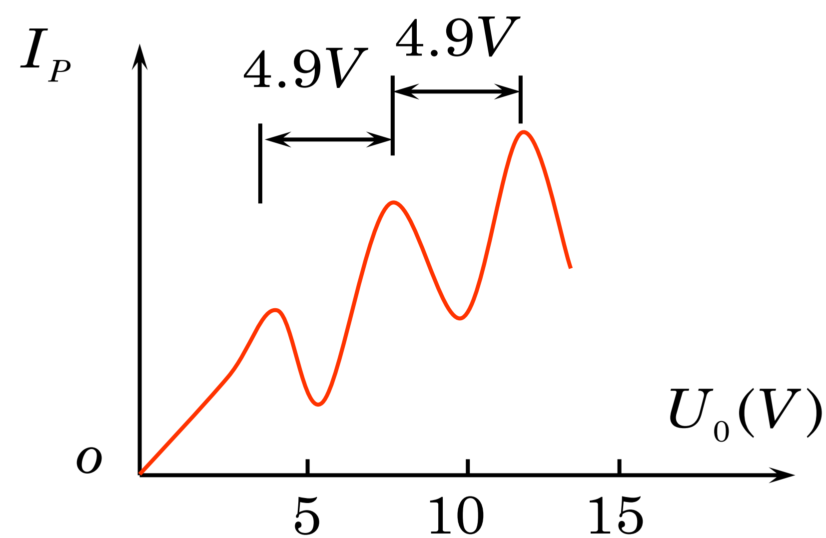


实验原理

- K、G 之间加正向电压，电子在 $\boldsymbol{E}$ 作用下向 G 运动。

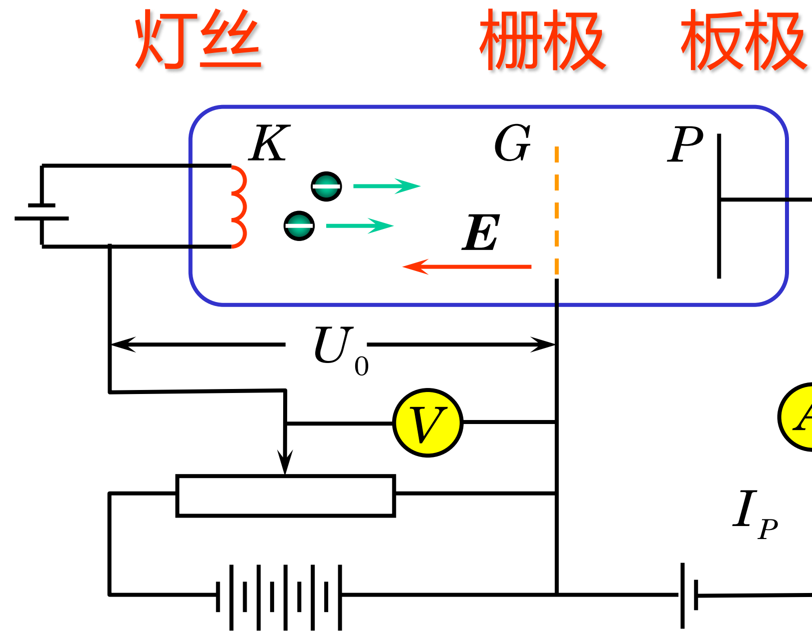
- G、P 之间加反向电压，电子穿过 G 达到 P 形成电流,作$I_P \sim U_0$图。





- 汞原子基态为 E_1，
- **第一激发态 E_2**

1. 电子动能E_k<E_2–E_1



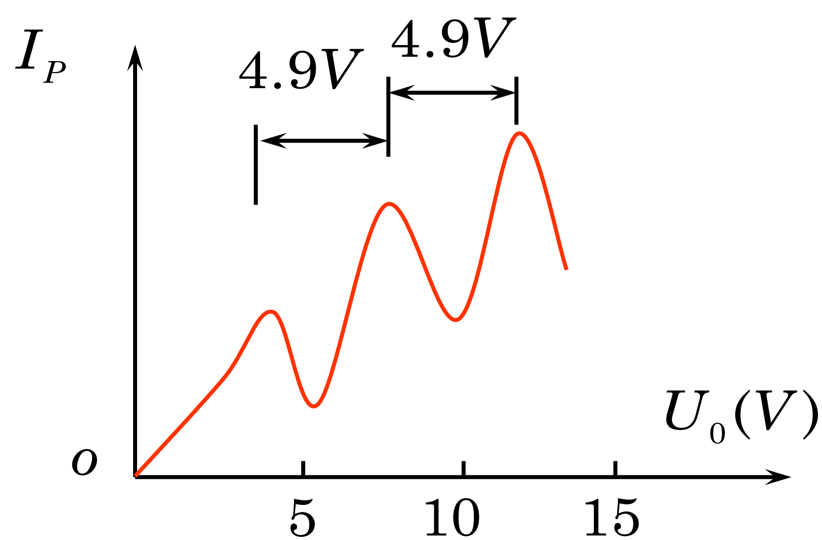
电子不能使 Hg原子激发到第一激发态，电子与 Hg 原子碰撞无能量损失，速率不变。

2. $U_0 \uparrow \longrightarrow E_k > E_2 - E_1$

Hg 原子从 $E_1 \longrightarrow E_2$

电子$E_k \downarrow \longrightarrow v \downarrow \longrightarrow I_P \downarrow$

$\longrightarrow$ 第一个波峰



3. $U_0 \uparrow \longrightarrow$

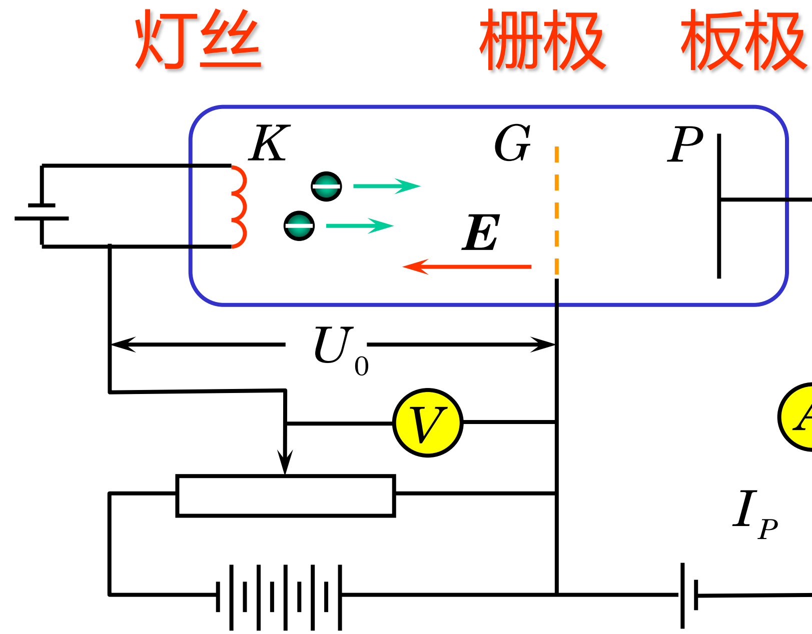
电子第一次使 Hg 激发后，在 U_0 的加速下又 $E_k > E_2 - E_1$

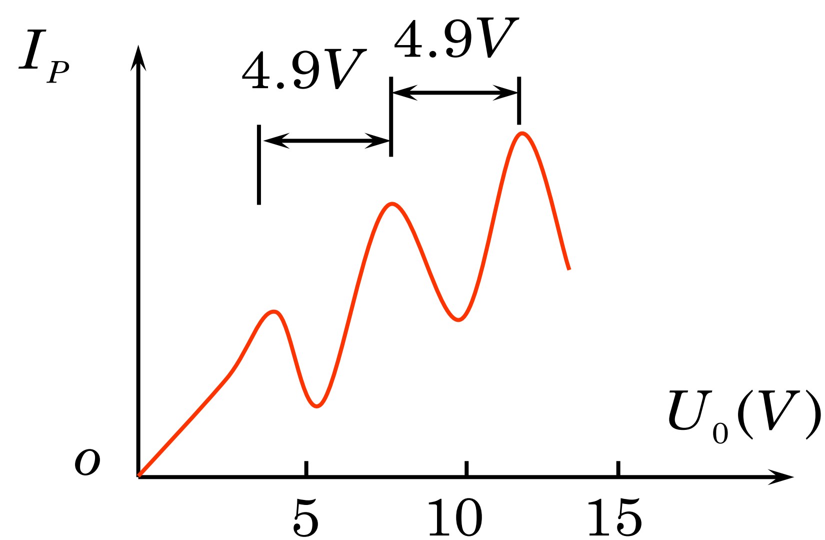
Hg 原子第二次从

$E_1 \longrightarrow E_2$

电子 $E_k \downarrow \longrightarrow v \downarrow \longrightarrow I_P \downarrow$

$\longrightarrow$ 第二个波峰





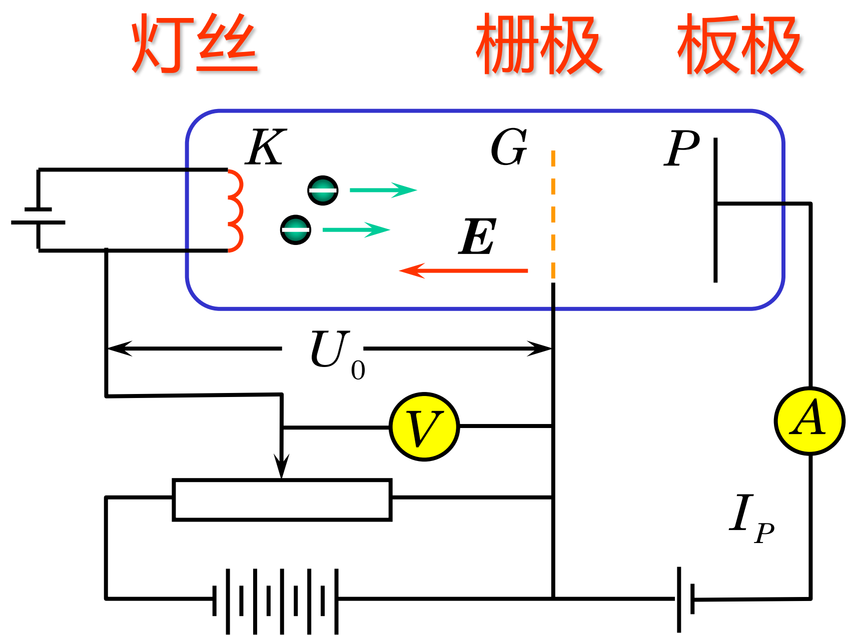
4.Hg 原子第一激发态与基态能量之差

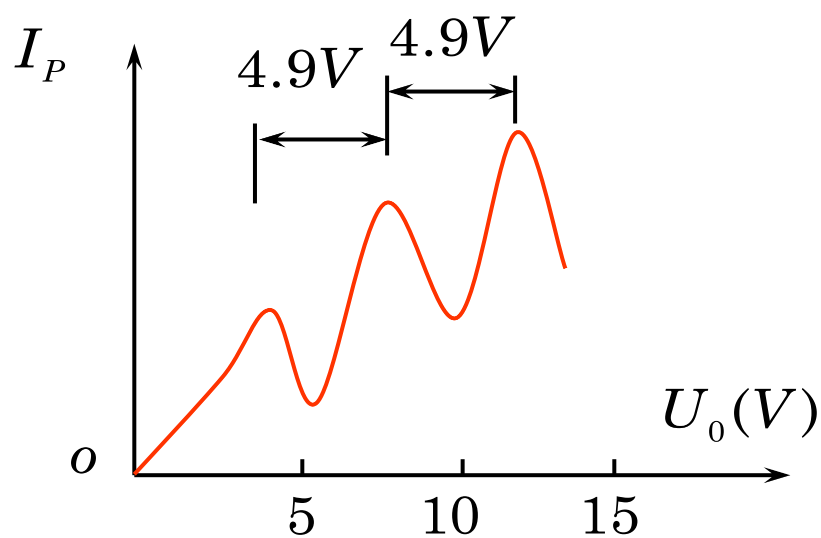
$$E_2 - E_1 = 4.9\text{eV}$$

5.实验中可观察到光谱，受激 Hg 原子从高能态跳回低能态放出光子。

$$\lambda = 2537\ \mathring{A}$$

$$h\nu = \frac{hc}{\lambda} = 4.89ev$$





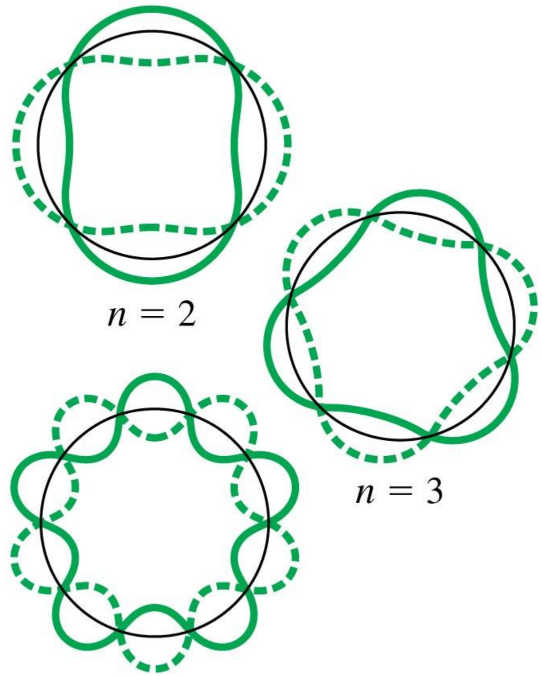
27-13 de Broglie's Hypothesis Applied to Atoms

De Broglie's hypothesis is the one associating a wavelength with the momentum of a particle. He proposed that only those orbits where the wave would be a circular standing wave will occur. This yields the same relation that Bohr had proposed.

In addition, it makes more reasonable the fact that the electrons do not radiate, as one would otherwise expect from an accelerating charge.

27-13 de Broglie's Hypothesis Applied to Atoms

These are circular standing waves for n = 2, 3, and 5.



Photon：

$$E = mc^2 = h\nu$$

$$\boldsymbol{p = mc = \frac{h}{\lambda}}$$

质量为*m*，速度为u的实物粒子可以用一定的频率和一定的波长来描述，它们的关系如下：

de Broglie's formula

$$\begin{cases} E = mc^2 = h\nu \\ p = mu = \dfrac{h}{\lambda} \end{cases}$$

$u \neq \lambda\nu$需两个方程

28-1 Quantum Mechanics—A New Theory

Quantum mechanics incorporates wave-particle duality, and successfully explains energy states in complex atoms and molecules, the relative brightness of spectral lines, and many other phenomena.

It is widely accepted as being the fundamental theory underlying all physical processes.

28-1 Quantum Mechanics—A New Theory

Quantum mechanics is essential to understanding atoms and molecules, but can also have effects on larger scales.

28-2 The Wave Function and Its Interpretation; the Double-Slit Experiment

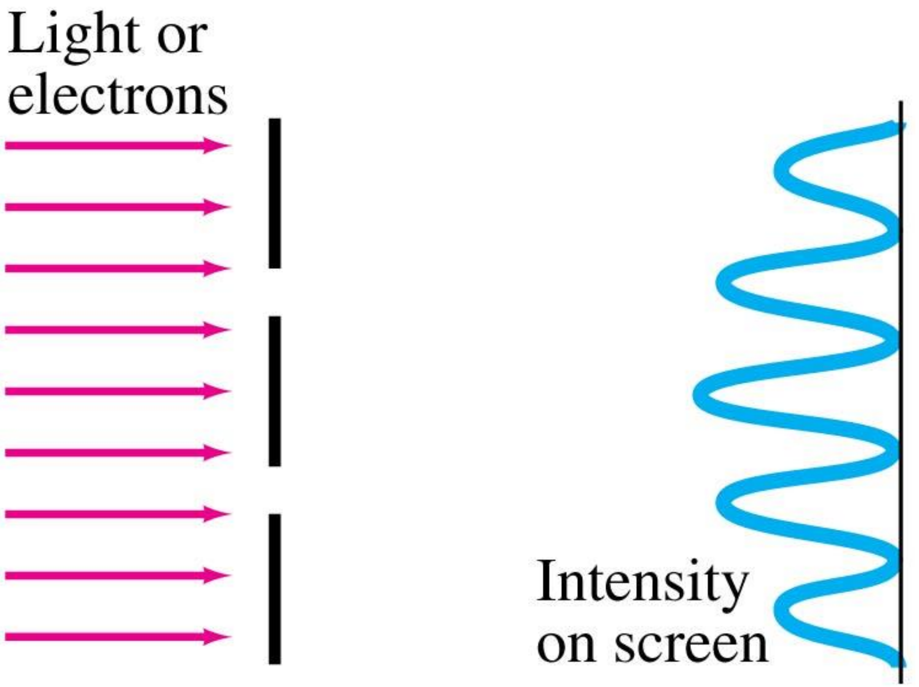
An electromagnetic wave has oscillating electric and magnetic fields. What is oscillating in a matter wave?

This role is played by the wave function, Ψ. The square of the wave function at any point is proportional to the number of electrons expected to be found there.

For a single electron, the wave function is the probability of finding the electron at that point.

28-2 The Wave Function and Its Interpretation; the Double-Slit Experiment

For example: the interference pattern is observed after many electrons have gone through the slits.



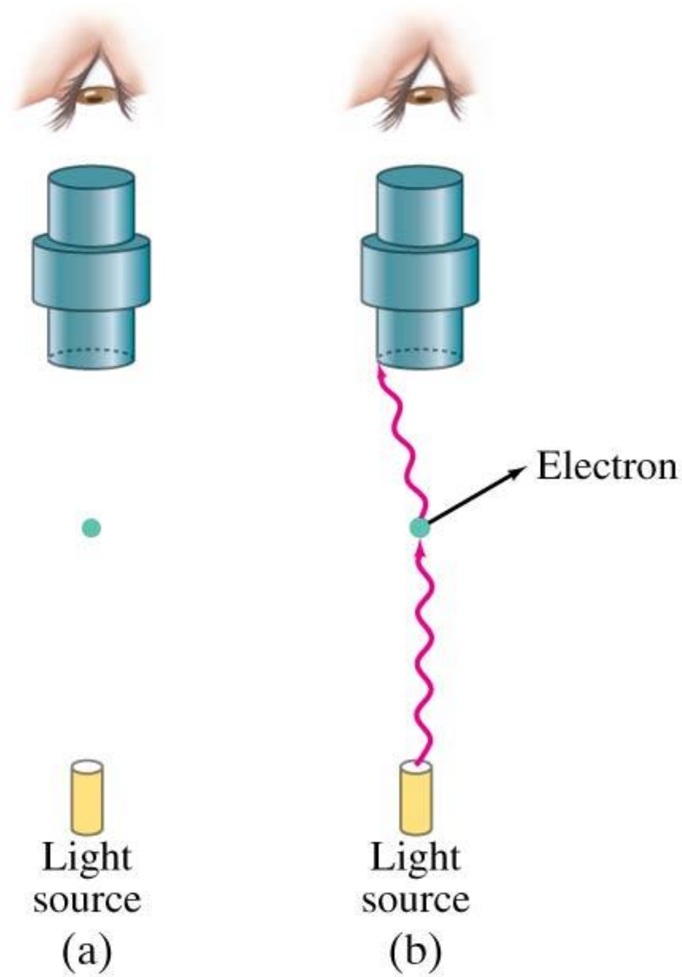
If we send the electrons through one at a time, we cannot predict the path any single electron will take, but we can predict the overall distribution.

28-3 The Heisenberg Uncertainty Principle

Quantum mechanics tells us there are limits to measurement—not because of the limits of our instruments, but inherently.

This is due to the wave-particle duality, and to interaction between the observing equipment and the object being observed.

28-3 The Heisenberg Uncertainty Principle

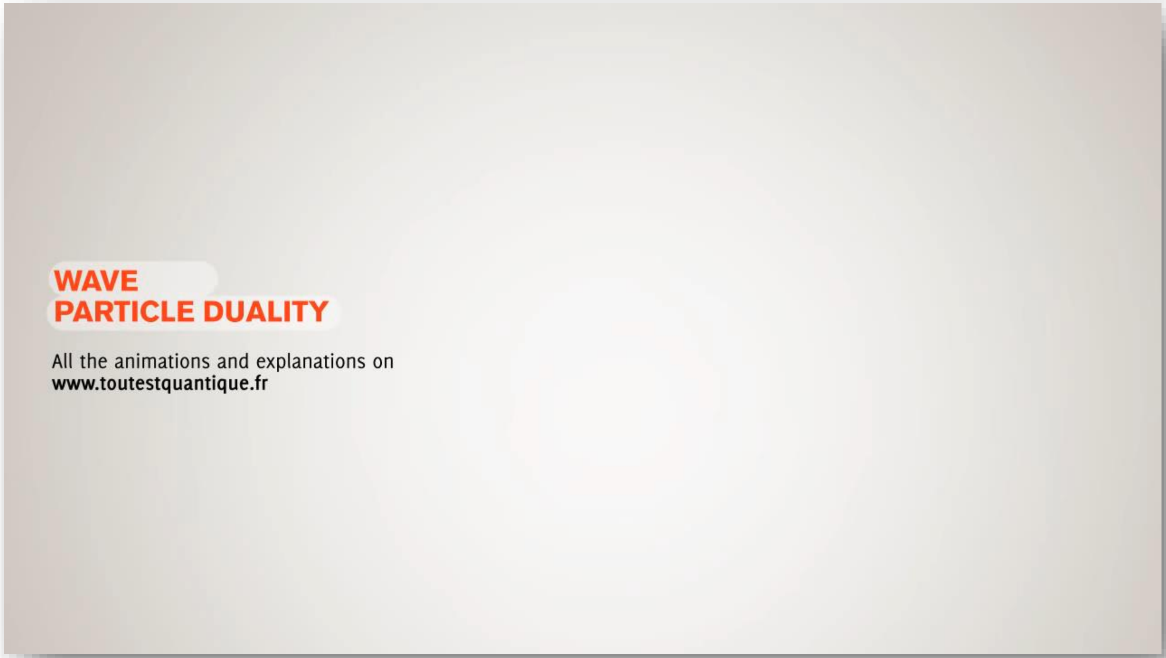


Imagine trying to see an electron with a powerful microscope. At least one photon must scatter off the electron and enter the microscope, but in doing so it will transfer some of its momentum to the electron.

28-3 The Heisenberg Uncertainty Principle

The uncertainty in the momentum of the electron is taken to be the momentum of the photon—it could transfer anywhere from none to all of its momentum.

In addition, the position can only be measured to about one wavelength of the photon.



28-3 The Heisenberg Uncertainty Principle

Combining, we find the combination of uncertainties:

$$(\Delta x)(\Delta p_x) \gtrsim \frac{h}{2\pi}. \qquad (28\text{-}1)$$

This is called the Heisenberg uncertainty principle.

It tells us that the position and momentum cannot simultaneously be measured with precision.

28-3 The Heisenberg Uncertainty Principle

This relation can also be written as a relation between the uncertainty in time and the uncertainty in energy:

$$(\Delta E)(\Delta t) \gtrsim \frac{h}{2\pi}. \qquad (28\text{-}2)$$

This says that if an energy state only lasts for a limited time, its energy will be uncertain. It also says that conservation of energy can be violated if the time is short enough.

28-4 Philosophic Implications; Probability versus Determinism

The world of Newtonian mechanics is a deterministic one. If you know the forces on an object and its initial velocity, you can predict where it will go.

Quantum mechanics is very different—you can predict what masses of electrons will do, but have no idea what any individual one will.

§ 28.3 The wave function Schrodinger equation

The task of quantum mechanics is to study how the state of microscopic particles changes with time。

一、微观粒子的状态怎么描述?

经典力学用 $[\vec{r}(t),\vec{v}(t)]$ 或 $[q(t),\ p(t)]$ 描述牛顿粒子的状态。

麦克斯韦电磁理论用时空函数E(r,t)，B(r,t)来描述电磁场的状态。

必须找到创新的方法来描述微观粒子的状态，才能反映微观粒子波粒二象性的特征。迄今为止，物理学家们已经找到了至少四种方法来描述微观粒子的状态。

四种方法：薛定谔、海森伯、狄拉克、费曼

薛定谔的方法：将德布罗意关系同某种波函数结合起来。

例： 一维自由粒子的描述

从粒子性看：具有确定的能量E，动量P

从德布罗意关系：具有确定的 ν，λ 属于单色平面波

以坐标原点为参考点，

设$\varphi=0$，波以速率u沿$+x$方向传播。

$$\Psi=\Psi_0\cos\omega(t-\frac{x}{u})=\Psi_0\cos 2\pi(\nu t-\frac{x}{\lambda})$$

将德布罗意关系组合进去可得：

$$\Psi = \Psi_0 \cos\omega(t - \frac{x}{u}) = \Psi_0 \cos 2\pi(\nu t - \frac{x}{\lambda})$$

$$= \Psi_0 \cos 2\pi (\frac{E}{h} t - \frac{x}{h/p}) = \Psi_0 \cos \frac{1}{\hbar}(Et - p_x \cdot x)$$

上式既有反映波动性的波函数(作为时空的函数)的形式，又有能够反映粒子性质的能量E和P。因此它不再是经典意义下的波函数，已经是量子力学中描述自由粒子状态的波函数了。

沿着这一思路，薛定谔假设不仅自由粒子可以用这样的波函数来描述状态，一般微观粒子也可以用类似的波函数来描述。

注意

Wave function is one of the fundamental postulates of quantum mechanics。

在量子力学中，常把波函数写成复数形式：

$$\boxed{\Psi(x,t)=\Psi_0 e^{-\frac{i}{\hbar}(Et-p_x\cdot x)}}$$ （取实部）

推广：三维自由粒子波函数 $$\boxed{\Psi(\vec{r},t)=\Psi_0 e^{-\frac{i}{\hbar}(Et-\vec{p}\cdot\vec{r})}}$$

波函数模的平方 波的强度

$$|\Psi|^2=\Psi\cdot\Psi^*$$ 波函数与其共轭复数的积

例：一维自由粒子

$$|\Psi(x,t)|^2=\Psi\cdot\Psi^*=\Psi_0 e^{-\frac{i}{\hbar}(Et-p_x\cdot x)}\cdot\Psi_0 e^{+\frac{i}{h}(Et-p_x\cdot x)}=\Psi_0^2$$

所谓系统的状态，是指系统全部性质的总和。如果波函数Ψ(r,t)能描述微观粒子的状态，则通过Ψ(r,t)便应能计算得到微观粒子的全部性质。

如何通过Ψ(r,t)计算微观粒子的各性质？ Ψ(r,t)反映了微观粒子的哪些性质呢？

____即Ψ(r,t)的物理意义是什么呢？

薛定谔本人运用波函数描述微观粒子的方法，成功计算出了与实验观测一致的氢原子光谱，但他没有指出这样的波函数Ψ(r,t)的物理意义是什么。

德国物理学家玻恩提出了一种理解方法，即所谓的玻恩解释，得到了物理学界的普遍承认。

波恩受到爱因斯坦解释光的波粒二象性的方法的启发，他意识到：微观粒子遵从的统计性规律是同波函数的物理意义相联系的。

$$I = N\,h\nu$$

他写道："爱因斯坦的想法仍然是具有指导性的，他把光波振幅平方看成是光出现的概率密度，并试图用这种方法把粒子和波的两重性解释清楚。这种思想可直接地运用于波函数，$\Psi^2(r,t)$应代表粒子t时刻出现在r处的概率密度"。

由于玻恩不能证明以上思路的正确性，只能以假设的形式提出来。

注意

玻恩假设的基本内容可以用数学形式表述如下：

$$|\Psi(x,y,z,t)|^2 = \Psi \cdot \Psi^* \propto \frac{\mathrm{d}N}{N \cdot \mathrm{d}V}$$

$|\Psi(x,y,z,t)|^2$ 的物理意义：

- t 时刻，出现在空间（x,y,z）点附近单位体积内的粒子数与总粒子数之比

- t 时刻，粒子出现在空间（x,y,z）点附近单位体积内的概率

- t 时刻，粒子在空间的概率密度分布

注意

1、描述微观粒子状态的波函数Ψ(r,t),其意义是通过它的模方表现出来。

2、在量子力学中，微观粒子仍然是分立的“质点”，只不过这些微观粒子出现在周围空间各位置的概率为不同，其大小由波函数决定。物质波是一种概率波，正是这种波决定了微观粒子在空间各位置出现的概率。

3、这种波不同于经典的波，经典波伴随着能量的传递，而伴随着概率波的微观粒子的能量是不会弥散开的。

注意

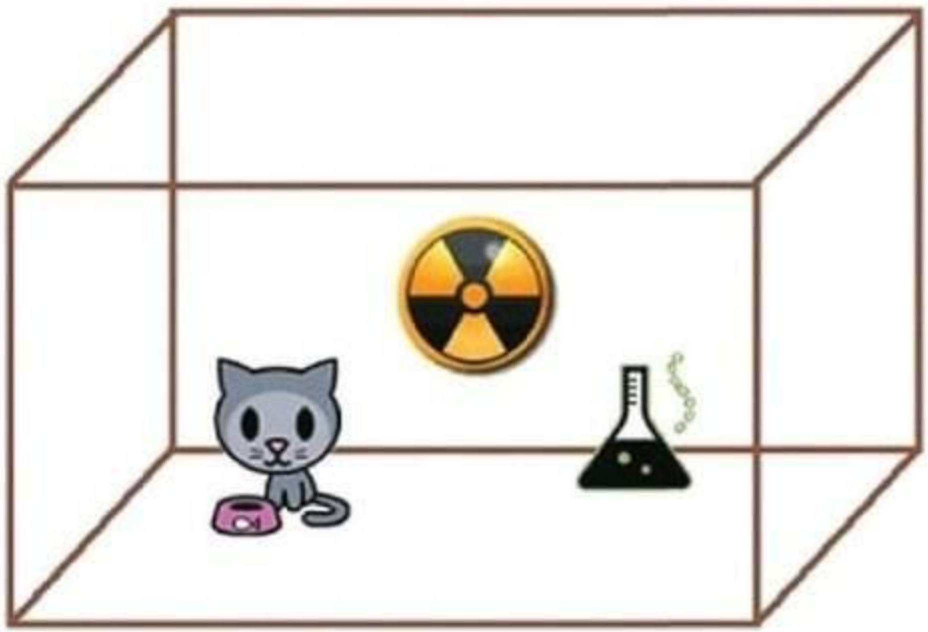
4、物质波的波函数不描述介质中运动状态（相位）传播的过程。

5、 Ψ(r,t)与c Ψ(r,t)描述同一概率波，即重要的不是Ψ(r,t)^{2}的绝对大小，而是其在空间各点的相对大小。

6、 Ψ(r,t) 遵从迭加原理。

$$\Psi = \Psi_1 + \Psi_2$$

$$|\Psi|^2 = |\Psi_1 + \Psi_2|^2 = \Psi_1 \cdot \Psi_1 * + \Psi_2 \cdot \Psi_2 * + \underbrace{\Psi_1 \cdot \Psi_2 * + \Psi_1 * \cdot \Psi_2}_{\text{干涉项}}$$



$$|\Psi|^2 = |\Psi_1 + \Psi_2|^2 = \Psi_1 \cdot \Psi_1^* + \Psi_2 \cdot \Psi_2^* + \underbrace{\Psi_1 \cdot \Psi_2^* + \Psi_1^* \cdot \Psi_2}_{\text{干涉项}}$$

注意

7、波函数的归一化条件和标准条件

① 归一化条件

粒子在整个空间出现的概率为1

$$\int_V |\Psi|^2 \mathrm{d}V = \int_V \frac{\mathrm{d}N}{N\mathrm{d}V} \cdot \mathrm{d}V = \frac{\int \mathrm{d}N}{N} = \frac{N}{N} = 1$$

② 标准条件

Ψ是单值、有限、连续的。

对微观客体的量子力学描述：

脱离日常生活经验，避免借用经典语言引起的表观矛盾，将波粒二象性统一到一起。

二、薛定谔方程

物理学的目的，就是通过一定的理论体系预见未来。即在已知系统的边界条件和初始状态的情况下，导出任意时刻的状态。这一目的是通过建立动力学方程来实现的。用波函数来描述微观粒子的状态，则：

微观粒子遵从的动力学方程应是关于 $\partial\psi(\vec{r},t)/\partial t=?$ 的微分方程

实事上，薛定谔本人也从未详尽阐述过，他是如何建立他的动力学方程的，薛定谔是把他的动力学方程做为一种假设纳入他的量子力学体系的。

$$\partial\psi(\vec{r},t)/\partial t=\hat{L}\psi(\vec{r},t)$$

量子力学的又一基本假设

一维自由粒子波函数:

$$\Psi(x,t)=\Psi_0 e^{-\frac{i}{\hbar}(Et-p_x\cdot x)}$$

对时间的一阶微分为:

$$\frac{\partial\Psi(x,t)}{\partial t}=-\frac{i}{\hbar}E\Psi_0 e^{-\frac{i}{\hbar}(Et-p_x\cdot x)}=-\frac{i}{\hbar}E\Psi(x,t)$$

对x的二阶微分:

$$\frac{\partial^2\Psi(x,t)}{\partial x^2}=-\frac{1}{\hbar^2}P_x{}^2\Psi_0 e^{-\frac{i}{\hbar}(Et-p_x\cdot x)}=-\frac{1}{\hbar^2}P_x{}^2\Psi(x,t)$$

对自由粒子：*v<<c*

$$E = E_{\mathrm{k}} = \frac{1}{2} m v_x^2 = \frac{p_x^2}{2m}$$

消去*E*和*P*可得：

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} = \hat{H} \psi(x,t)$$

如果： $E^2 = c^2 p^2 + m_0{}^2 c^4$

$$\hbar^2 \frac{\partial \Psi^2(x,t)}{\partial t^2} = c^2 \hbar^2 \frac{\partial^2 \Psi(x,t)}{\partial x^2} - m_0{}^2 c^4 \Psi(x,t)$$

*克莱因-戈登方程（P175）

三、定态薛定谔方程

若粒子是不自由的，而是在某种势场U中运动，且U不随时间发生变化，则相应的薛定谔方程称为定态薛定谔方程。

一维定态薛定谔方程

一维情况下波函数仍然满足以下公式：

$$\psi(x,t)=\psi(x)\cdot e^{-\frac{i}{\hbar}Et}$$

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}=\frac{-p_x^{\;2}}{\hbar^2}\psi(x)$$

只需求出振幅函数就可求振幅模的平方，以及整个波函数的形式。

粒子在力场中运动，且势能不随时间变化

$$E = E_{\mathrm{k}} + E_{\mathrm{p}} = \frac{p_x^2}{2m} + U$$

$$p_x^2 = 2m(E - U)$$

代入 $$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = \frac{-p_x^2}{\hbar^2}\psi(x)$$*

得 $$\boxed{\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - U)\psi(x) = 0}$$

即 一维定态薛定谔方程