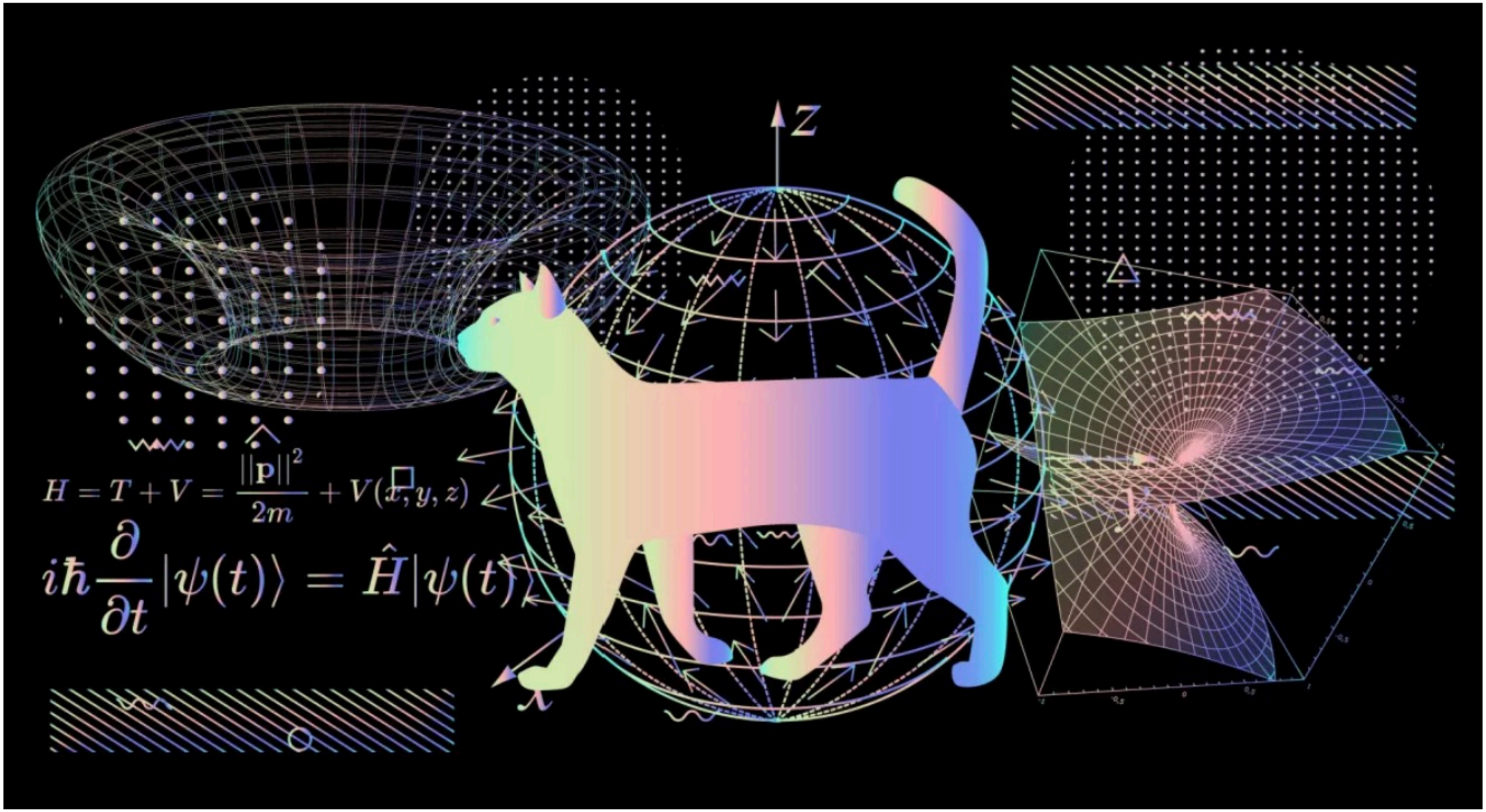
Quantum mechanics

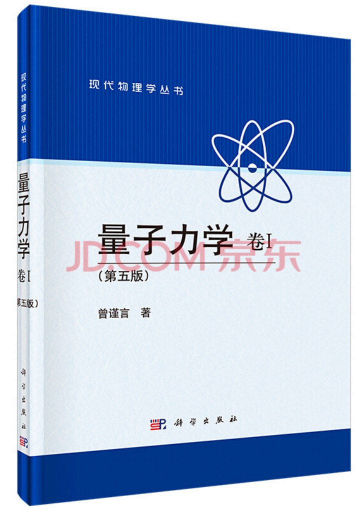
Chapter I Introduction



Class requirements

✓ Quiz+Homework (40%)

✓ Final examination (60%)



✓References

J. J. Sakura and Jim Napolitano, Modern Quantum Mechanics

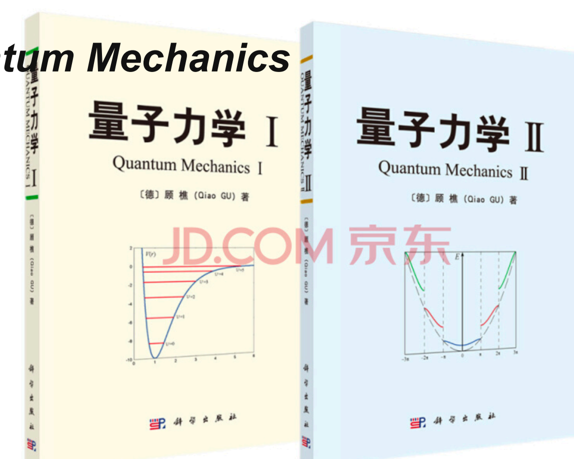
S. Weinberg, Lectures on Quantum Mechanics

D. J. Griffiths and D. F. Schroeder, Introduction to Quantum Mechanics

曾谨言，量子力学 第四版

苏汝铿，量子力学 第二版

顾 樵，量子力学 I II



Group works

1. The Heisenberg's Matrix Mechanics
2. How to solve the harmonies oscillator in momentum space
3. The mathematical basis of quantum mechanics
4. The pictures of quantum mechanic
5. The quantum computing methods
6. The Hydrogen solved by Machine learning
7. The algebra solution of hydrogen
8. The approximated methods in quantum mechanics

Prior knowledge

Mechanics

Optics

Thermodynamics

Atomic Physics

Linear Algebra

Differential equation

Origins of quantum mechanics

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Classical physics – (pre 1900)

Mechanics – Newton

Thermodynamics – Boltzmann, Gibbs et al.

Electromagnetics – Maxwell et al.

Scientists believed that:

The physical universe was deterministic.

Light consisted of waves, ordinary matter was composed of particles.

Physical quantities (energy, momentum, etc) could be treated as continuous variables.

There exists an objective physical reality independent of any observer.

What happens to those ideas?

Before we get into the details, let's see what the development of quantum mechanics meant for those four "certainties" of classical physics:

Classical ⇒ The physical universe is deterministic.

Modern ⇒ The physical universe is not deterministic.

At the scale of atomic particles, the best that we can do is find the probability of the outcome of an experiment. We can't predict exact results with certainty. Uncertainty is an intrinsic property of matter at this level.

Classical $\Rightarrow$ Light consists of waves, while ordinary matter is composed of particles.

Modern $\Rightarrow$ Both light and matter exhibit behavior that seems characteristic of both particles and wave. (wave-particle duality)

Classical $\Rightarrow$ Physical quantities (energy, momentum, etc) can be treated as continuous variables.

Modern $\Rightarrow$ Under certain circumstances, some physical quantities are quantized, meaning that they can take on only certain discrete values.

Origins of quantum mechanics

Classical ⇒ There exists an objective physical reality independent of any observer.

Modern ⇒ It appears that the observer always affects the experiment. It is impossible to disentangle the two.

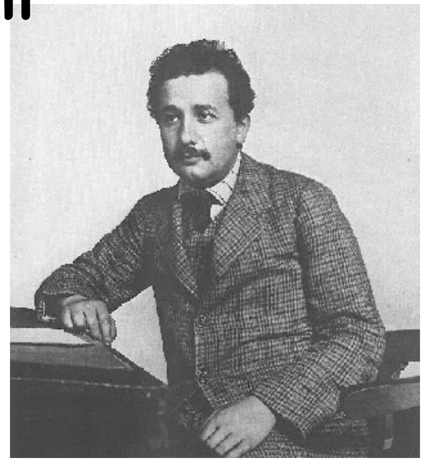
Outstanding problems c. 1900

Black-body radiation

The nature of light

The structure of the atom

Planck



Einstein

Bohr

The fifth Solvay conference

Timeline of quantum mechanics

1897 - Pieter Zeeman shows that light is radiated by the motion of charged particles in an atom, and Joseph John Thomson discovers the electron.

1900 Max Planck explains blackbody radiation in the context of quantized energy emission: Quantum theory is born.

1905 Albert Einstein proposes that light, which has wavelike properties, also consists of discrete quantized bundles of energy, which are later called photons.

1911 Ernest Rutherford proposes the nuclear model of the atom.

1913 Niels Bohr proposes his planetary model of the atom, along with the concept of stationary energy states, and accounts for the spectrum of hydrogen.

Atoms go quantum. In 1913, Niels Bohr ushered quantum physics into world of atoms.

1914 James Franck and Custav Hertz confirm the existence of stationary states through an electron scattering experiment.

Timeline of quantum mechanics

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1923 Arthur Compton observes that x-rays behave like miniature billiard balls in their interactions with electrons. Thereby providing further evidence for the particle nature of light.

1923 Louis De Broglie generalizes wave-particle duality by suggesting that particles of mater are also wavelike.

1924 Satyendra Nath Bose and Albert Einstein find a new way to count quantum particles, later called Bose-Einstein statistics, and they predict that extremely cold atoms should condense into a single quantum state, later known as a Bose-Einstein condensate.

1925 Wolfgang Pauli enunciates the exclusion principle.

1925 Werner Heisenberg, Max Born, and Pascual Jordan develop matrix mechanics, the first version of quantum mechanics, and make an initial step toward quantum field theory.

1926 Erwin Schrödinger develops a second description of quantum physics, called wave mechanics. It includes what becomes one of the most famous formulae of science, which is later known as the Schrödinger equation.

Timeline of quantum mechanics

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1926 Enrico Fermi and Paul A. M. Dirac find that quantum mechanics requires a second way to count particles, Fermi-Dirac statistics, opening the way to solid state physics.

1926 Dirac publishes a seminal paper on the quantum theory of light.

1927 Heisenberg states his uncertainty principle, that it is impossible to exactly measure the position and momentum of a particle at the same time.

Unknowable reality. Werner Heisenberg articulated one of the most societally absorbed ideas of quantum physics: the Uncertainty Principle.

Timeline of quantum mechanics

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1928 Dirac presents a relativistic theory of the electron that includes the prediction of antimatter.

1932 Carl David Anderson discovers antimatter, an antielectron called the positron.

1948 Richard Feynman, Julian Schwinger, and Sinitiro Tomonaga develop the first complete theory of the interaction of photons and electrons, quantum electrodynamics, which accounts for the discrepancies in the Dirac theory.

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Blackbody Radiation

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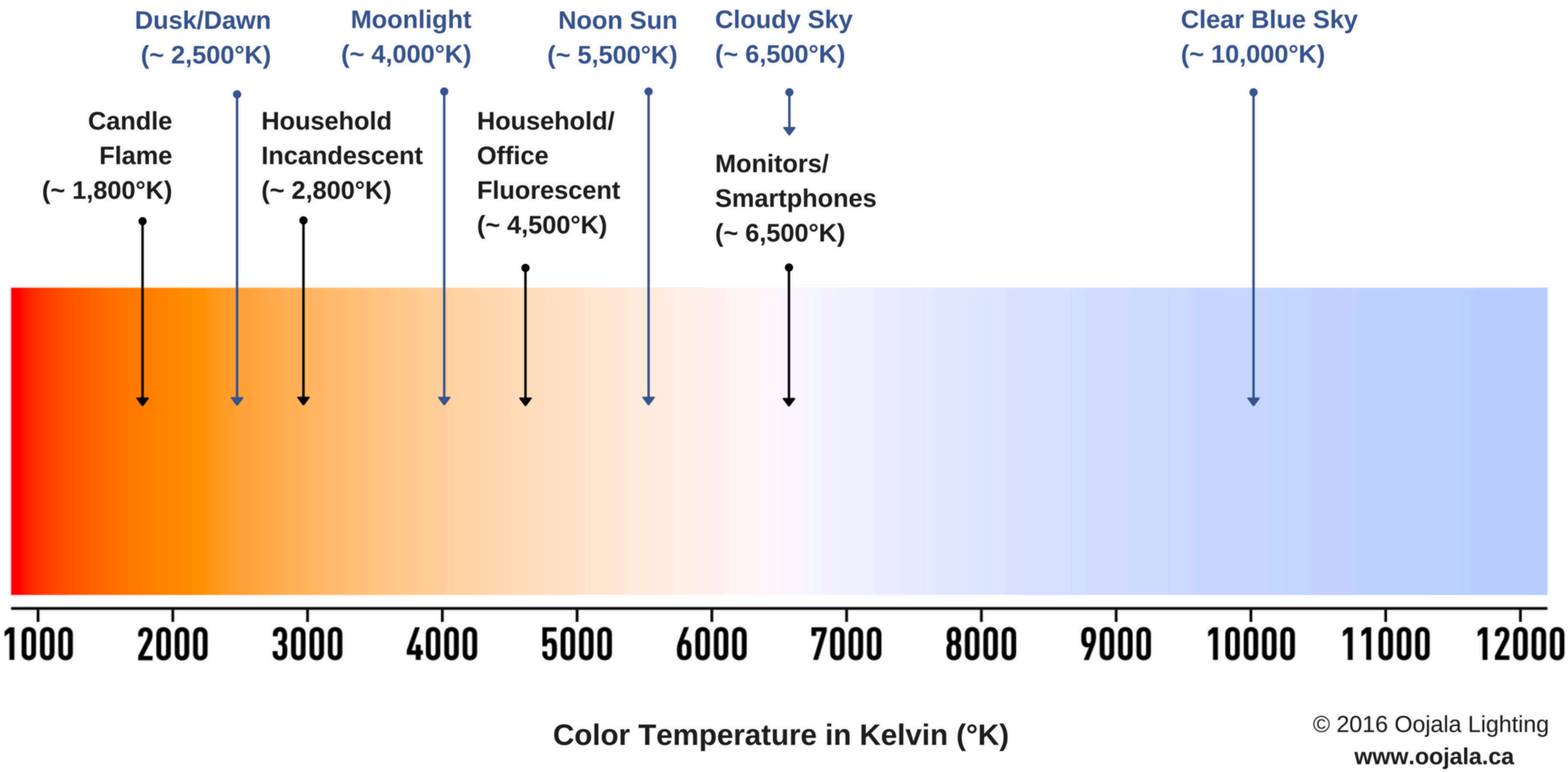
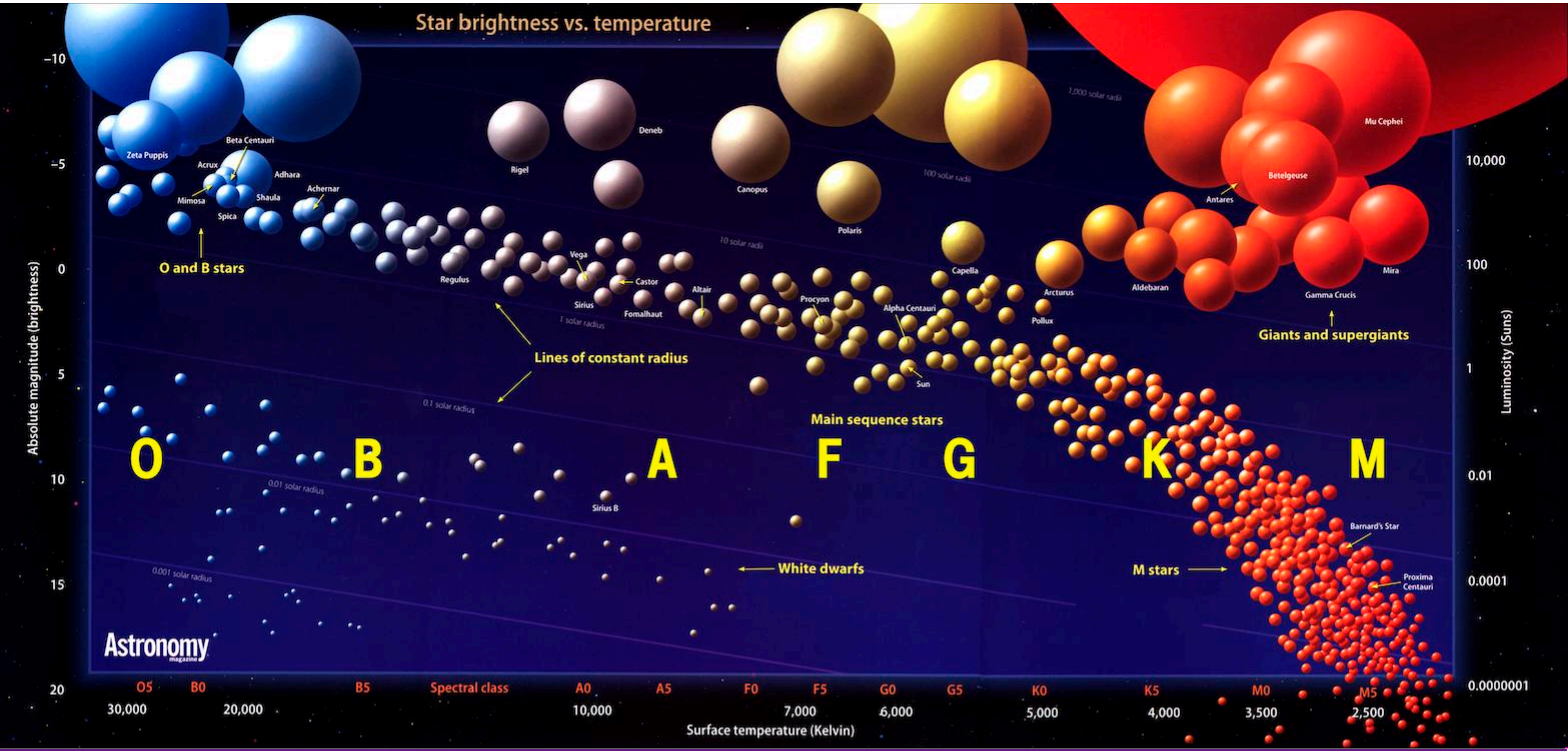
If the temperature were increased still further, the color would progress through orange, yellow, and finally white.



The spectrum of star

Hertzsprung-Russell diagram is a plot of stars showing the relationship between the stars' luminosities versus their effective temperatures.



Blackbody Radiation

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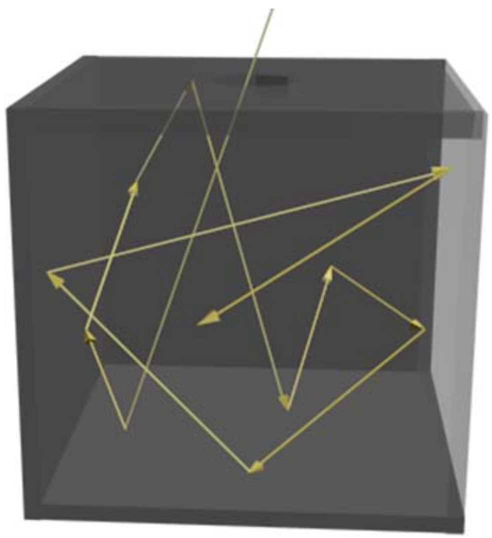
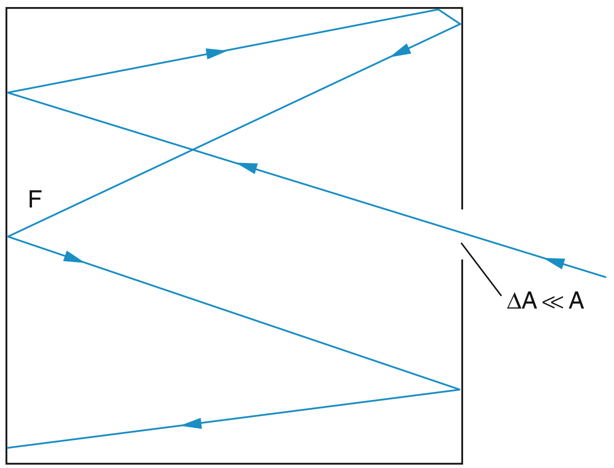
Thermal equilibrium: one body absorbs thermal energy at the same rate as it emits it.

Blackbody: a body absorbs all the radiations falling upon it and emits all the radiations when heated.

The simplest way to construct a blackbody is to drill a small hole in the wall of a hollow container.





The Kirchhoff's law: for a given temperature, the composition of the equilibrium radiation inside the enclosure is exactly the same regardless of the nature of matter.

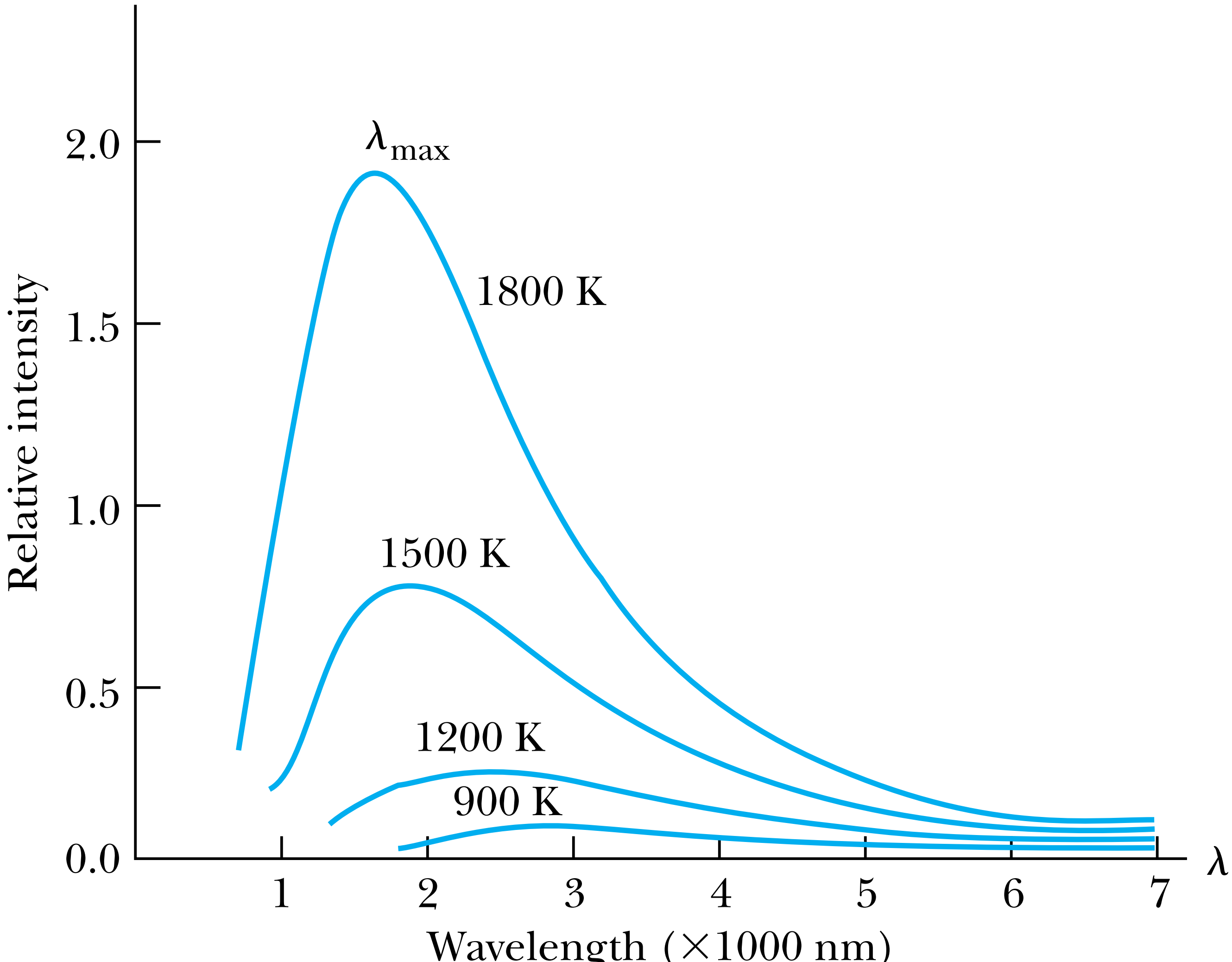
Spectral distribution: properties of intensity versus wavelength at fixed temperatures.

The intensity:

$$e_f = J(f, T)$$

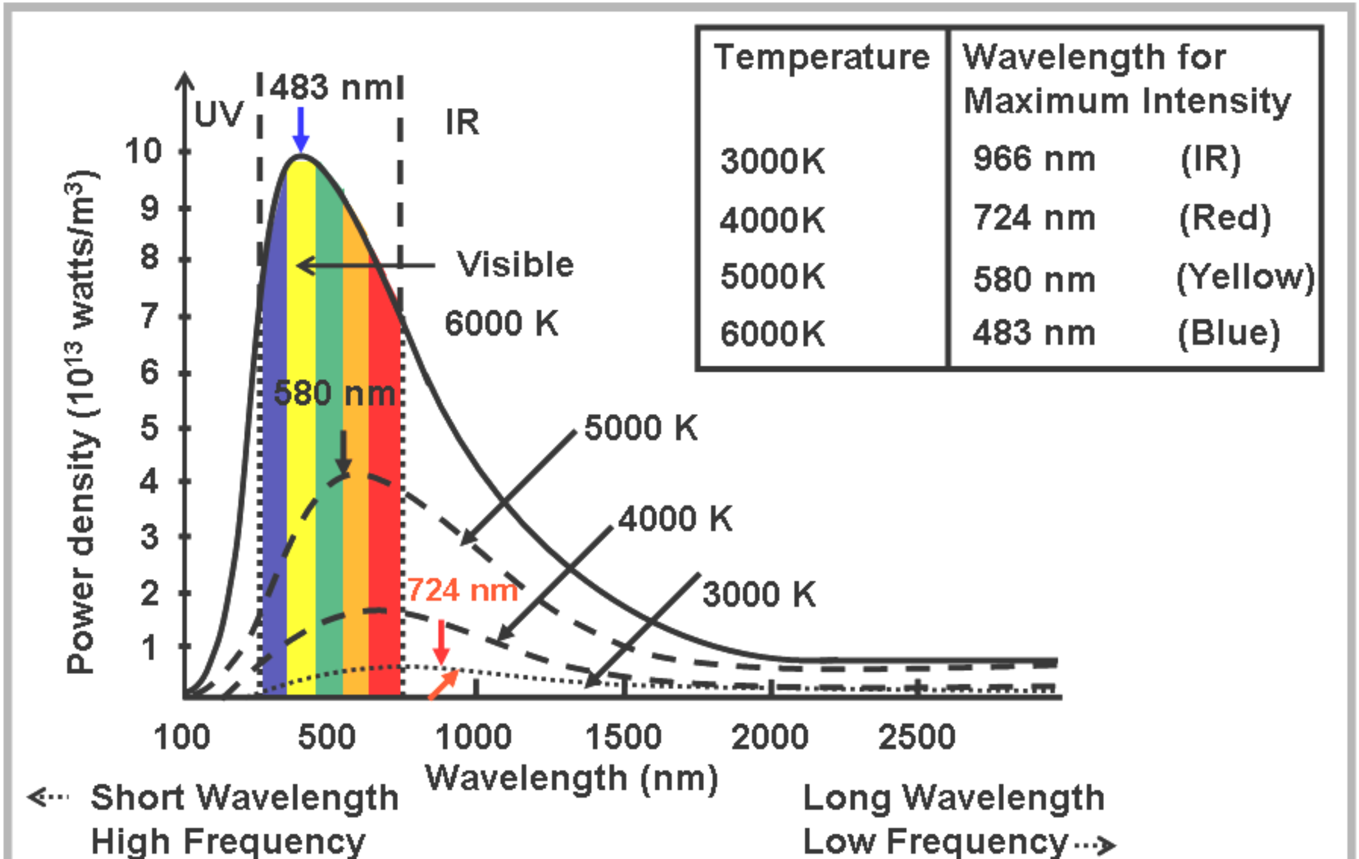
is the total power radiated per unit area per unit wavelength at a given temperature.

Measurements of intensity for a blackbody are displayed



Blackbody Radiation

Measurements of intensity for a blackbody are displayed



Temperature	Wavelength for Maximum Intensity	
3000K	966 nm	(IR)
4000K	724 nm	(Red)
5000K	580 nm	(Yellow)
6000K	483 nm	(Blue)

Fig. Spectral intensity distribution of Blackbody Radiation vs Wavelength Intensity Maximum shifts to shorter wavelengths as temperature increases.

Two important observations should be noted:

1. The maximum of the distribution shifts to smaller wavelengths as the temperature is increased.
2. The total power radiated increases with the temperature.

The first observation is expressed in Wien's displacement law:

$$\lambda_{\max} T = 2.898 \times 10^{-3}\ \mathrm{m \cdot K}$$

where λ_{max} is the wavelength of the peak of the spectral distribution at a given temperature.

Wilhelm Wien received the Nobel Prize in 1911 for his discoveries concerning radiation.

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We can quantify the second observation by integrating the quantity intensity over all wavelengths to find the power per unit area at temperature T:

$$e_{\text{total}} = \int_0^{\infty} e_f \, df = \sigma T^4$$

Stefan-Boltzmann law:

$$e_{\text{total}} = a\sigma T^4$$

with the constant

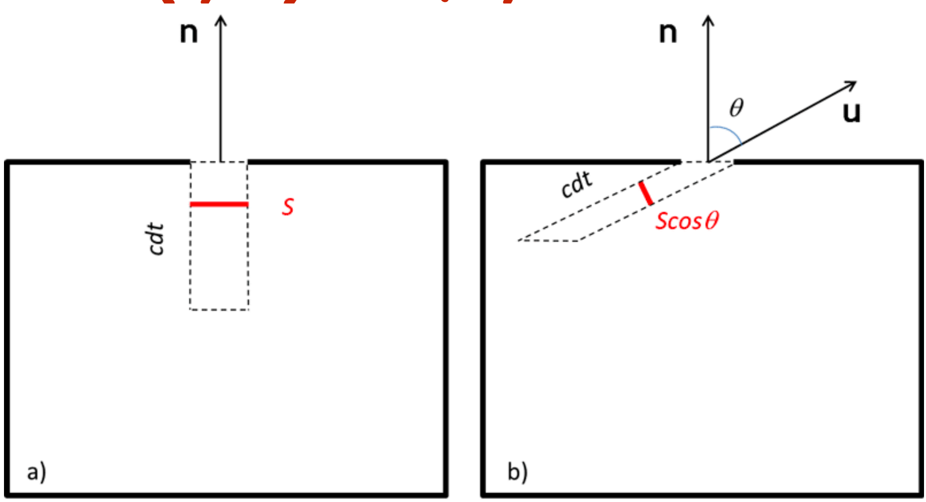
$$\sigma = 5.6705 \times 10^{-8} \ \mathrm{W/(m^2 \cdot K^4)}$$

The emissivity a is simply the ratio of the emissive power of an object to that of an ideal blackbody and is always less than 1.

It is more convenient to consider the spectral energy density, or energy per unit volume per unit frequency of the radiation within the blackbody cavity, u(f, T).

Because the cavity radiation is isotropic and unpolarized, one can average over direction to show that the constant of proportionality between J(f, T) and u(f, T) is c/4, where c is the speed of light. Therefore,

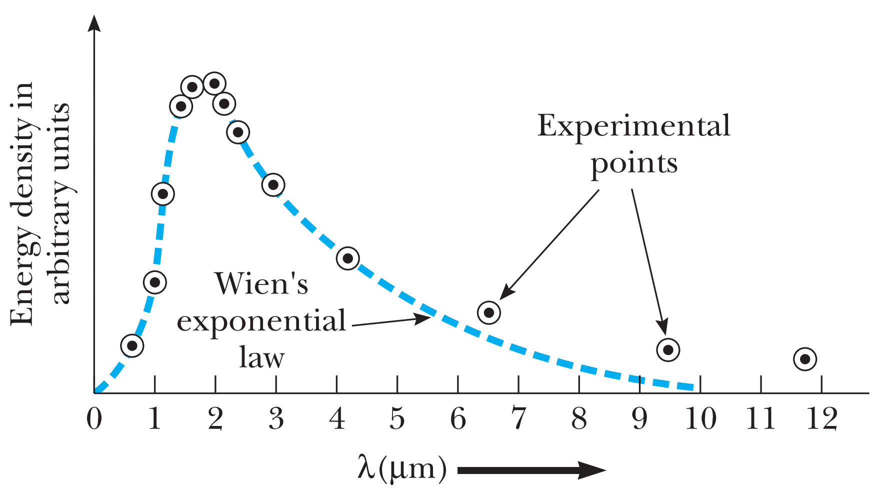
$$J(f, T) = u(f, T)\, c/4$$



An important guess as to the form of the universal function u(f, T) was made in 1893 by Wien and had the form

$$u(f, T) = Af^3 e^{-\beta f/T}$$

where A and β are constants. This result was known as Wien's exponential law; it resembles and was loosely based on Maxwell's velocity distribution for gas molecules.



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By considering the conditions leading to equilibrium between the wall resonators and the radiation in the blackbody cavity, the spectral energy density u(f, T) could be expressed as the product of the number of oscillators having frequency between f and f+df, denoted by N(f) df, and the average energy emitted per oscillator, E. Thus we have the important result

$$u(f, T)\, df = \overline{E} N(f)\, df$$

In the classical case considered by Rayleigh, an oscillator could have any energy E in a continuous range from 0 to ∞

$$\overline{E} = \frac{\displaystyle\int_0^\infty E e^{-E/k_B T} dE}{\displaystyle\int_0^\infty e^{-E/k_B T}\, dE} = k_B T$$

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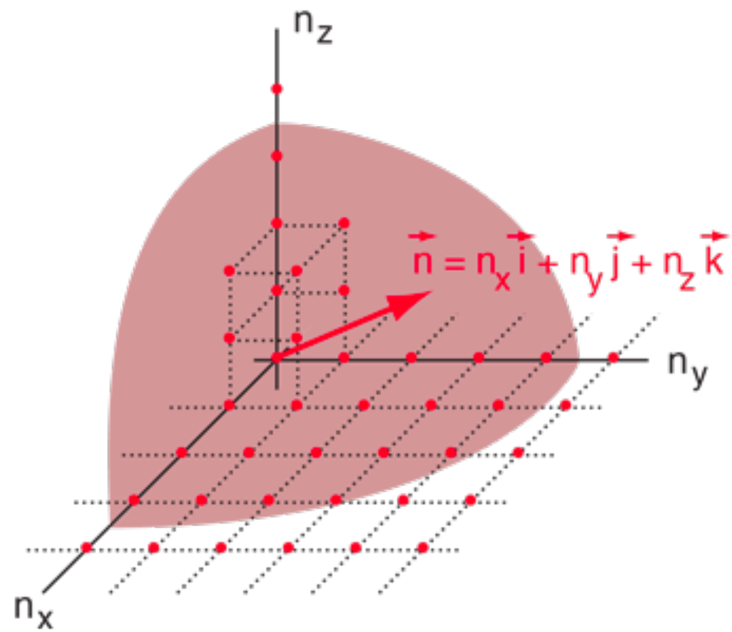
The density of modes, N(f) df is



$$N(f)\,df = \frac{8\pi f^2}{c^3}\,df$$

or in terms of wavelength,

$$N(\lambda)\,d\lambda = \frac{8\pi}{\lambda^4}\,d\lambda$$

The spectral energy density is simply the density of modes multiplied by $k_B T$, or

$$u(f,T)\,df = \frac{8\pi f^2}{c^3}\,k_B T\,df$$

Rayleigh-Jeans formula:

$$u(\lambda,\, T)\, d\lambda = \frac{8\pi}{\lambda^4}\, k_{\mathrm{B}} T\, d\lambda$$

It is the best formulation that classical theory can provide to describe blackbody radiation.

When

$$\lambda \rightarrow 0$$

the total energy of all configurations is infinite. In 1911 Paul Ehrenfest dubbed this situation the "ultraviolet catastrophe," and it was one of the outstanding exceptions that classical physics could not explain.

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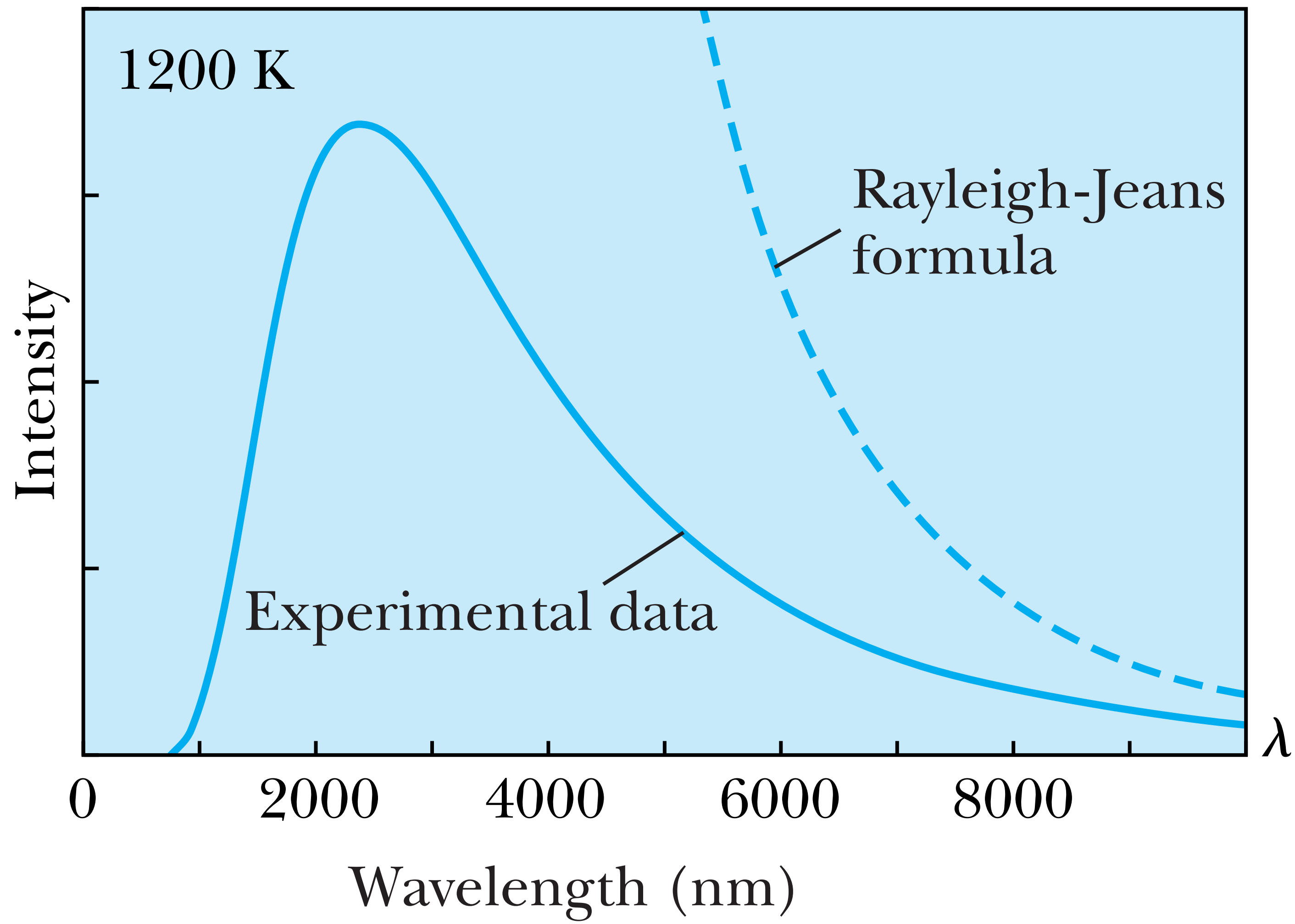
1200 K
Rayleigh-Jeans formula
Experimental data
Intensity
λ
0
2000
4000
6000
8000
Wavelength (nm)

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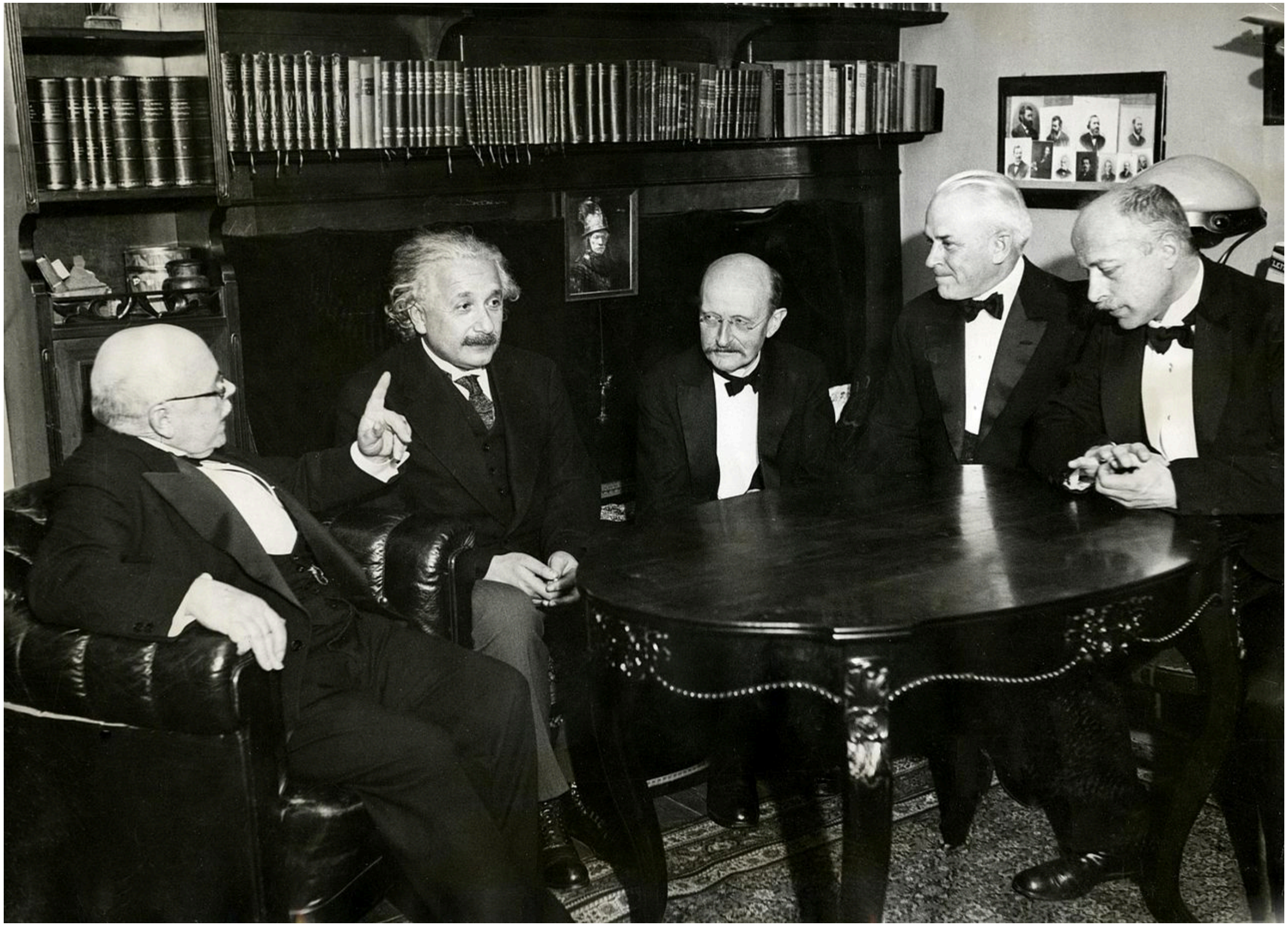
Max Plank



W. Nernst, A. Einstein, **M. Planck**, R.A. Millikan and von Laue

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Planck's radiation law:

$$u(f, T) = \frac{8\pi h f^3}{c^3}\left(\frac{1}{e^{hf/k_{\mathrm{B}}T} - 1}\right)$$

He could arrive at agreement with the experimental data only by making two important modifications of classical theory:

1. The oscillators (of electromagnetic origin) can only have certain discrete energies determined by

$$E_{\text{resonator}} = nhf \qquad n = 1, 2, 3, \ldots$$

where n is an integer, f is the frequency, and h is called Planck's constant and has the value

$$h = 6.6261 \times 10^{-34} \mathrm{J \cdot s}$$

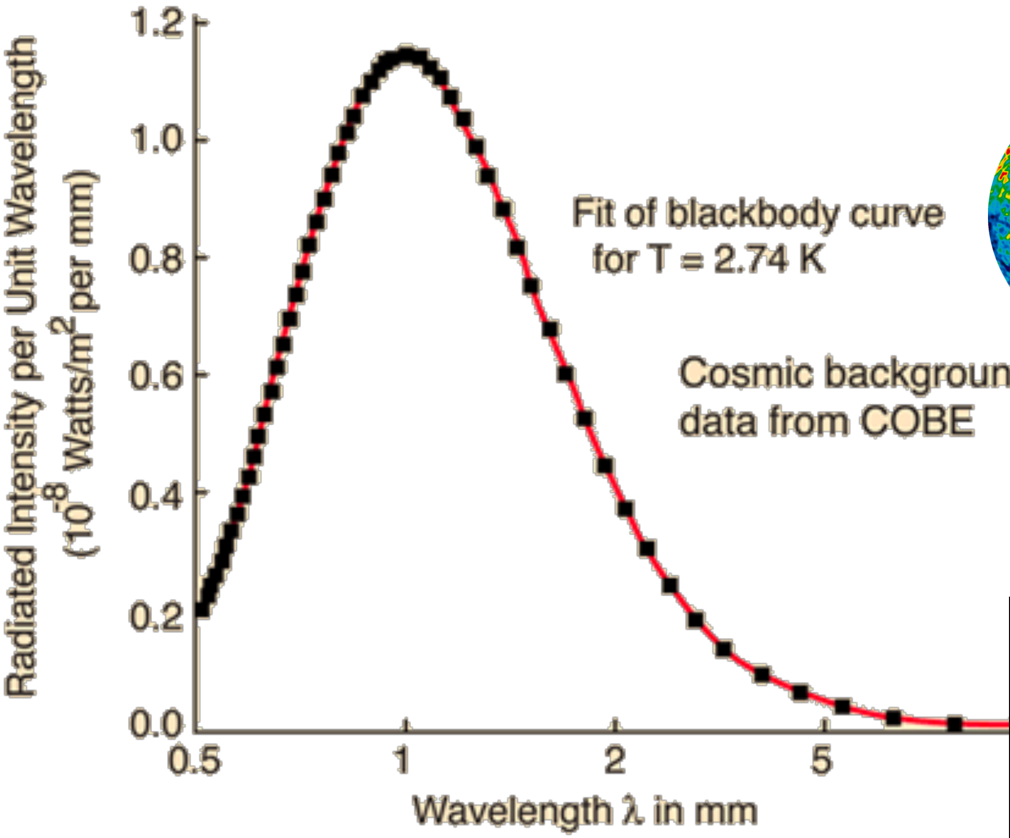
$$\bar{E} = \frac{\sum E \cdot P(E)}{\sum P(E)}$$

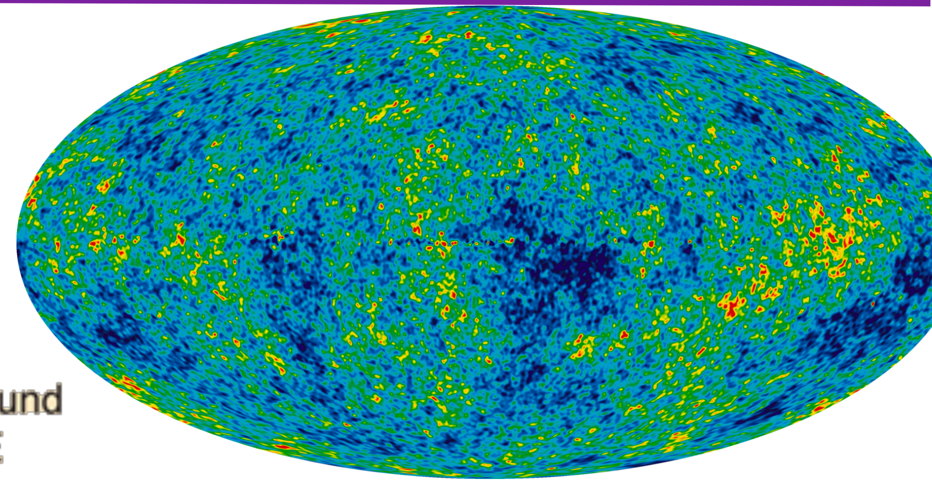
2. The oscillators can absorb or emit energy in discrete multiples of the fundamental quantum of energy given by

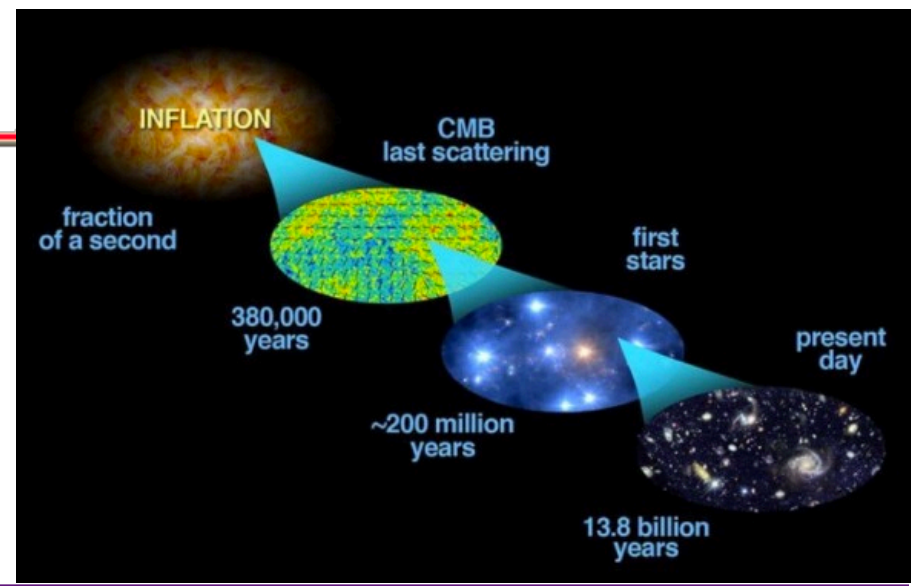
$$\Delta E = hf$$

Planck found these results quite disturbing and spent several years trying to find a way to keep the agreement with experiment while letting $h \rightarrow 0$. Each attempt failed, and Planck's quantum result became one of the cornerstones of modern science.

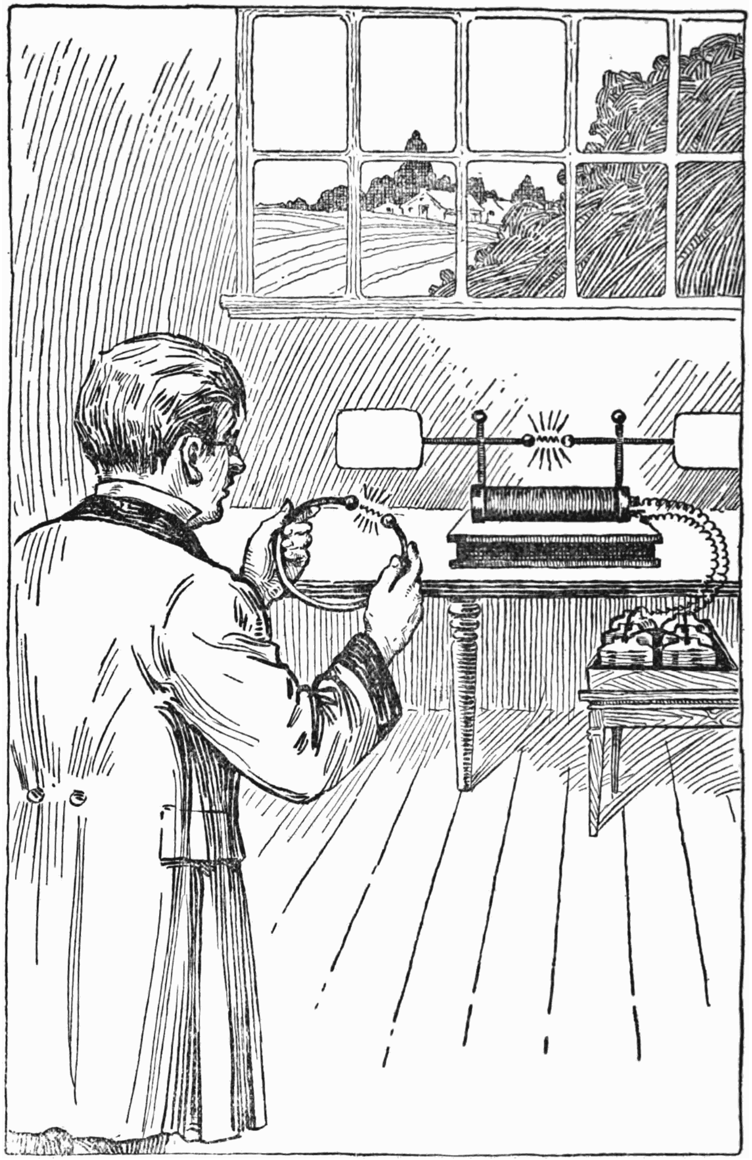
Cosmic microwave background







While Heinrich Hertz was performing his famous experiment in 1887 that confirmed Maxwell's electromagnetic wave theory of light, he noticed that when ultraviolet light fell on a metal electrode, a charge was produced that separated the leaves of his electroscope.



Photoelectric Effect

Photoelectric Effect

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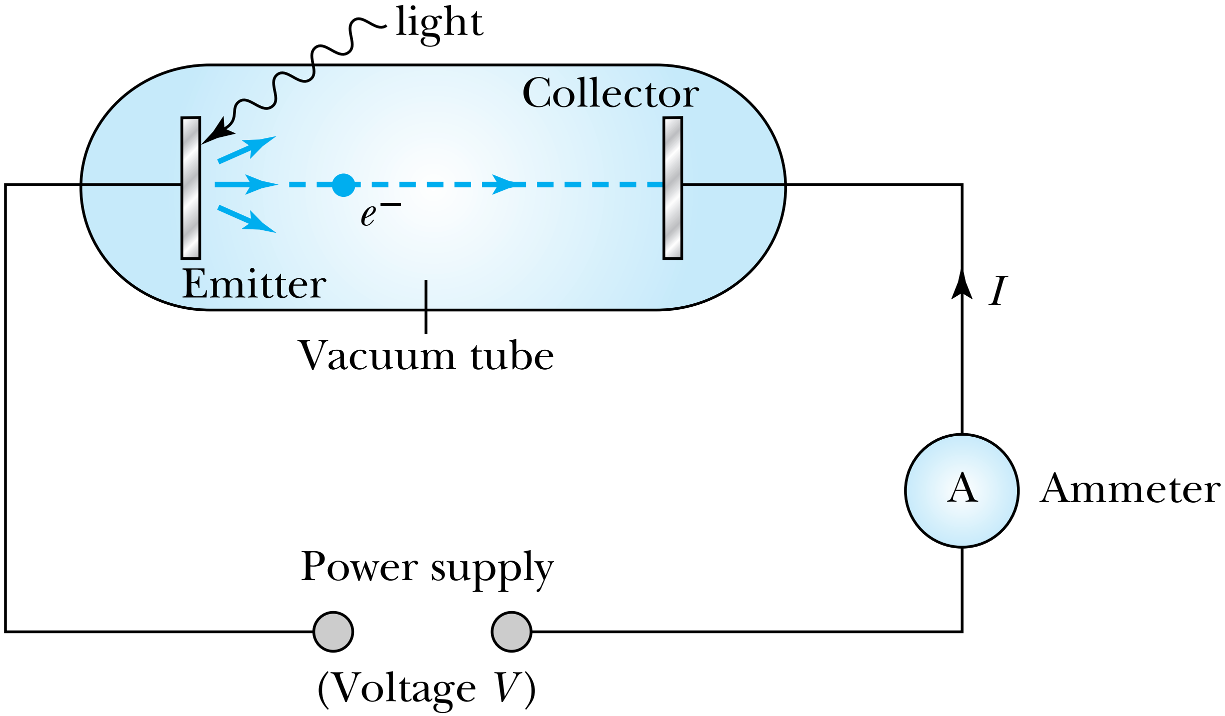
The photoelectric effect is one of several ways in which electrons can be emitted by materials.

The methods known now by which electrons can be made to completely leave the material include:

1. Thermionic emission: Application of heat allows electrons to gain enough energy to escape.
2. Secondary emission: The electron gains enough energy by transfer from a high-speed particle that strikes the material from outside.
3. Field emission: A strong external electric field pulls the electron out of the material.
4. Photoelectric effect: Incident light (electromagnetic radiation) shining on the material transfers energy to the electrons, allowing them to escape.

Experimental Results

Incident light falling on the emitter ejects electrons. Some of the electrons travel toward the collector (also called the anode), where either a negative (retarding) or positive (accelerating) applied voltage V is imposed by the power supply.



Photoelectric Effect

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We call the ejected electrons photoelectrons. The minimum extra kinetic energy that allows electrons to escape the material is called the work function ϕ. The work function is the minimum binding energy of the electron to the material

Element	ϕ (eV)	Element	ϕ (eV)	Element	ϕ (eV)
Ag	4.64	K	2.29	Pd	5.22
Al	4.20	Li	2.93	Pt	5.64
C	5.0	Na	2.36	W	4.63
Cs	1.95	Nd	3.2	Zr	4.05
Cu	4.48	Ni	5.22		
Fe	4.67	Pb	4.25		

Experimental Results

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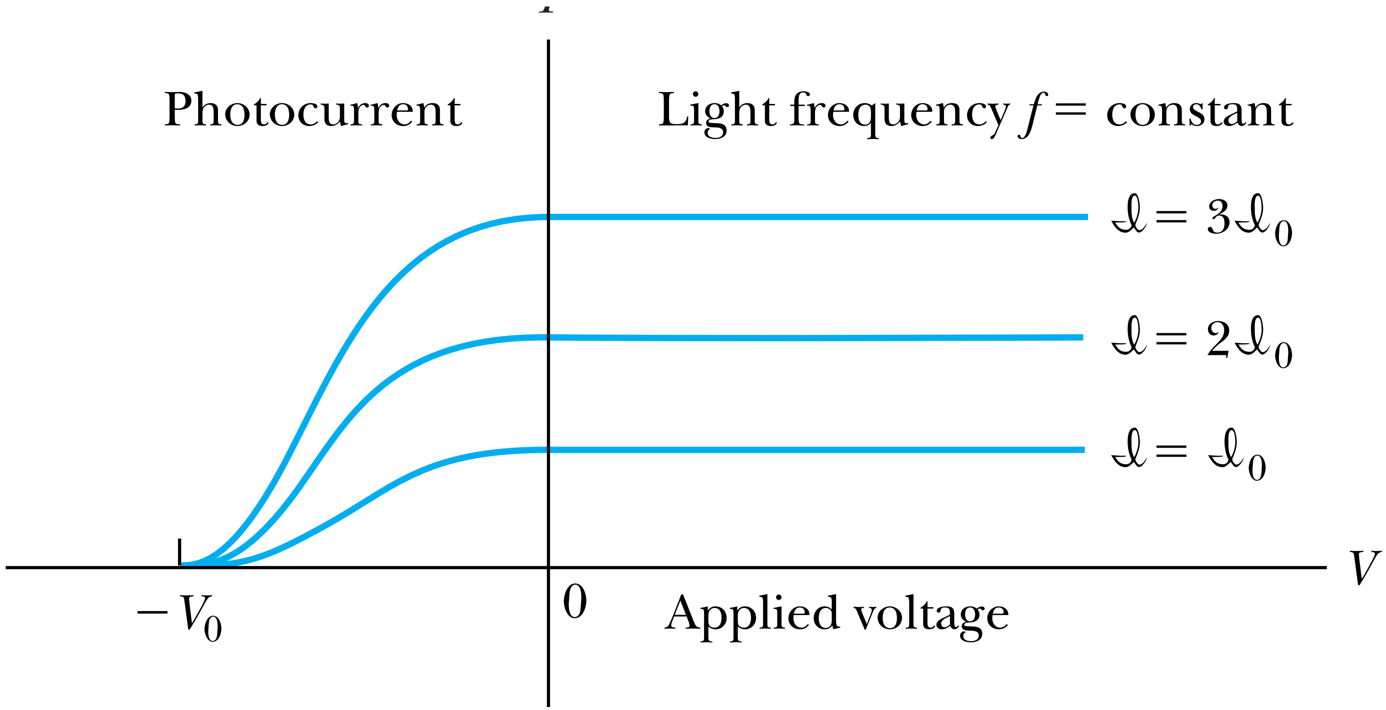
The pertinent experimental facts about the photoelectric effect are these:

1. The kinetic energies of the photoelectrons are independent of the light intensity.



Experimental Results

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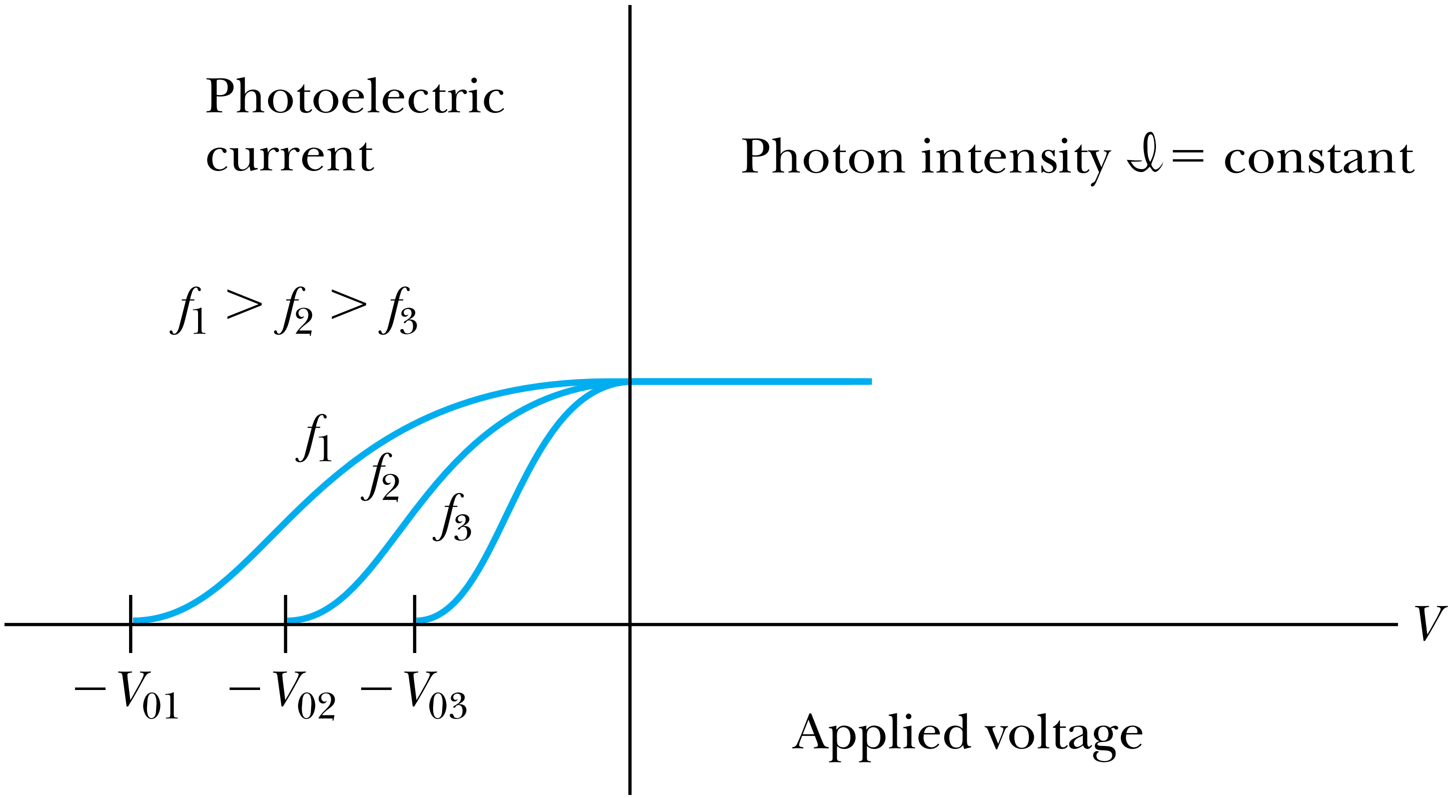
2. The maximum kinetic energy of the photoelectrons, for a given emitting material, depends only on the frequency of the light.



Experimental Results

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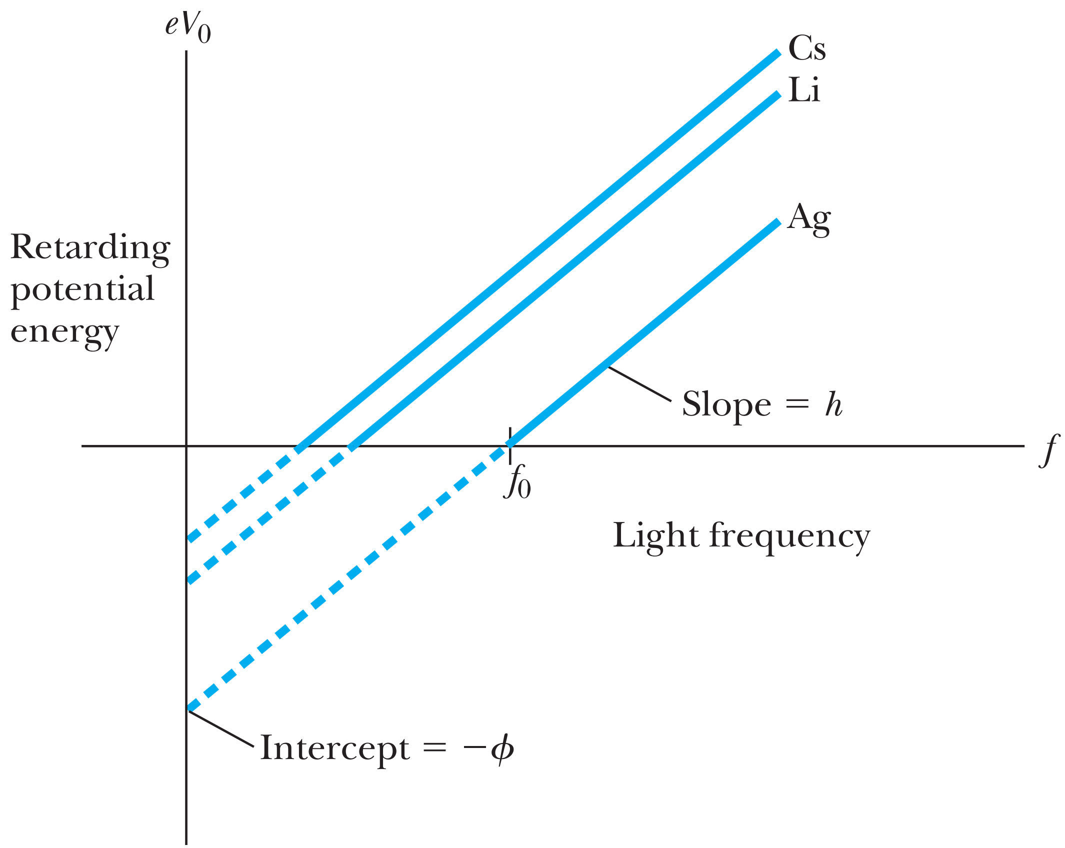
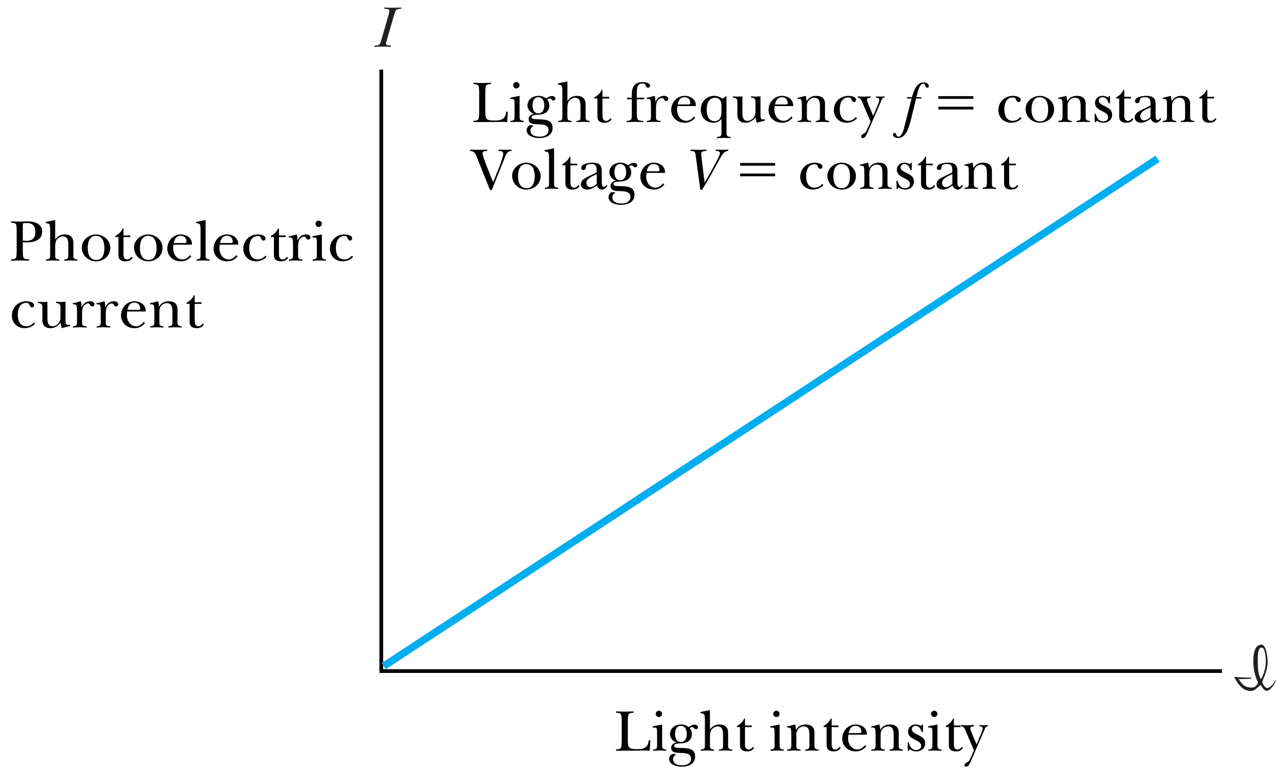
3. The smaller the work function ϕ of the emitter material, the lower is the threshold frequency of the light that can eject photoelectrons.



4. When the photoelectrons are produced, however, their number is proportional to the intensity of light



Experimental Results

5. The photoelectrons are emitted almost instantly ($3*10^{-9}$s) following illumination of the photocathode, independent of the intensity of the light.

Except for result 5, these experimental facts were known in rudimentary form by 1902, primarily due to the work of Philipp Lenard, who had been an assistant to Hertz in 1892 after Hertz had moved from Karlsruhe to Bonn.

Lenard, who extensively studied the photoelectric effect, received the Nobel Prize in Physics in 1905 for this and other research on the identification and behavior of electrons.

Classical Interpretation

1. Classical theory allows electromagnetic radiation to eject photoelectrons from matter.
2. Classical theory predicts that the total amount of energy in a light wave increases as the light intensity increases.
3. Classical theory cannot explain that the maximum kinetic energy of the photoelectrons depends on the value of the light frequency ν and not on the intensity.
4. The existence of a threshold frequency is completely inexplicable in classical theory.
5. Classical theory does predict that the number of photoelectrons ejected will increase with intensity.

Einstein's Theory

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1. Albert Einstein was intrigued by Planck's hypothesis that the electromagnetic radiation field must be absorbed and emitted in quantized amounts.

2. Einstein took Planck's idea one step further and suggested that the electromagnetic radiation field itself is quantized

3. We now call these energy quanta of light photons. According to Einstein each photon has the energy quantum

$$E = h\nu$$

where ν is the frequency of the electromagnetic wave associated with the light, and h is Planck's constant.

4. Einstein proposed that in addition to its well-known wavelike aspect, amply exhibited in interference phenomena, light should also be considered to have a particle-like aspect.

The conservation of energy requires that

$$h\nu = \phi + E_k$$

We want to experimentally detect the maximum value of the kinetic energy.

$$h\nu = \phi + \frac{1}{2}mv_{\max}^2$$

The retarding potentials are thus the opposing potentials needed to stop the most energetic electrons.

$$eV_0 = \frac{1}{2}mv_{\max}^2$$

Quantum Interpretation

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The kinetic energy of the electrons depends only on the light frequency and the work function of the material.

$$\frac{1}{2}mv_{\max}^2 = eV_0 = h\nu - \phi$$

which proposed by Einstein in 1905, predicts that the stopping potential will be linearly proportional to the light frequency, The slope is independent of the metal used to construct the photocathode. This equation can be rewritten as

$$eV_0 = \frac{1}{2}mv_{\max}^2 = h(\nu - \nu_0)$$

The frequency ν_0 represents the threshold frequency for the photoelectric effect. (when the kinetic energy of the electron is precisely zero).

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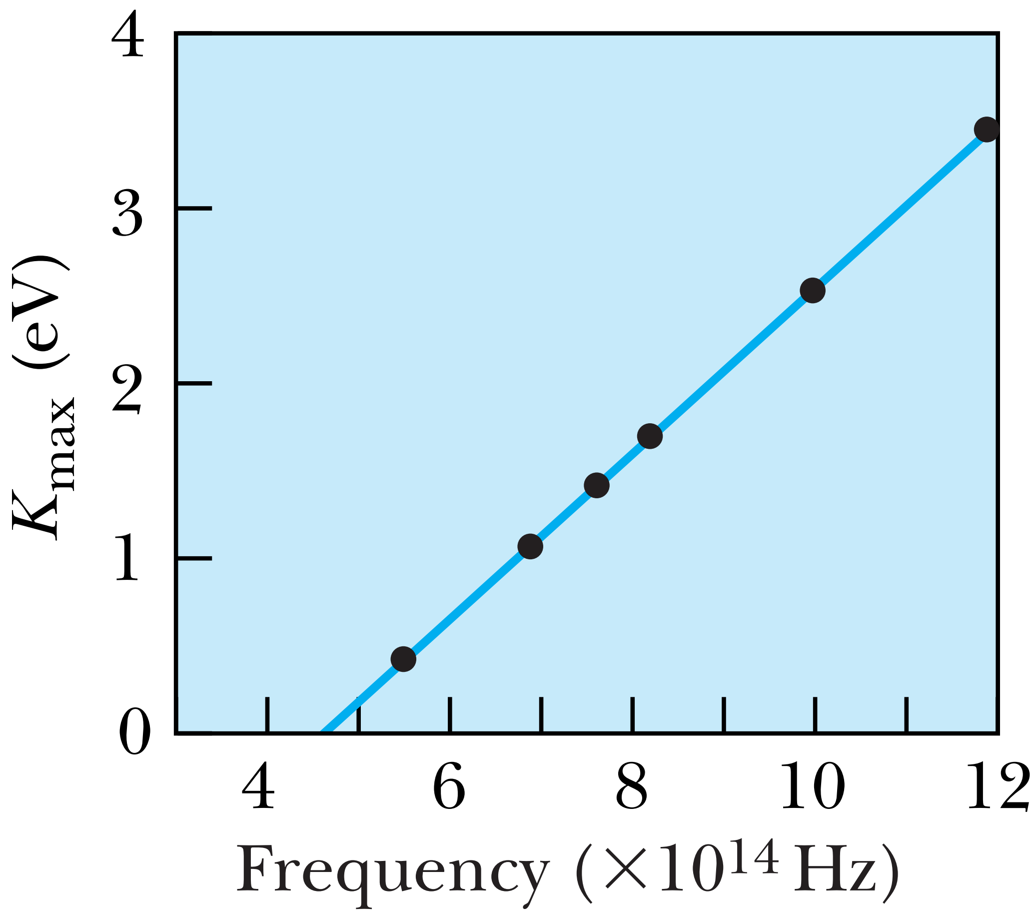
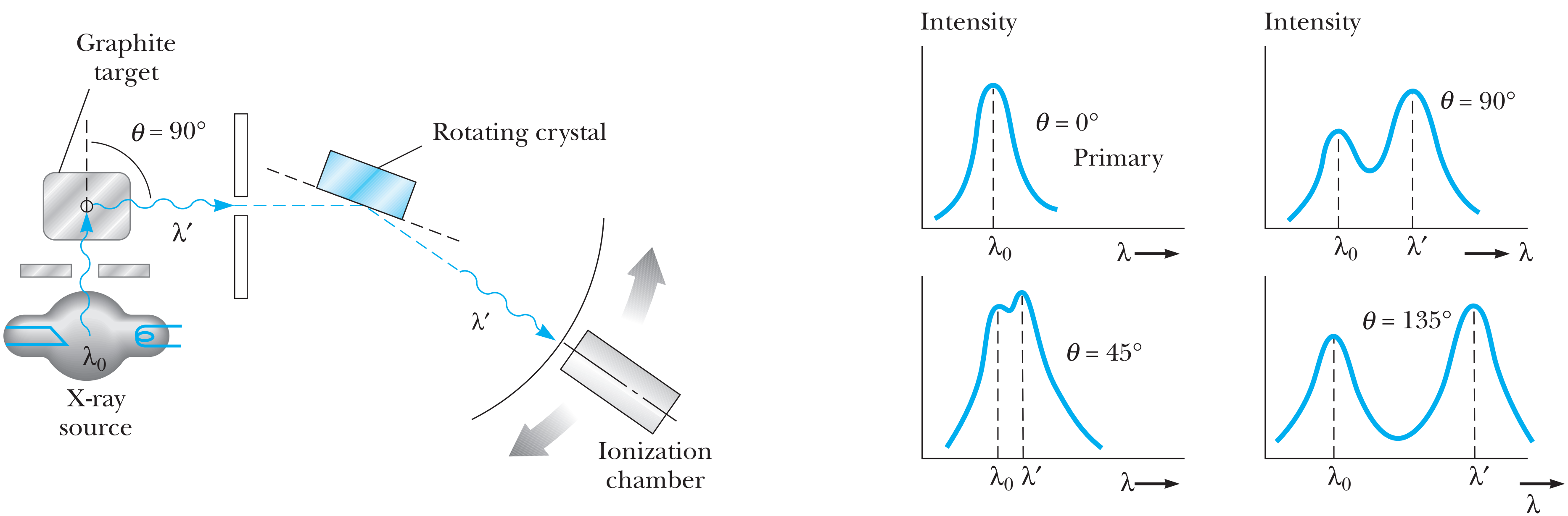
In 1916 Millikan reported data that confirmed Einstein's prediction.



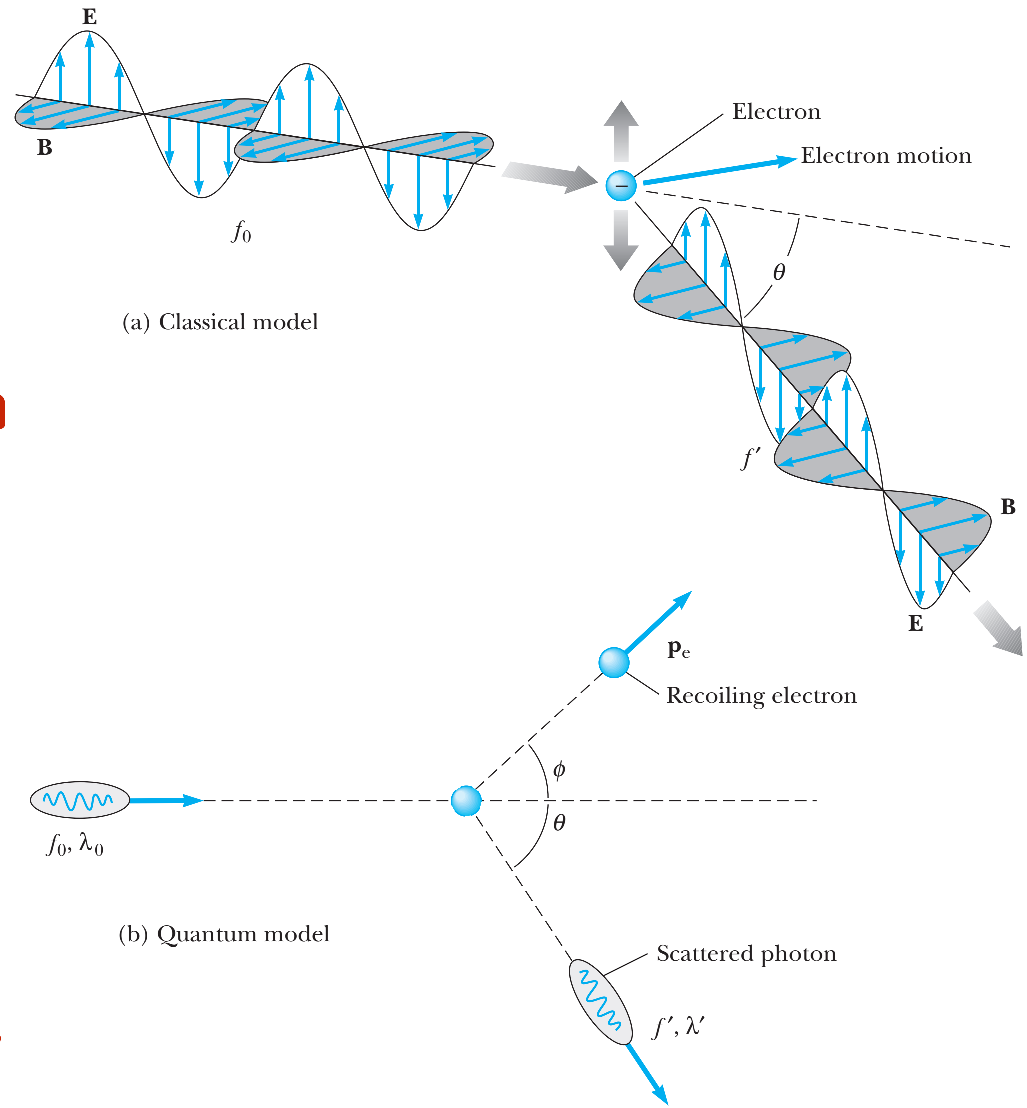
The Compton Effect



The Compton effect was observed in 1923 by Arthur Holly Compton. He demonstrated another experimental observation toward the validation of the particle nature of light.

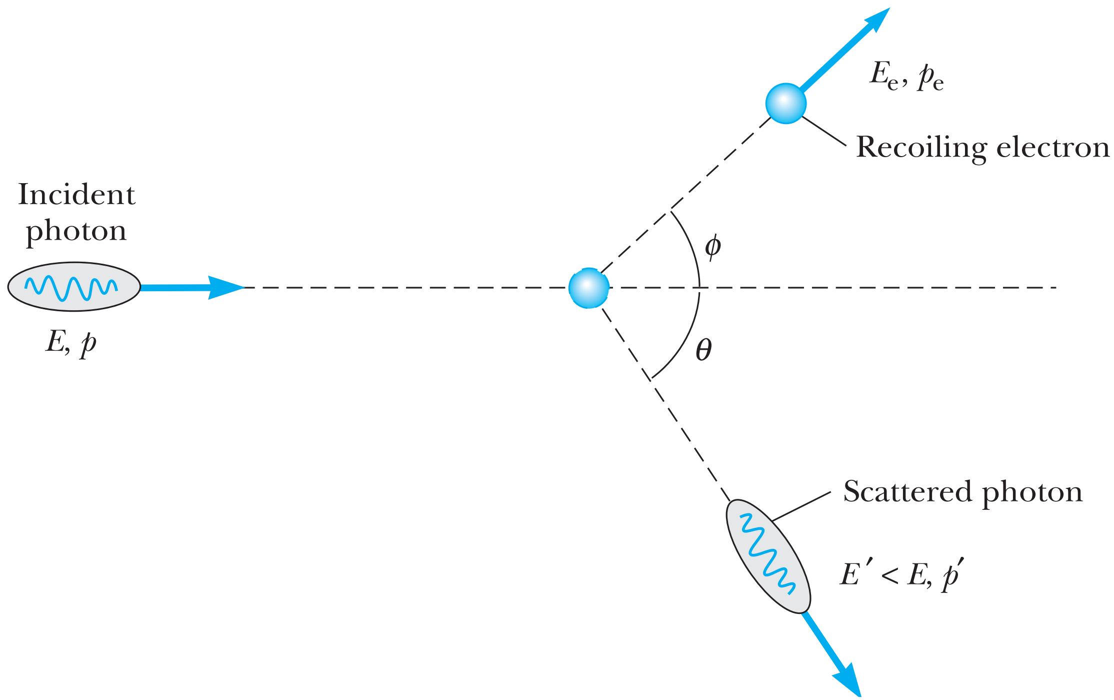
The Compton Effect

In particular, classical theory predicted that incident radiation of frequency f_0 should accelerate an electron in the direction of propagation of the incident radiation, and that it should cause forced oscillations of the electron and reradiation at frequency f', where $f' < f_0$



The Compton Effect

Also, according to classical theory, the frequency or wavelength of the scattered radiation should depend on the length of time. The electron was exposed to the incident radiation as well as on the intensity of the incident radiation.



The expression for conservation of energy gives

$$E + m_e c^2 = E' + E_e$$

where E is the energy of the incident photon, E is the energy of the scattered photon, $m_e c^2$ is the rest energy of the electron, and E_e is the total relativistic energy of the electron after the collision. Likewise, from momentum conservation we have

$$p = p' \cos\theta + p_e \cos\phi$$

$$p' \sin\theta = p_e \sin\phi$$

where p is the momentum of the incident photon, p′ is the momentum of the scattered photon, and p_e is the recoil momentum of the electron.

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The momentum of electron is

$$p_e^2 = (p')^2 + p^2 - 2pp' \cos\theta$$

If we assume that a photon obeys the relativistic expression

$$E^2 = p^2c^2 + m^2c^4$$

and that a photon has a mass of zero, we have

$$p_{\text{photon}} = \frac{E}{c} = \frac{hf}{c} = \frac{h}{\lambda}$$

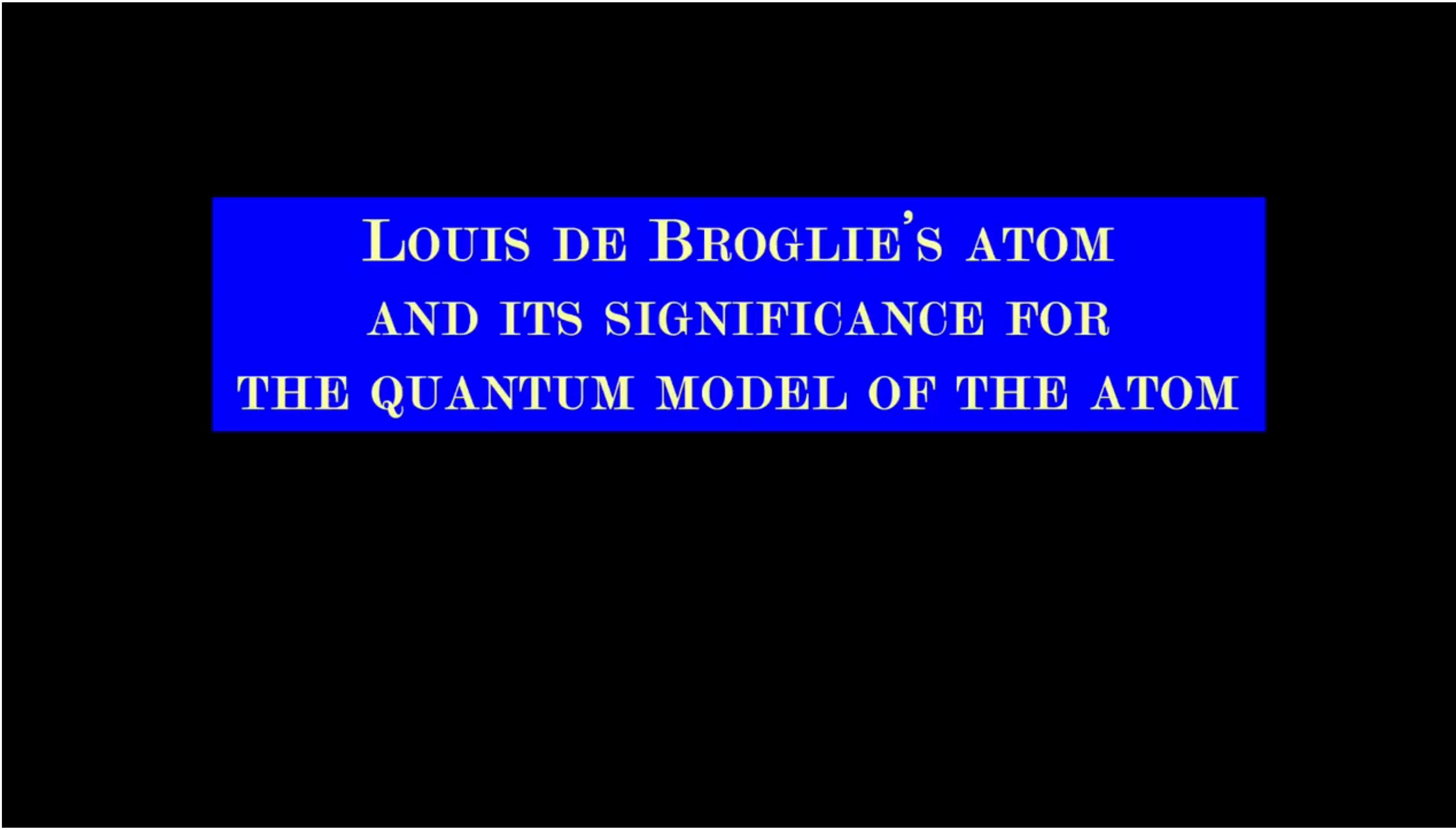
Therefore

$$E_e = hf - hf' + m_e c^2$$

$$\lambda' - \lambda_0 = \frac{h}{m_e c}(1 - \cos\theta)$$

$$p_e^2 = \left(\frac{hf'}{c}\right)^2 + \left(\frac{hf}{c}\right)^2 - \frac{2h^2ff'}{c^2}\cos\theta$$

Wave properties of matter



Wave properties of matter

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1924, De Broglie established the wave properties of particles. His fundamental relationship is the prediction

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

That is, the wavelength to be associated with a particle is given by Planck's constant divided by the particle's momentum. For a photon in Einstein's special theory of relativity

$$E = pc$$

and quantum theory

$$E = h\nu$$

so

$$pc = h\nu = \frac{hc}{\lambda}$$

Wave properties of matter

De Broglie extended this relation for photons to all particles. Particle waves were called matter waves by de Broglie, and the wavelength is now called the de Broglie wavelength of a particle.

Example: Calculate the de Broglie wavelength of

(a) a tennis ball of mass 57 g traveling 25 m/s and

(b) an electron with kinetic energy 50 eV.

Solution:

(a) For the tennis ball $\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34}}{0.057 \times 25} = 4.7 \times 10^{-34}\text{m}$

(b) For the electron

$$\lambda = \frac{h}{p} = \frac{hc}{\sqrt{2mc^2E}} = \frac{1240 \text{ ev} \cdot \text{nm}}{\sqrt{2 \times 0.511 \times 10^6 \times 50 \text{ (eV)}^2}} = 0.17\text{nm}$$

Represent the electron as a standing wave in an orbit around the proton. The condition for a standing wave in this configuration is that the entire length of the standing wave must just fit around the orbit's circumference.

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

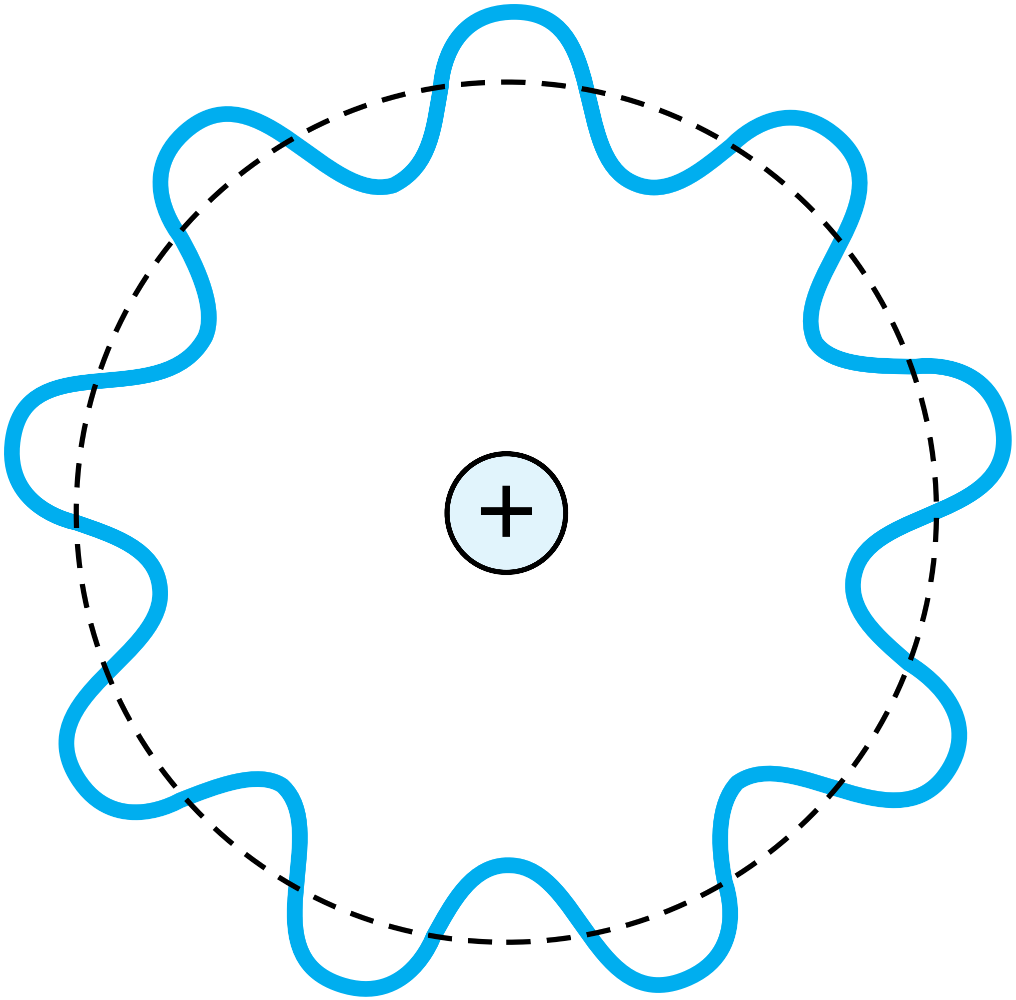
where r is the radius of the orbit. Now we use the de Broglie relation for the wavelength and obtain

$$n\lambda = 2\pi r = n\frac{h}{p}$$

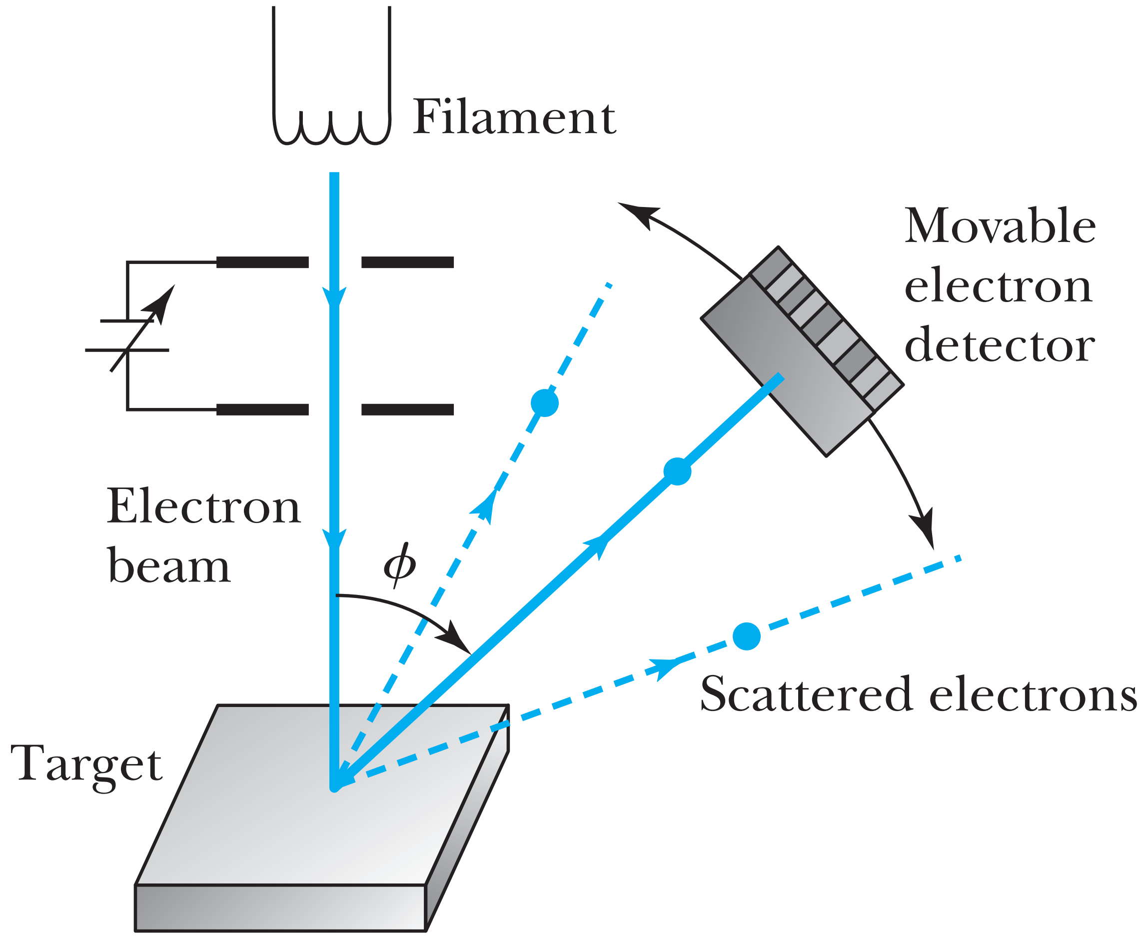
The angular momentum of the electron in this orbit is L=rp, so we have, using the above relation,

$$L = rp = \frac{nh}{2\pi} = n\hbar$$

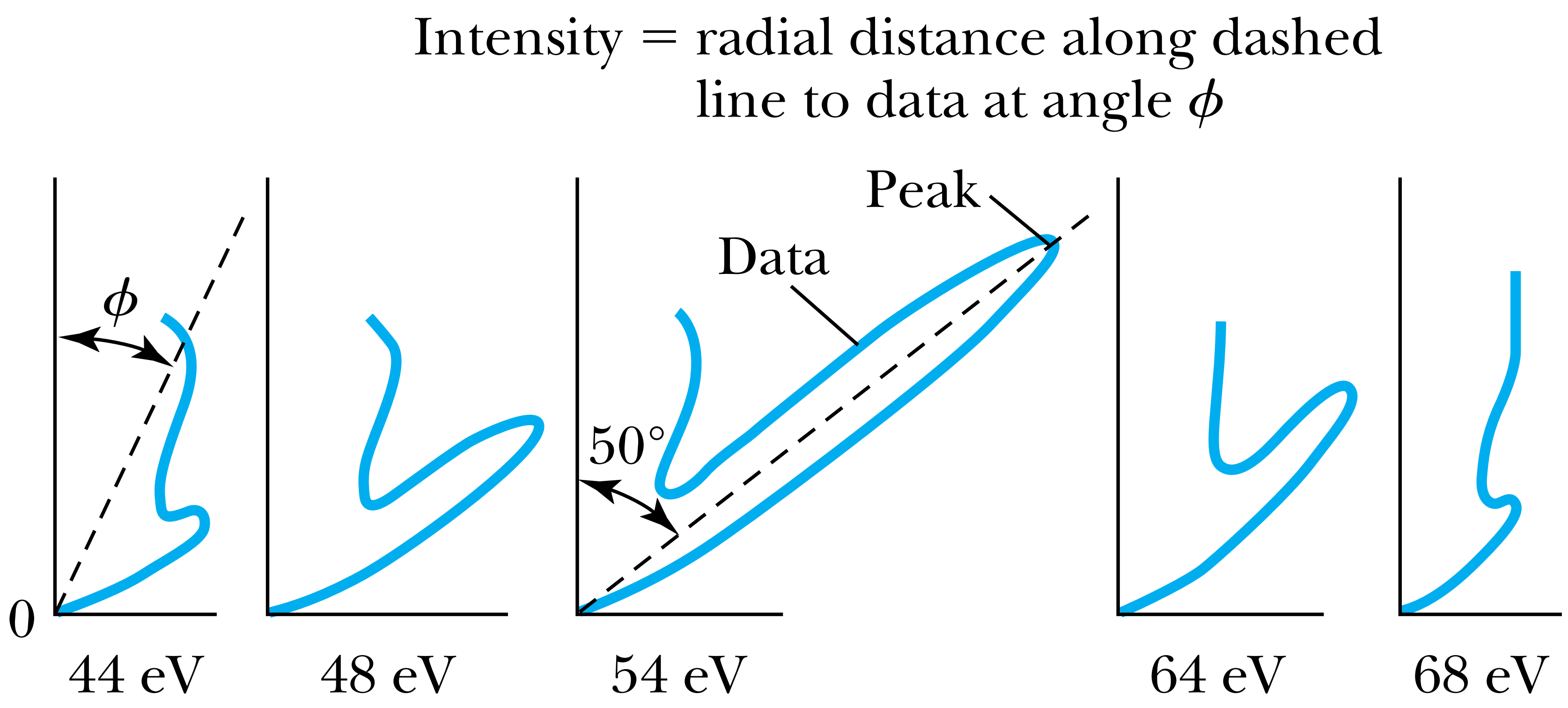
$$\oint p_a \, dq_a = n_a h \ ,$$



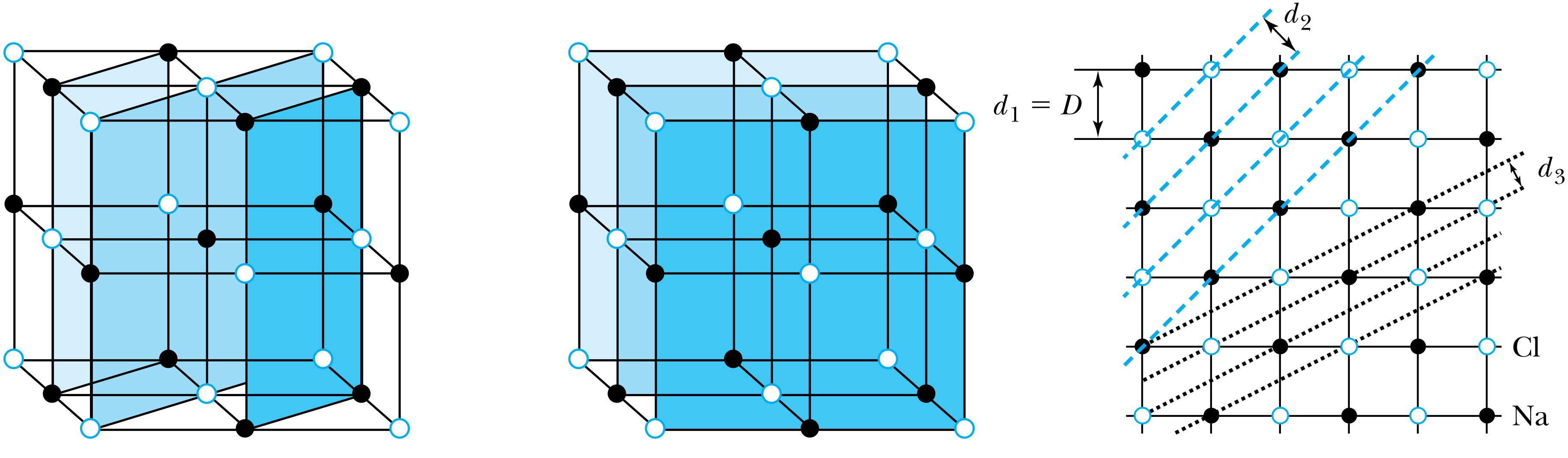
In 1925 a laboratory accident led to experimental proof for de Broglie's wavelength hypothesis by C. Davisson and L. H. Germer.



The relationship between the incident electron beam and the nickel crystal scattering planes is shown



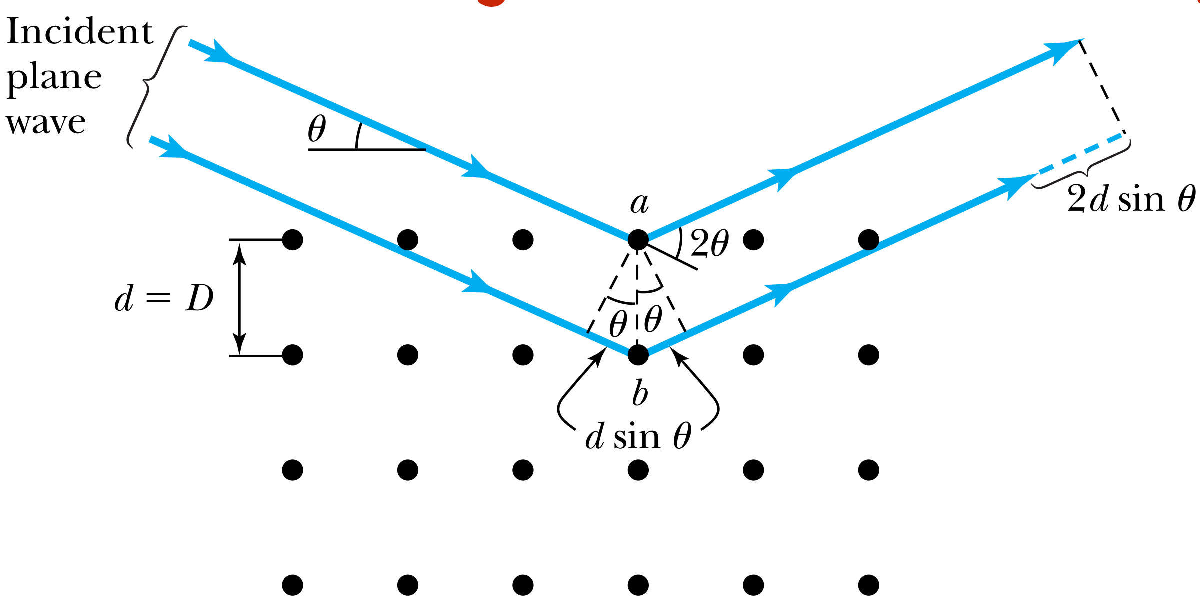
The atoms of crystals like NaCl form lattice planes, called **Bragg planes**. It is possible to have many Bragg planes in a crystal, each with different densities of atoms.



Bragg Law

There are two conditions for constructive interference of the scattered matter wave of electron:

1. The angle of incidence must equal the angle of reflection of the outgoing wave.
2. The difference in path lengths (2d sinθ) shown lower panel must be an integral number of wavelengths.



Bragg's Law with condition 2

$$n\lambda = 2d\sin\theta$$

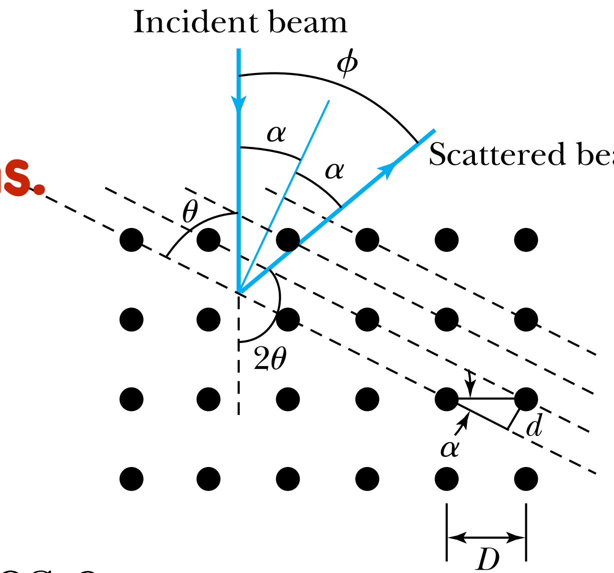
The integer n is called the order of reflection, following the terminology of ruled diffraction gratings in optics.

In the Bragg law, 2θ is the angle between the incident and exit beams. Therefore

$$\phi = \pi - 2\theta = 2\alpha$$

So

$$n\lambda = 2d\cos\alpha = 2D\sin\alpha\cos\alpha$$
$$= D\sin\phi$$



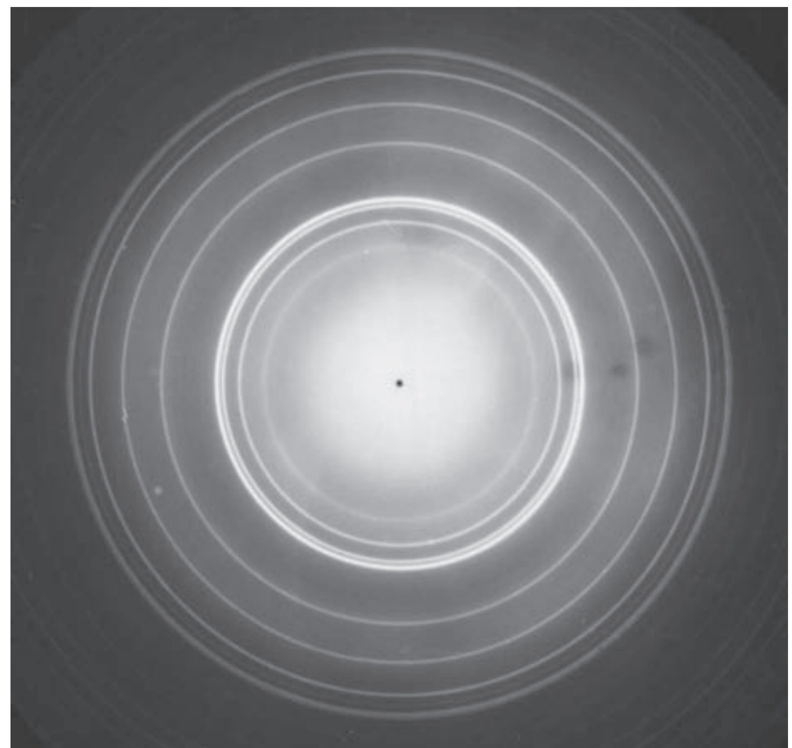
Electron scattering

For nickel the interatomic distance is D=0.215 nm. If the peak found by Davisson and Germer at 50° was n=1, then the electron wavelength should be

$$\lambda = 0.215 \sin(50\pi/180) = 0.165 \text{ nm}$$

Courtesy of David Follstaedt, Sandia National Laboratory

(a)



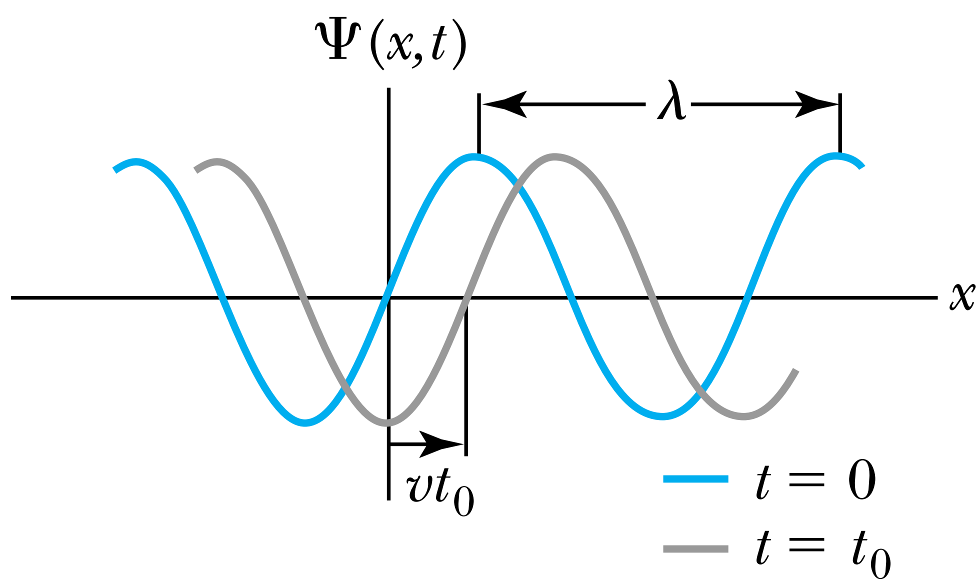
Omikron/Photo Researchers, Inc.

(b)

The simplest form of wave has a sinusoidal form; at a fixed time (say, t=0) its spatial variation looks like

$$\Psi(x,t)|_{t=0} = A\sin\left(\frac{2\pi}{\lambda}x\right)$$

The function $\Psi(x, t)$ represents the instantaneous amplitude or displacement of the wave as a function of position x and time t.



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As time increases, the position of the wave will change, so the general expression for the wave is

$$\Psi(x,t) = A\sin\left[\frac{2\pi}{\lambda}(x - vt)\right]$$

A traveling wave satisfies the wave equation

$$\frac{\partial^2\Psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2\Psi}{\partial t^2}$$

We can write wave function more compactly by defining the wave number k and angular frequency ω by

$$k \equiv \frac{2\pi}{\lambda} = \frac{2\pi}{vT}, \quad \text{and}, \quad \omega = \frac{2\pi}{T}$$

as

$$\Psi(x,t) = A\sin\left[kx - \omega t + \phi\right]$$

Phase constant

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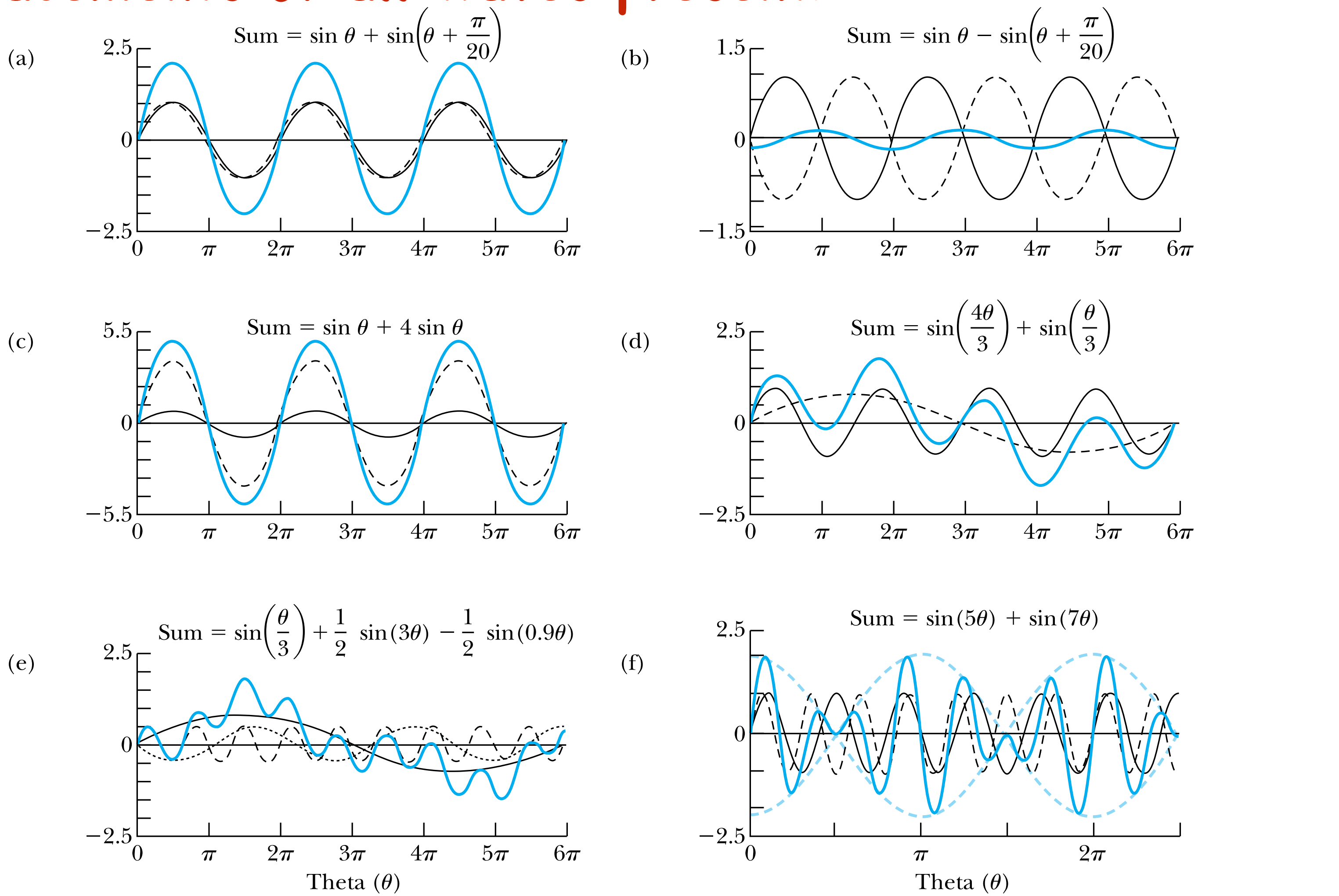
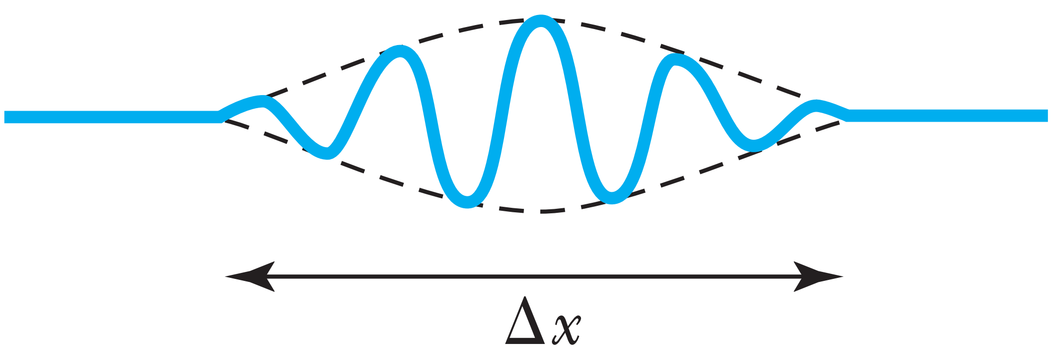
According to the principle of superposition, we add the displacements of all waves present.



If we add many waves of different amplitudes and frequencies in particular ways, it is possible to obtain what is called a wave packet.

The important property of the wave packet is that its net amplitude differs from zero only over a small region Δx



We can localize the position of a particle in a particular region by using a wave packet description

Wave packet

Localized wave packets can be constructed by superposing, in the same region of space, waves of slightly different wavelengths, but with phases and amplitudes chosen to make the superposition constructive in the desired region and destructive outside it. Mathematically, we can carry out this superposition by means of *Fourier transforms*.

We can construct the packet ψ(x,t) by superposing plane waves (propagating along the x -axis) of different frequencies (or wavelengths):

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i(kx-\omega t)} dk;$$

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The simplest form of the angular frequency is when it is *proportional* to the wave number k; this case corresponds to a *nondispersive* propagation.

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ik(x-v_0 t)} dk. \qquad \omega = v_0 k$$

However, since we are interested in wave packets that describe particles, we need to consider the more general case of *dispersive* media which transmit harmonic waves of different frequencies at different velocities. This means that is a *function* of k:

$$\omega = \omega(k)$$

Wave packet

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We can Taylor expand ω(k) about k_0:

$$\begin{aligned}\omega(k) &= \omega(k_0) + (k-k_0)\left.\frac{d\omega(k)}{dk}\right|_{k=k_0} + \frac{1}{2}(k-k_0)^2\left.\frac{d^2\omega(k)}{dk^2}\right|_{k=k_0} + \cdots \\ &= \omega(k_0) + (k-k_0)v_g + (k-k_0)^2\alpha + \cdots\end{aligned}$$

where

$$v_g = \left.\frac{d\omega(k)}{dk}\right|_{k=k_0} \text{ and } \alpha = \frac{1}{2}\left.\frac{d^2\omega(k)}{dk^2}\right|_{k=k_0}$$

Therefore,

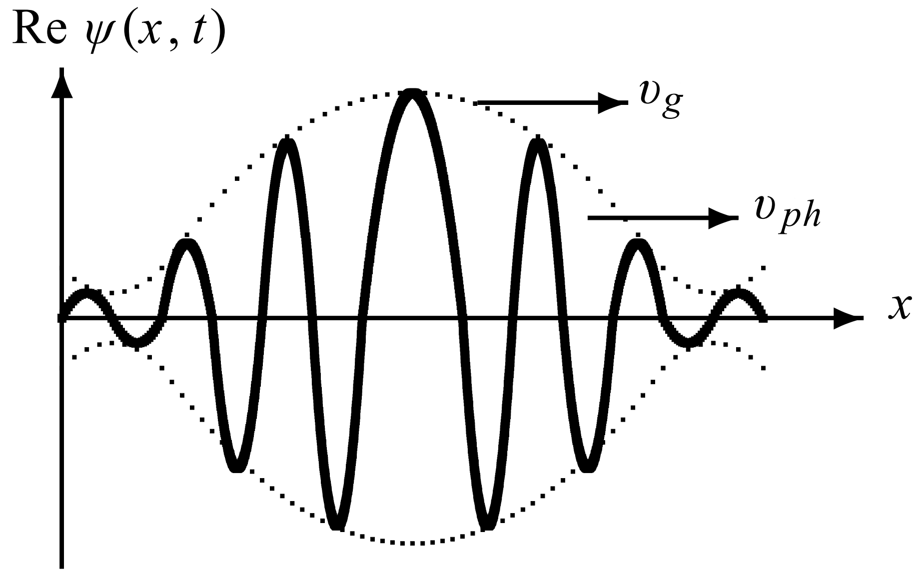
$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} e^{ik_0(x-v_{ph}t)} \int_{-\infty}^{+\infty} g(k-k_0) e^{i(k-k_0)(x-v_g t)} e^{-i(k-k_0)^2\alpha t + \cdots} dk$$

And

$$\boxed{v_g = \frac{d\omega(k)}{dk}, \qquad v_{ph} = \frac{\omega(k)}{k};}$$

v_{ph} and v_g are respectively the *phase* velocity and the *group* velocity.

Wave packet



When we superimpose many waves of different amplitudes and frequencies, we can obtain a wave packet or pulse which travels at the group velocity v_g; the *individual* waves that constitute the packet, however, move with different speeds; each wave moves with its own phase velocity v_{ph}.

The difference between the group velocity and the phase velocity can be understood quantitatively by deriving a relationship between them.

$$v_g = \frac{d\omega}{dk} = v_{ph} + k\frac{dv_{ph}}{dk} = v_{ph} - \lambda\frac{dv_{ph}}{d\lambda},$$

Consider the case of a particle traveling in a *constant potential V*; its total energy is $E=p^2/2m+V$. We can obtain

$$v_g = \frac{dE(p)}{dp}, \qquad v_{ph} = \frac{E(p)}{p},$$

and

$$v_g = \frac{d}{dp}\left(\frac{p^2}{2m}+V\right) = \frac{p}{m} = v_{particle}, \qquad v_{ph} = \frac{1}{p}\left(\frac{p^2}{2m}+V\right) = \frac{p}{2m}+\frac{V}{p}.$$

The group velocity of the wave packet is thus equal to the classical velocity of the particle.

Wave packet

In what follows we want to look at the form of the packet at a given time. Choosing this time to be t=0

$$\psi_0(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} dk,$$

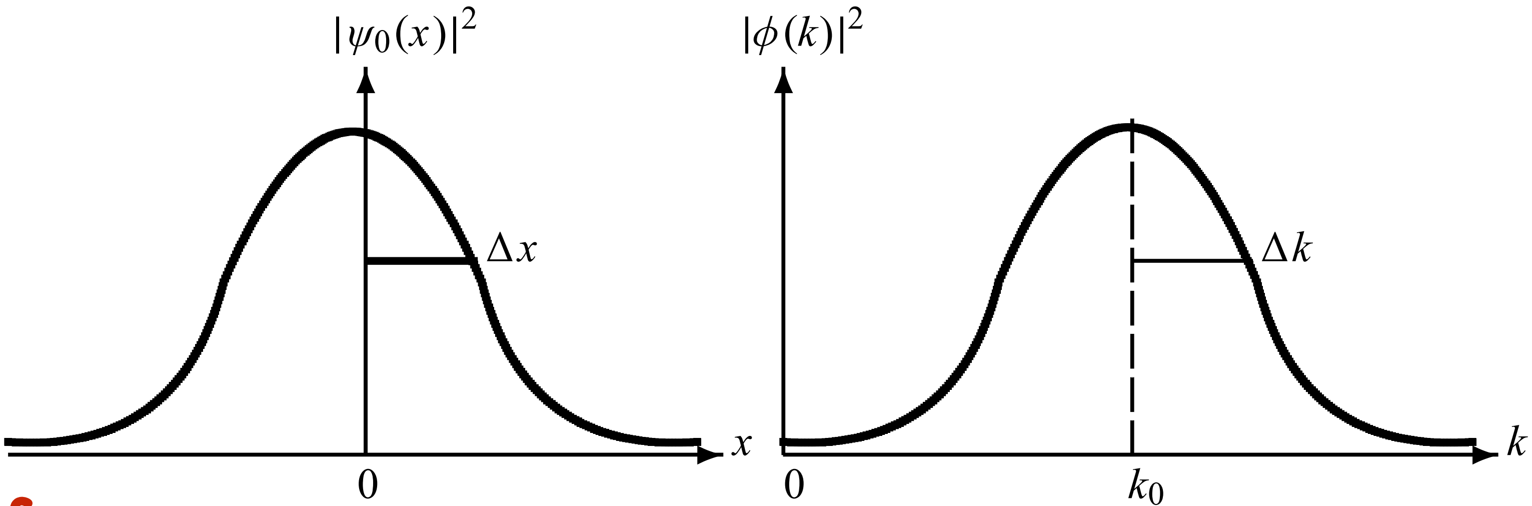
For a Gaussian wave packet

$$\psi_0(x) = \left(\frac{2}{\pi a^2}\right)^{1/4} e^{-x^2/a^2} e^{ik_0 x}, \qquad \phi(k) = \left(\frac{a^2}{2\pi}\right)^{1/4} e^{-a^2(k-k_0)^2/4}.$$

It is convenient to define the half-widths Δx and Δk as corresponding to the half-maxima of packet amplitudes

$$\frac{|\psi(\pm\Delta x,\ 0)|^2}{|\psi(0,\ 0)|^2} = e^{-1/2}, \qquad \frac{|\phi(k_0 \pm \Delta k)|^2}{|\phi(k_0)|^2} = e^{-1/2}.$$

Wave packet



Therefore,

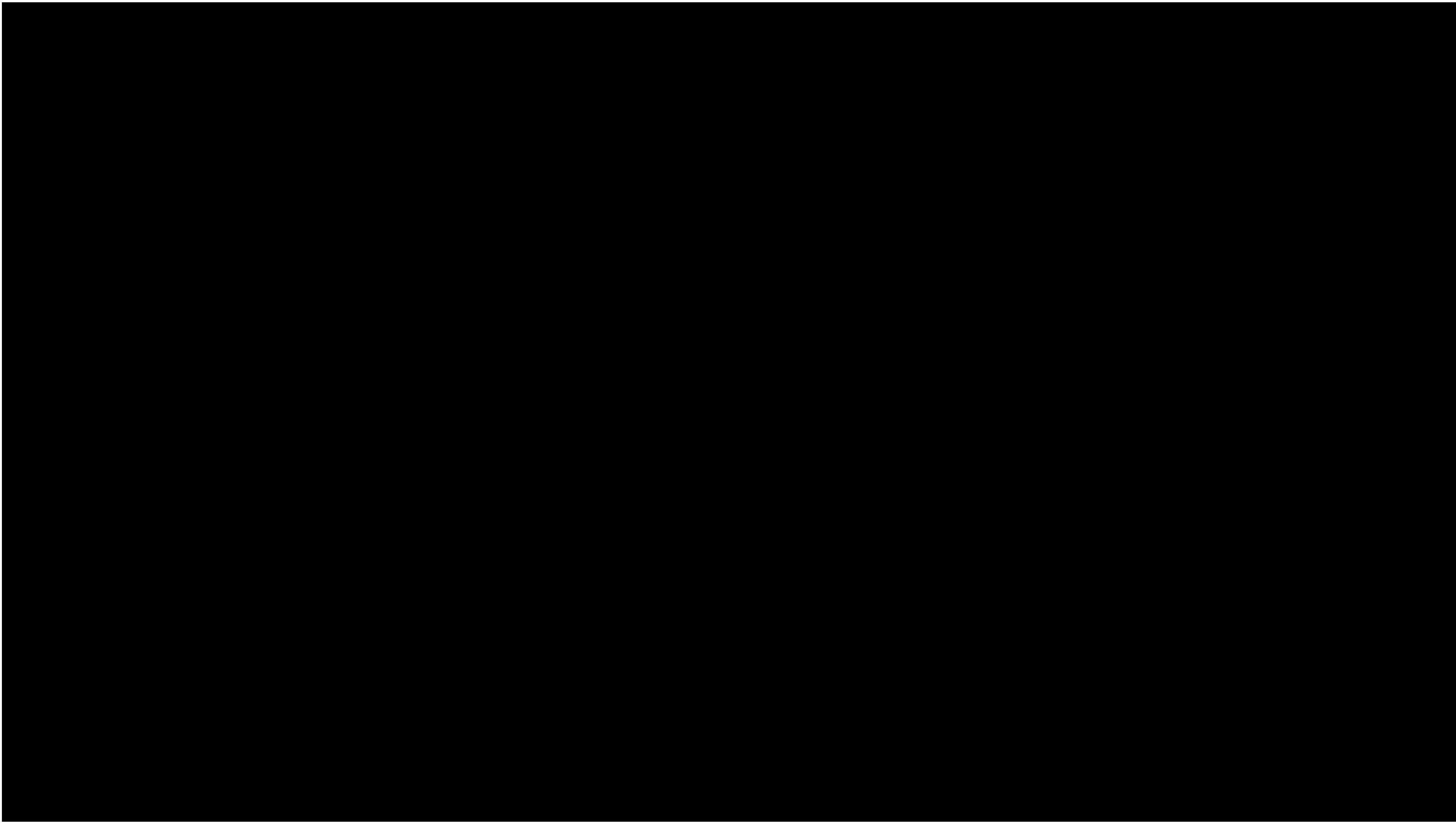
$$\Delta x = \frac{a}{2}, \qquad \Delta k = \frac{1}{a};$$

And

$$\Delta x \, \Delta k = \frac{1}{2}.$$

This relation shows that if the packet's width is narrow in x-space, its width in momentum space must be very broad, and vice versa.

Uncertainty Principle




35
Breaking
56
Bad

We learned that it is impossible to measure simultaneously, with no uncertainty, the precise values of k and x for the same particle. The wave number k may be rewritten as

$$k = \frac{p}{\hbar}$$

in the case of the Gaussian wave packet,

$$\Delta p \Delta x = \frac{\hbar}{2}$$

Heisenberg's uncertainty principle can therefore be written

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

It is possible to have a greater uncertainty in the values of p_x and x, but it is not possible to know them with more precision than allowed by the uncertainty principle.

The Gaussian wave packet yields an *equality*, not an *inequality* relation. It is the *lowest limit* of Heisenberg's inequality. As a result, the Gaussian wave packet is called the *minimum uncertainty* wave packet. All other wave packets yield higher values for the product of the x and p uncertainties:

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

We have now seen how the wave packet concept offers a heuristic way of deriving Heisenberg's uncertainty relations; a more rigorous derivation is given later.

Uncertainty Principle

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Consider a particle for which the location is known within a width of l along the x axis. The uncertainty principle specifies that Δp is limited by

$$\Delta p \geq \frac{\hbar}{2\Delta x} \geq \frac{\hbar}{l}$$

the minimum value of the kinetic energy ,

$$E_{\min} = \frac{p_{\min}^2}{2m} \geq \frac{(\Delta p)^2}{2m} \geq \frac{\hbar^2}{2ml^2}$$

Note that this equation indicates that if we are uncertain as to the exact position of a particle, for example, an electron somewhere inside an atom of diameter l, the particle can't have zero kinetic energy.

Electron Double-Slit Experiment

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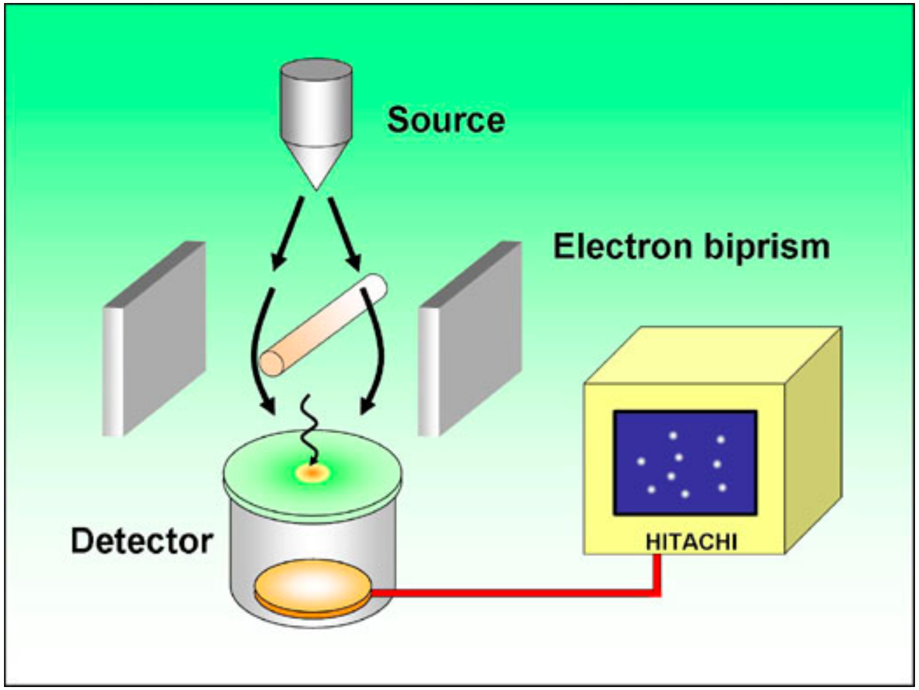
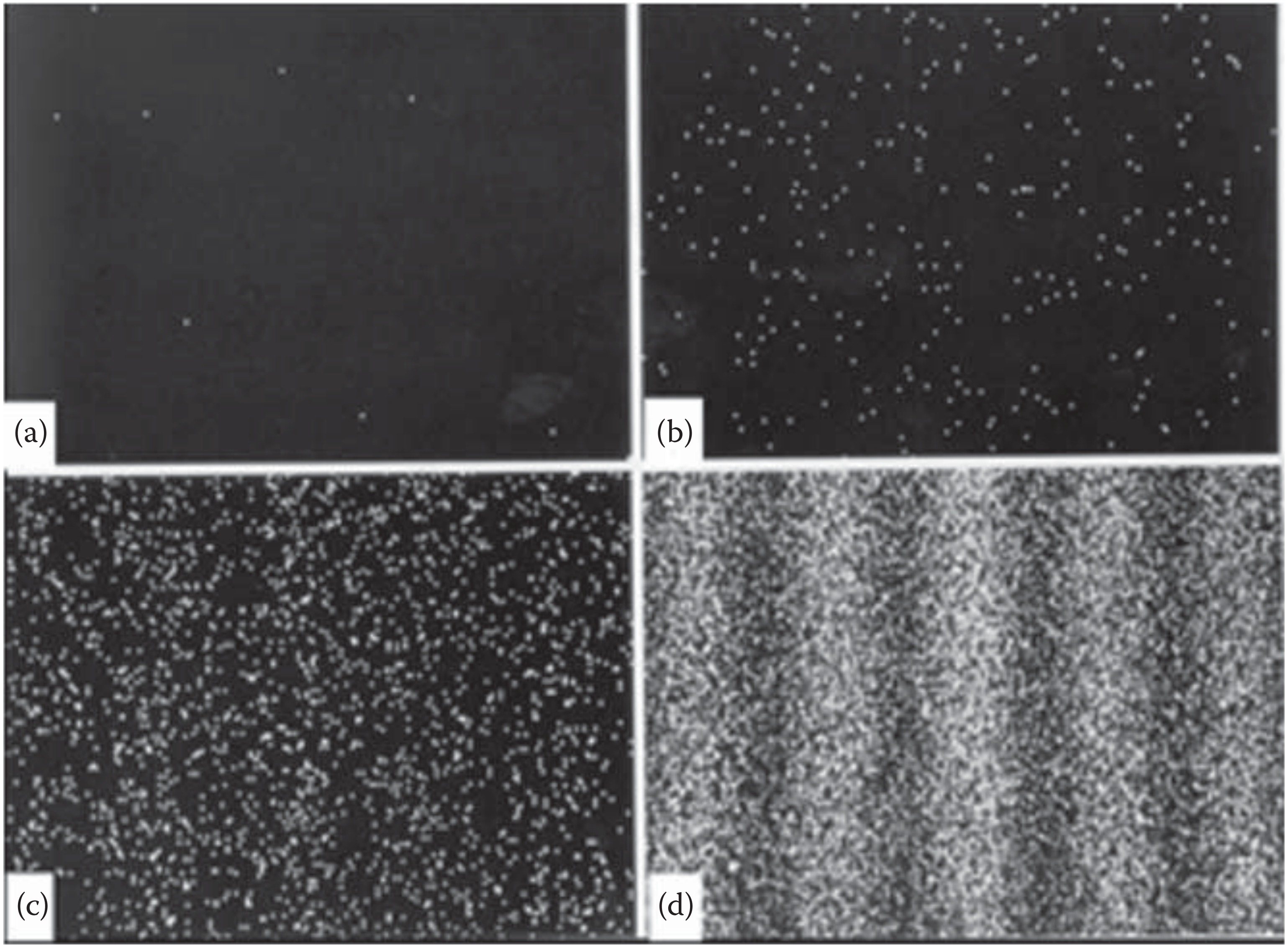
In 1989, a team led by Akira Tonomura at Hitachi performed a double slit experiment. For this experiment, each single electron passed through a single slit one at a time and arrived at the screen of a detector as a single particle as a "dot."



https://www.hitachi.com/rd/research/materials/quantum/doubleslit/index.html

Electron Double-Slit Experiment

Electron Double-Slit Experiment



Electron Double-Slit Experiment

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Particle double-slit experiment

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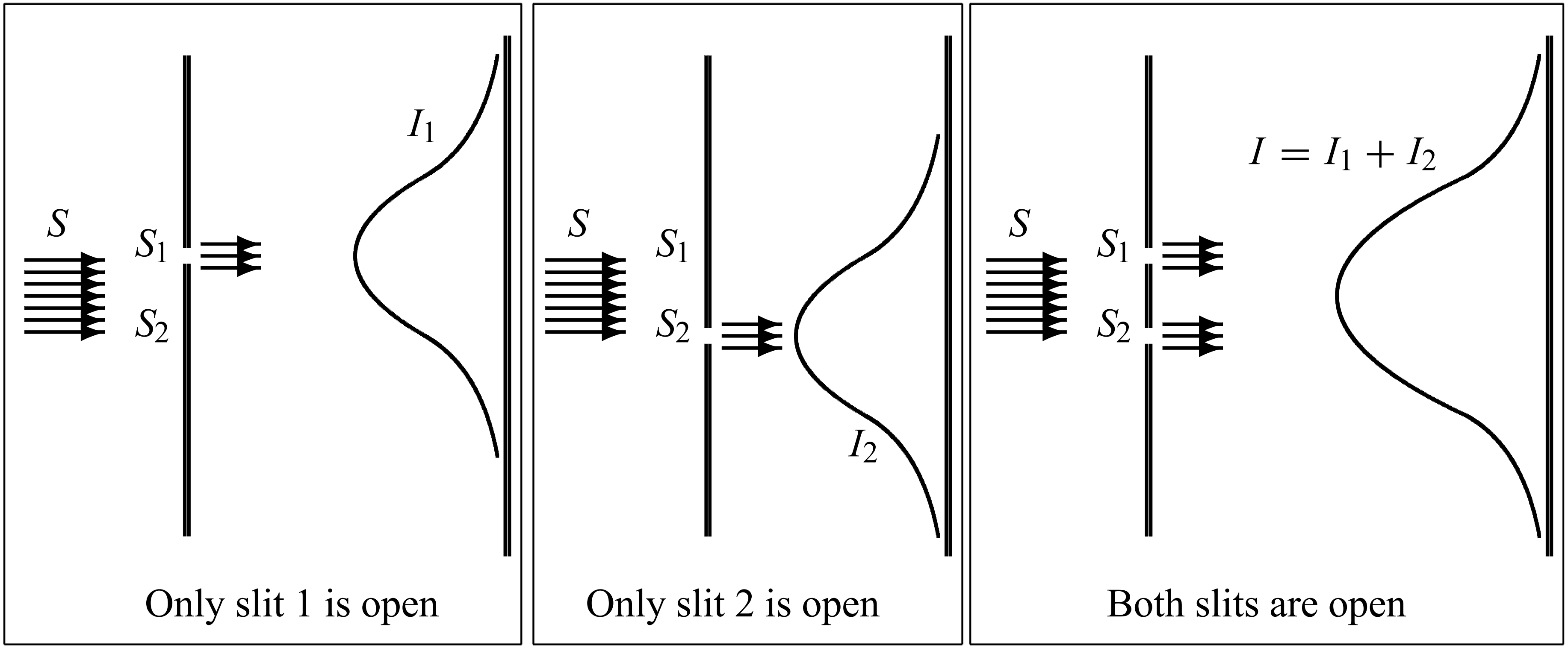
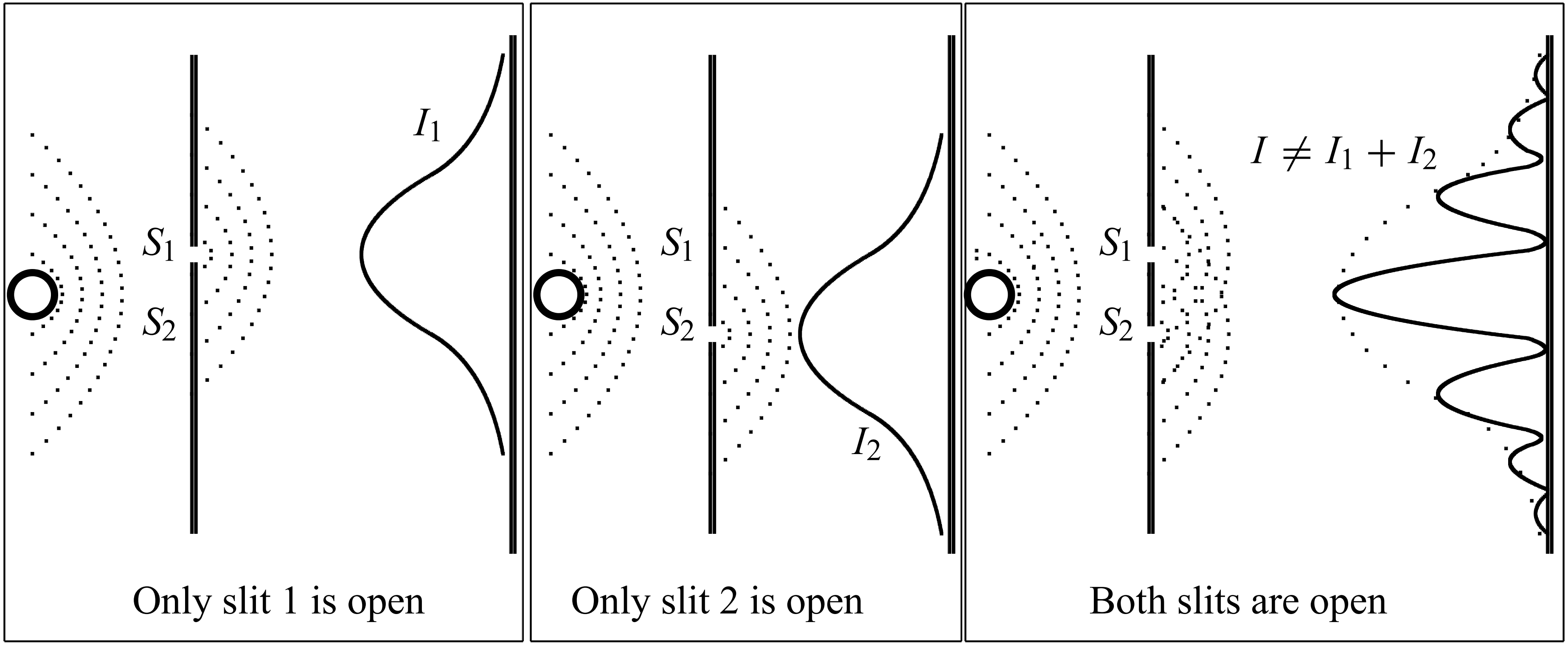
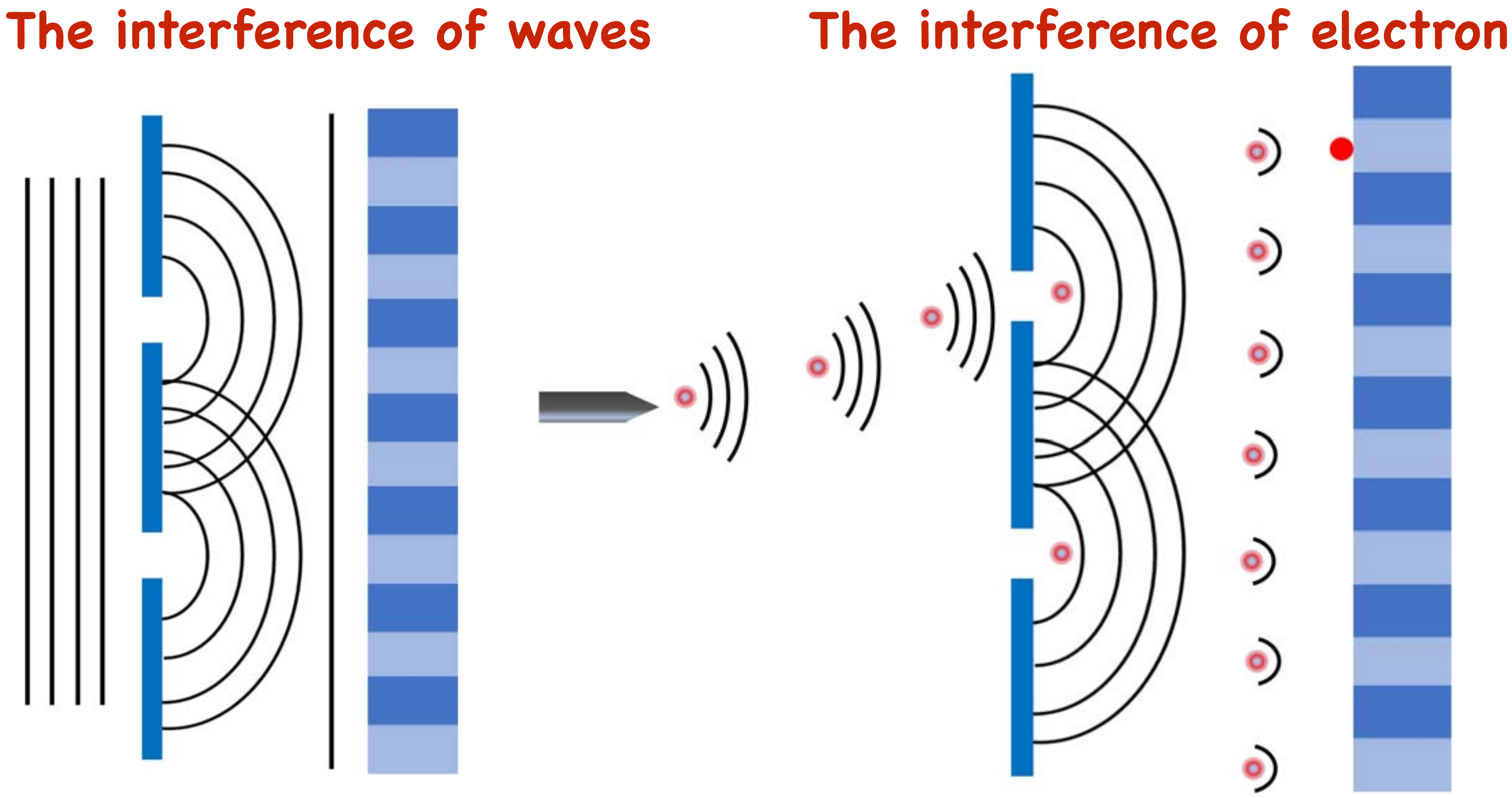
$$I = I_1 + I_2.$$



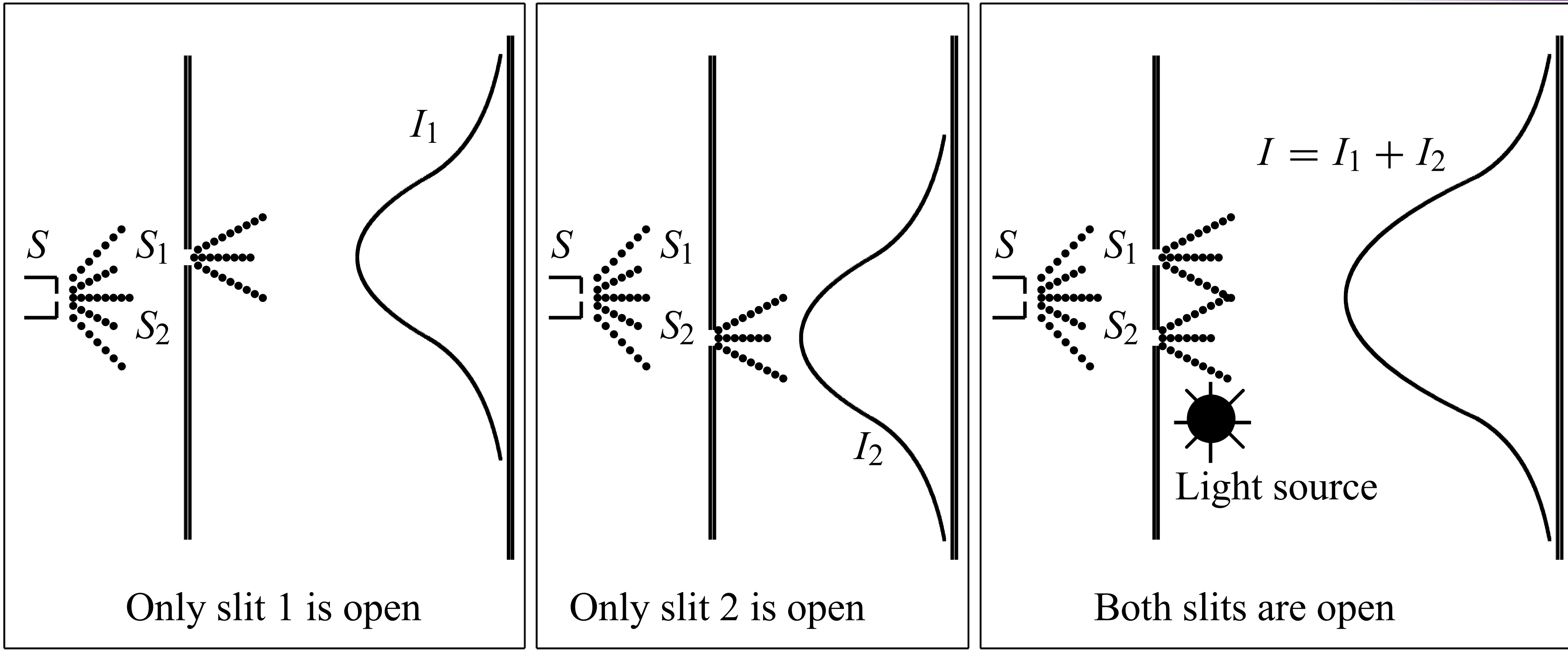
Wave double-slit experiment



Electron Double-Slit Experiment



Electron Double-Slit Experiment



It is impossible to design an apparatus which allows us to determine the slit that the electron went through without disturbing the electron enough to destroy the interference pattern.

Consider the interference of classic waves, for a wave entering slit 1, the mathematical function that describes such a wave is:

$$f_1(r, t) = A_1 e^{i(k_1 r - \omega t + \phi_1)}$$

where A_1 is the amplitude of the wave and ω is the angular frequency, k_1 is the wave vector. Similarly, the wave entering through slit 2 can be described as:

$$f_2(r, t) = A_2 e^{i(k_2 r - \omega t + \phi_2)}$$

The corresponding intensities of the two waves are the absolute squares of the above functions, and thus:

$$I_1 = |A_1|^2, \quad I_2 = |A_2|^2$$

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After entering slit 1 and slit 2, these two waves superpose on each other:

$$f(r,t) = A_1 e^{i(k_1 r - \omega t + \phi_1)} + A_2 e^{i(k_2 r - \omega t + \phi_2)}$$

and as a result their intensities sum as follows:

$$I_{12} = |f(r,t)|^2 = |A_1|^2 + |A_2|^2 + 2A_1A_2\cos\theta$$

where

$$\theta = (k_1 - k_2)\cdot r + (\phi_1 - \phi_2)$$

Such that:

$$I_{12} \neq I_1 + I_2$$

The total intensity reaches maxima of constructive interference, when:

$$\theta = 0,\ \pm 2\pi,\ \pm 4\pi,\ \ldots\ldots$$

Electron Double-Slit Experiment

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The wave function of an electron that has matter wave associated with it is a complex function and very similar to the function of classical wave

$$\psi_1(r, t) = B_1 e^{i(k_1 r - \omega t + \phi_1)}$$

The above equation describes the wave function of the electron entering through slit 1. Here B_1 is not the amplitude of the intensity of the matter wave of the electron, but rather is referred to as the "probability amplitude."

We used a function $\Psi(r, t)$ named as wave function to denote the superposition of many waves to describe the wave packet. The quantity

$$P_1(r) = |\,\psi_1(r, t)|^2$$

is called the probability density and represents the probability of finding the particle in a given unit volume at a given instant of time

Postulate 1:

The wavefunction attempts to describe a quantum mechanical entity through its spatial location and time dependence

The wave function for the electron entering through slit 2 is:

$$\psi_2(r, t) = B_2 e^{i(k_2 r - \omega t + \phi_2)}$$

where

$$P_2(r) = |\psi_2(r, t)|^2$$

is the corresponding probability density. The probability densities of the electrons that have entered through slit 1 or slit 2 are:

$$|\psi_1|^2 = |B_1|^2, \quad |\psi_2|^2 = |B_2|^2$$

The probability distribution, which is also called the probability density of the electrons must be the sum of these probability densities. Thus:

$$|\psi_1|^2 + |\psi_2|^2 = P_{12}$$

However, if the probability densities add up in this way then there will be no observation of the interference of the probability distribution. In such a scenario, only two spots would be observed on the screen with no interference pattern. This is the same pattern that described above for particles.

Since the specific slit through which the electron has entered is not known, the wave function of the electron entering through the double slit will be the sum of the functions above. The superimposed wave function is:

$$\Psi(r) = \psi_1(r) + \psi_2(r)$$

and the probability densities of the electron add up in the same manner as waves as defined by the following relation:

$$|\Psi(r)|^2 = |\psi_1 + \psi_2|^2 = |B_1|^2 + |B_2|^2 + 2\,|B_1||B_2|\cos\theta$$

This equation describes the probability distribution of the electron on the screen, and the third term is very similar to the interference term of wave. This term causes uncertainty about where the electron will arrive on the screen. The probability distribution of the electrons has the interference pattern of maxima and minima as a result of this term.

Consider the motion of a free particle along the x-axis with momentum p. According to de Broglie's hypothesis, a wave of $\lambda = h/p$ is associated with the particle and hence we can assume a wave function $\psi(x,t)$ given by:

$$\psi(x,t) = Ae^{(kx-\omega t)}$$

The hypotheses of Planck and de Broglie suggest that $E = h\nu = \hbar\omega$ and $p = h/\lambda = \hbar k$. Therefore:

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

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On partial differentiation of above equation with respect to x and t, we obtain:

$$\frac{\partial\psi(x,t)}{\partial x} = \frac{ip}{\hbar}\psi(x,t) \longrightarrow \left[\frac{\partial}{\partial x} - \frac{ip}{\hbar}\right]\psi(x,t) = 0$$

$$\frac{\partial\psi(x,t)}{\partial t} = \frac{-iE}{\hbar}\psi(x,t) \longrightarrow \left[\frac{\partial}{\partial t} + \frac{iE}{\hbar}\right]\psi(x,t) = 0$$

They suggest that

$$p = -i\hbar\frac{\partial}{\partial x} \qquad\qquad E = i\hbar\frac{\partial}{\partial t}$$

For a non-relativistic free particle, we get

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

which is the Schrödinger equation for a free particle moving along the x-axis.

For a free particle moving along an arbitrary direction, the Schrödinger equation can be generalized to:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\psi(x,t)=i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

$$\longrightarrow -\frac{\hbar^2}{2m}\nabla^2\psi(x,t)=i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

For a particle moving under the influence of a field characterized by potential energy, V(r) , the Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(r)\right]\psi(x,t)=i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

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The linear combination of the wave function will also be the solution of Schrödinger equation

Therefore:

$$\psi(x,t)=\int A(k)e^{i(kx-\omega t)}\,dk$$

It means group of waves having different k-values. The group of waves is known as a wave packet. Each k corresponds to a wave and in principle, k can take any value in between $-\infty$ and ∞.

Hamilton–Jacobi equation

$$\frac{\partial S}{\partial t} + H(q, p, t) = 0$$

with

$$p_i = \partial S / \partial q_i,\ i = 1, \ldots s,$$

and S is the action with variable endpoint

$$S(q, t) = \int_{t_0}^{t} L(\tilde{q}, \dot{\tilde{q}}, \tilde{t}) d\tilde{t}$$

and the Hamiltonian can be written as

$$H(q, p, t) = \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L(q, \dot{q}, t)$$

For systems with constant energy E we can separate the time t from the coordinates q in the action as

$$S(q,t) = W(q) - Et$$

The momentum vector

$$\vec{p} = \nabla S = \nabla W$$

As a very simple example we solve here the problem for a free particle in 1-D. The Hamilton-Jacobi equation in that case is

$$\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 = -\frac{\partial S}{\partial t}$$

A separation ansatz with

$$S = W(x) - Et$$

gives

$$\left(\frac{\partial W}{\partial x}\right)^2 = \alpha^2 = \text{const}$$
$$-2mE = \alpha^2$$

with a constant α which (from the last equation) can obviously be chosen to be the momentum p of the particle. From the first equation we get

$$S = px - \frac{p^2}{2m}t + \text{const}$$

The Schrödinger Equation from action

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Without further proof we generalize the result to free particles in 3 dimension. The action in this case is

$$S = \vec{p}\cdot\vec{r} - Et$$

which is similar with the solution of classical wave

$$e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

Therefore, Schrödinger assume that the wave function of matter wave is

$$\psi = \exp\left[\frac{S}{K}\right]$$

and

$$\vec{\nabla}^2\psi - \frac{2m_{\rm e}}{K^2}(E-V)\psi = 0 \qquad\qquad K \to -i\hbar$$

Postulate 2:

The time-dependent Schrödinger equation governs the time evolution of a quantum mechanical system

The time-dependent Schrödinger equation, for a particle moving under the influence of a field defined by potential energy, V(r), is given

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})\right]\psi(\mathbf{r},t)=i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}$$

In the Schrödinger representation of quantum mechanics, the Hamiltonian,

$$H=-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})$$

Therefore, the Schrödinger equation can be written as

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=H\psi(\mathbf{r},t)$$

The Probability Density

Probability density is defined as

$$P = \left|\psi(\mathbf{r},t)\right|^2$$

Then charge density is given by $\rho = qP$, where q is charge on the particle. We have:

$$\frac{\partial P}{\partial t} = \frac{\partial\left|\psi\right|^2}{\partial t} = \frac{\partial}{\partial t}\left(\psi^*\psi\right) = \frac{\partial\psi^*}{\partial t}\psi + \psi^*\frac{\partial\psi}{\partial t}$$

The complex conjugation of Schrödinger equation is

$$-i\hbar\frac{\partial\psi^*(\mathbf{r},t)}{\partial t} = H^*\psi^*(\mathbf{r},t)$$

Therefore

$$\frac{\partial P}{\partial t} = \frac{1}{i\hbar}\left[\psi^*(H\psi) - (H\psi)^*\psi\right]$$

The Probability Density

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If V(r) is real, we then get:

$$\frac{\partial P}{\partial t} = \frac{1}{i\hbar}\left[-\psi^* \frac{\hbar^2}{2m}\left(\nabla^2\psi\right) + \psi^* V(\mathbf{r})\psi + \frac{\hbar^2}{2m}\left(\nabla^2\psi^*\right)\psi - \psi V(\mathbf{r})\psi^*\right]$$

$$= \frac{1}{i\hbar}\left[-\psi^* \frac{\hbar^2}{2m}\left(\nabla^2\psi\right) + \frac{\hbar^2}{2m}\left(\nabla^2\psi^*\right)\psi\right]$$

$$= -\frac{i\hbar}{2m}\nabla.\left[\psi\nabla\psi^* - \psi^*\nabla\psi\right]$$

which yields:

$$\frac{\partial P}{\partial t} + \frac{i\hbar}{2m}\nabla.\left[\psi\nabla\psi^* - \psi^*\nabla\psi\right] = 0$$

$$\Rightarrow \frac{\partial P}{\partial t} + \nabla.\mathbf{S} = 0$$

with

$$\mathbf{S} = \frac{i\hbar}{2m}\left[\psi\nabla\psi^{*} - \psi^{*}\nabla\psi\right]$$

S is called probability current, describing the flow of probability. This also implies:

$$\partial\rho / \partial t + \nabla.\mathbf{J} = 0$$

Here, we have defined current density J=S. This equation is a well-known continuity equation.

To understand more about probability current, let us consider a system completely confined to a volume V so that nothing is going in and out at the surface.

The Probability Density

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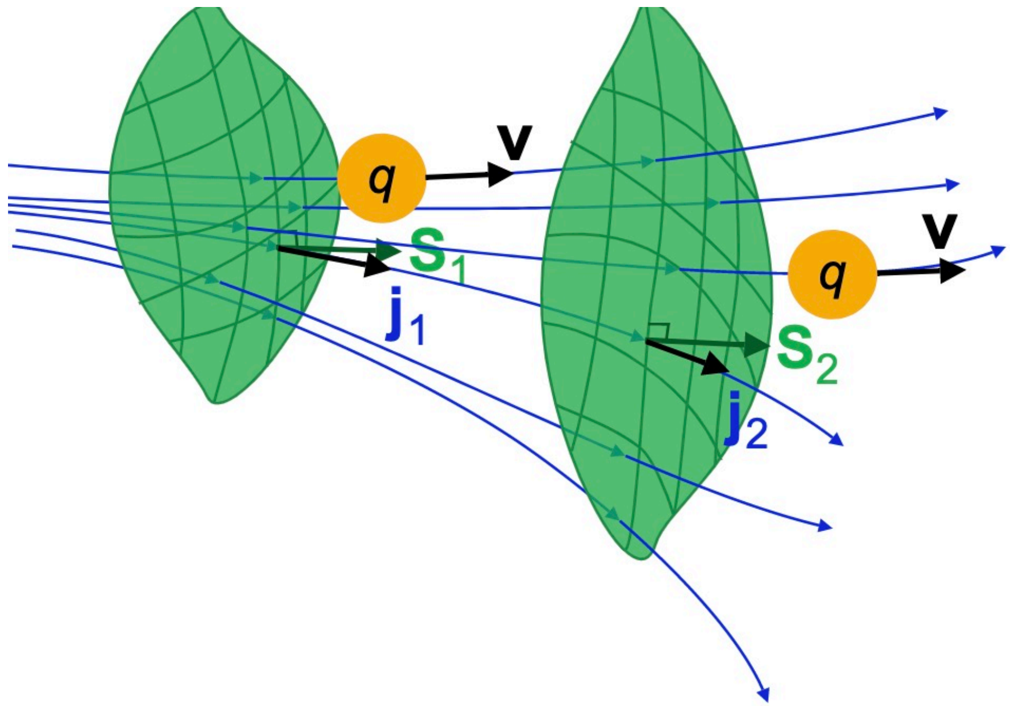
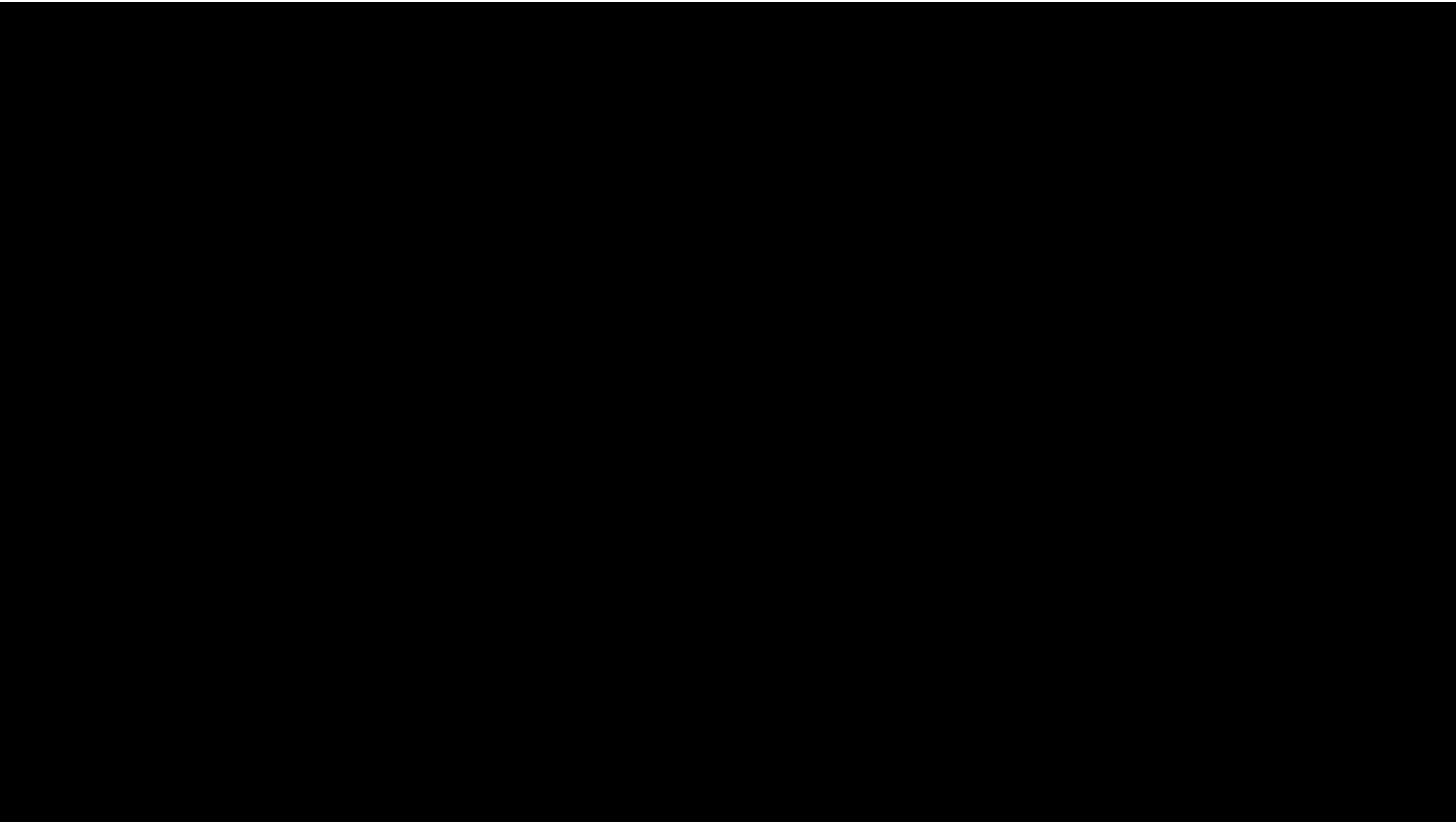


$$\frac{dq}{dt} + \oiint_S \mathbf{j} \cdot d\mathbf{S} = \Sigma$$

The Probability Density



The Probability Density

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On integrating both terms of the equation over the entire volume, we get:

$$\oint\left(\frac{\partial P}{\partial t}+\nabla.\mathbf{S}\right)d^3\mathrm{r}=0$$

$$\Rightarrow\oint\frac{\partial P}{\partial t}d^3r=-\oint\nabla.\mathbf{S}d^3r=-\oint\mathbf{S}.d\mathbf{s}$$

where, we used the Gauss theorem to convert volume integration to surface integration.

In this case, because we confined to system completely in the volume, there is nothing at the surface and therefore

$$\oint\mathbf{S}.d\mathbf{s}=0$$

On interchanging the order of the volume integral and the time derivative over P, we write;

$$\frac{\partial}{\partial t}\oint P d^3 r = 0$$

which states that

$$\oint P d^3 r$$

is constant or a conserved quantity. Actually, S(r) and P(r) are the current and density, respectively, of a conserved quantity.

The definition of probability density allows us to calculate expectation value of an observable (operator).

Exercises

1. According to displacement law, the wavelength of maximum thermal energy from a body at temperature "T" is mathematically described as, $\lambda_{max} T = 2.898 \times 10^{-3}$ m.K. For a human body at a temperature of about 21 °C, the wavelength of the thermal radiation emitted:

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1. According to displacement law, the wavelength of maximum thermal energy from a body at temperature "T" is mathematically described as, $\lambda_{max}T = 2.898\times10^{3}$ m.K. For a human body at a temperature of about 21 °C, the wavelength of the thermal radiation emitted:

$$\lambda_{\max} = \frac{2.898 \times 10^{-3}\ \mathrm{m.K}}{294\ \mathrm{K}}$$

$$\lambda_{\max} = 10.0 \times 10^{-6}\ \mathrm{m}$$

Thus, the wavelength of thermal radiation emitted by human body is about 10 microns.

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2. A light with a wavelength of about 10^{-7}m strikes a potassium metal plate (whose work functions is 2.2 eV). Determine the velocity of the photoelectrons released from the plate.

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2. A light with a wavelength of about 10^{-7}m strikes a potassium metal plate (whose work functions is 2.2 eV). Determine the velocity of the photoelectrons released from the plate.

$$\frac{1}{2}m_e v_e^2 = \frac{hc}{\lambda} - \phi$$

$$v_e = \sqrt{\frac{2}{m_e}\left(\frac{hc}{\lambda} - \phi\right)}$$

$$= \sqrt{\frac{2}{0.91 \times 10^{-30}\,\mathrm{kg}}\left(\frac{6.63 \times 3 \times 10^{-26}\,\mathrm{m.J}}{10^{-7}\,\mathrm{m}} - 2.2 \times 1.6 \times 10^{-19}\,\mathrm{J}\right)}$$

$$\Rightarrow v_e = 19 \times 10^5\,\mathrm{m/s}$$

Exercises

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3. An X-ray photon of wavelength 0.0300 nm strikes a free, stationary electron, and a scattered photon is deflected at 90^o from the initial position. Determine the momentum of the incident and scattered photon.

3. An X-ray photon of wavelength 0.0300 nm strikes a free, stationary electron, and a scattered photon is deflected at 90° from the initial position. Determine the momentum of the incident and scattered photon.

For the incident photon:

$$p_i = \frac{h}{\lambda} = \frac{6.63\times10^{-34}\,\mathrm{J.s}}{0.0300\times10^{-9}\,\mathrm{m}} = 2.21\times10^{-23}\mathrm{kg.m/s}$$

The momentum of the deflected photon can be obtained

$$\lambda' - \lambda = \frac{h}{m_e c}(1-\cos\theta)$$

$$\lambda' = \lambda + \frac{h}{m_e c}(1-\cos 90)$$

$$p_{sc} = \frac{h}{\lambda} = \frac{6.63\times10^{-34}\,\mathrm{J.s}}{0.0324\times10^{-9}\,\mathrm{m}} = 2.04\times10^{-23}\,\mathrm{kg.m/s}$$

$$= 3.0\times10^{-11} + \frac{6.63\times10^{-34}\,\mathrm{J.s}}{9.1\times3\times(10^{-31+8})\,\mathrm{kg.m/s}} \rightarrow 3.24\times10^{-11}$$