Química Quântica I (CQ115)

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Bibliografia

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- Levine, I. N. - *Physical Chemistry , 6th ed.* - McGraw-Hill, 2008
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- Keeler, J.; Wother, P. - *Chemical Structure and Reactivity, 2nd ed - Oxford University Press, 2015*
- *Baggott, J. - The Meaning of the Quantum Theory – Oxford University Press*
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Suporte Matemático

Cálculo diferencial e integral de uma e de várias variáveis (Cálculo I e II)

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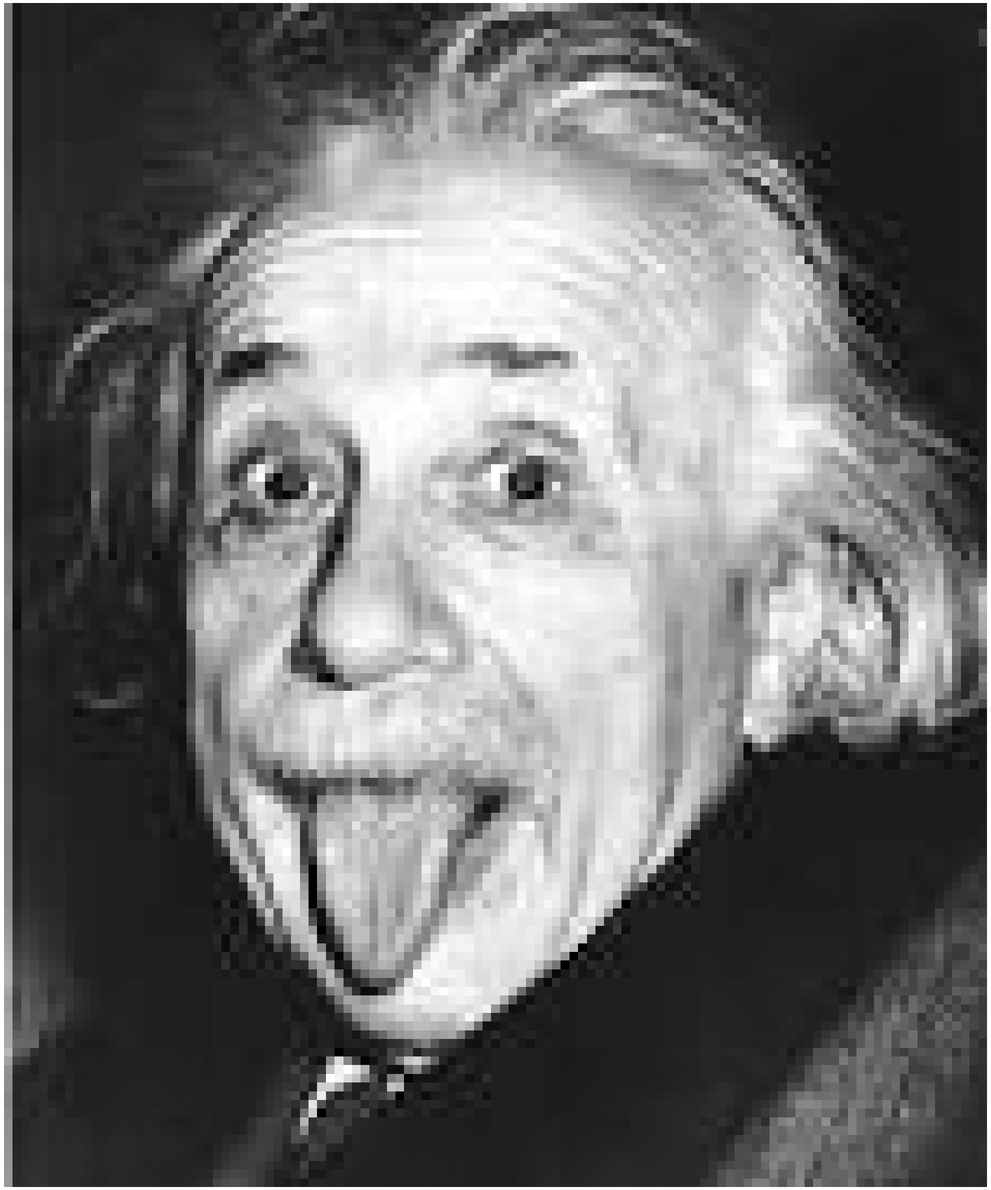
Bancos de Dados

http://webbook.nist.gov/chemistry/

W. M. Haymes - CRC Handbook of Physics and Chemistry - 95 th edition

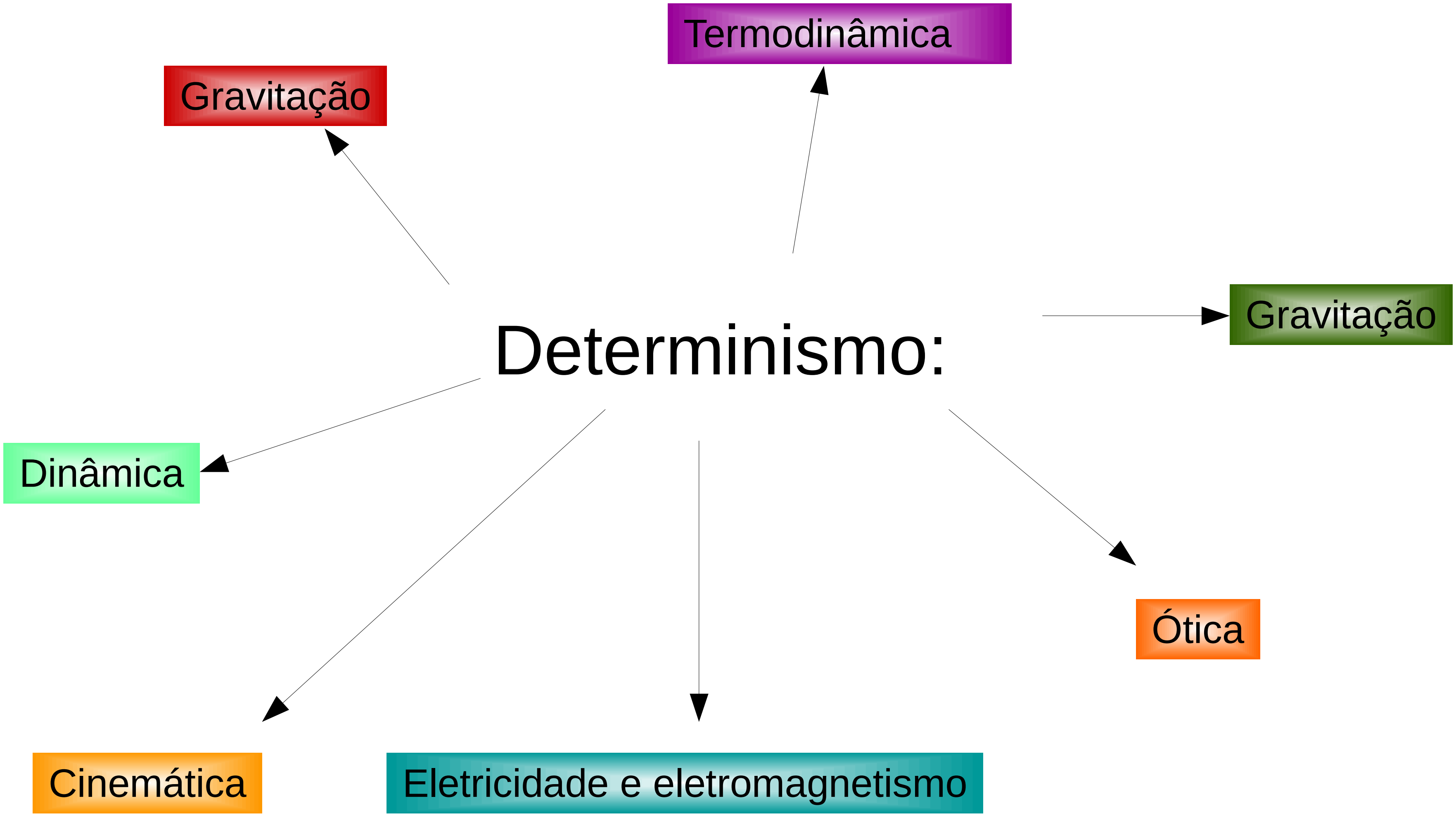
Atkins, P. W. - Physical Chemistry 10 th ed – Oxford University Press, 2014



Por que a mecânica quântica desperta tanto “temor” nas pessoas?

A Física Clássica no Final do Século XIX:

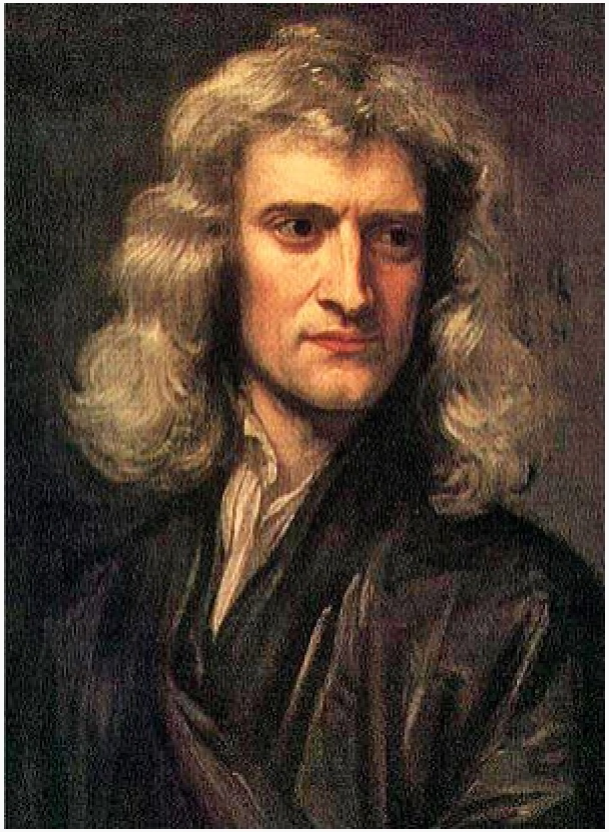
A ciência havia chegado ao seu ápice!!



Bases da Física Clássica

Galileu Galilei, por Justus Sustermans 1636.

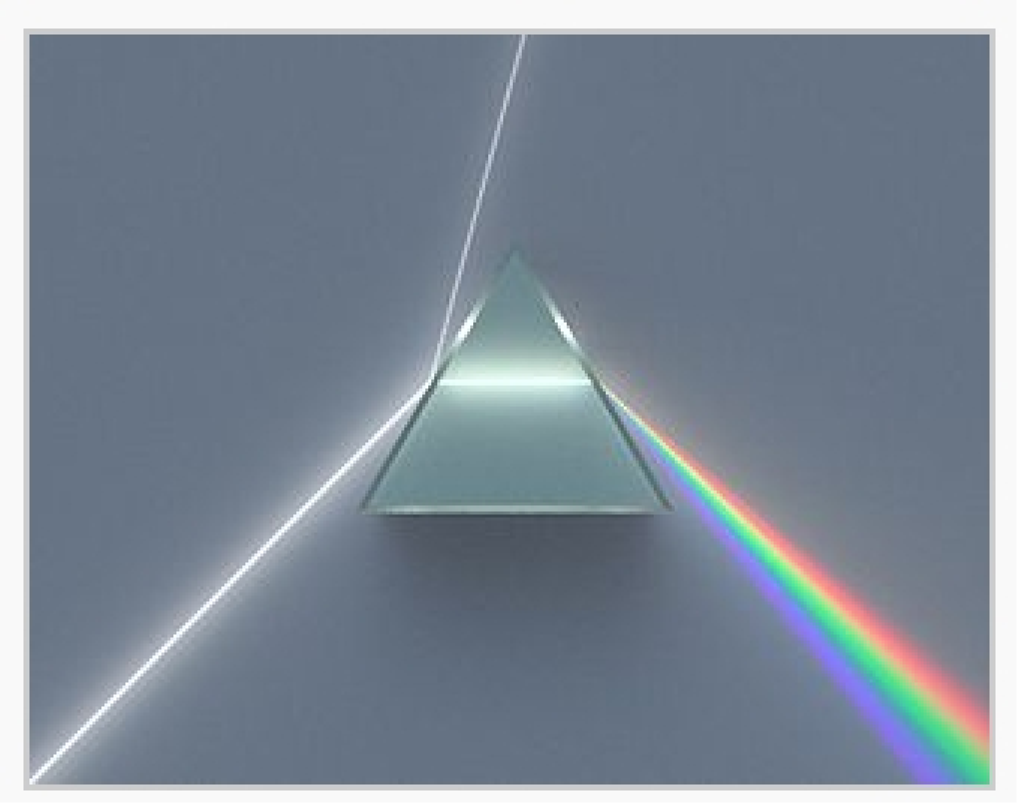
15/02/1564 –08/01/1642



Newton retratado por Godfrey Kneller, 1689 (com 46 anos de idade)

04/01/1643 – 31/03/1727

A natureza da Luz



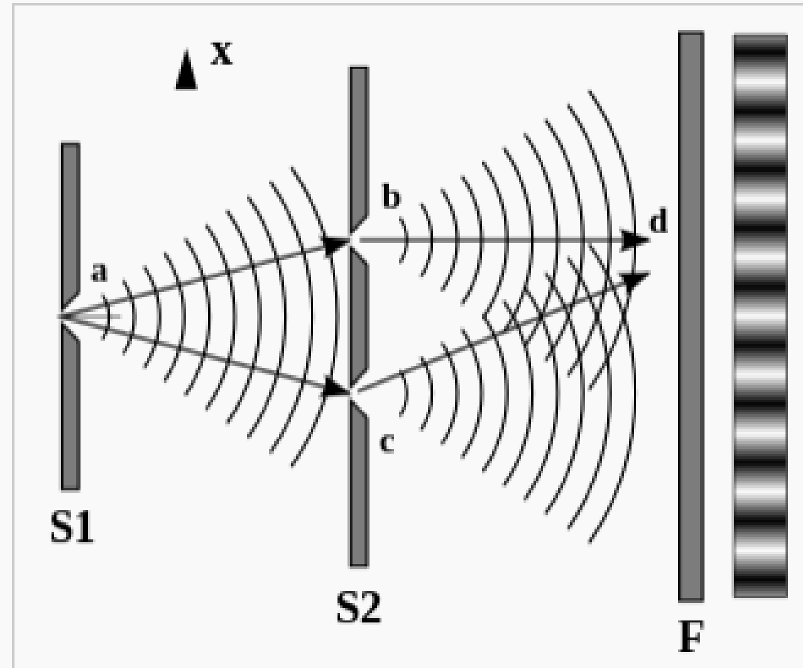
Onda ou partícula?

Newton: corpuscular

E todos aceitavam, porque era, afinal de contas, Newton quem estava dizendo

Christiaan Huygens

Thomas Young

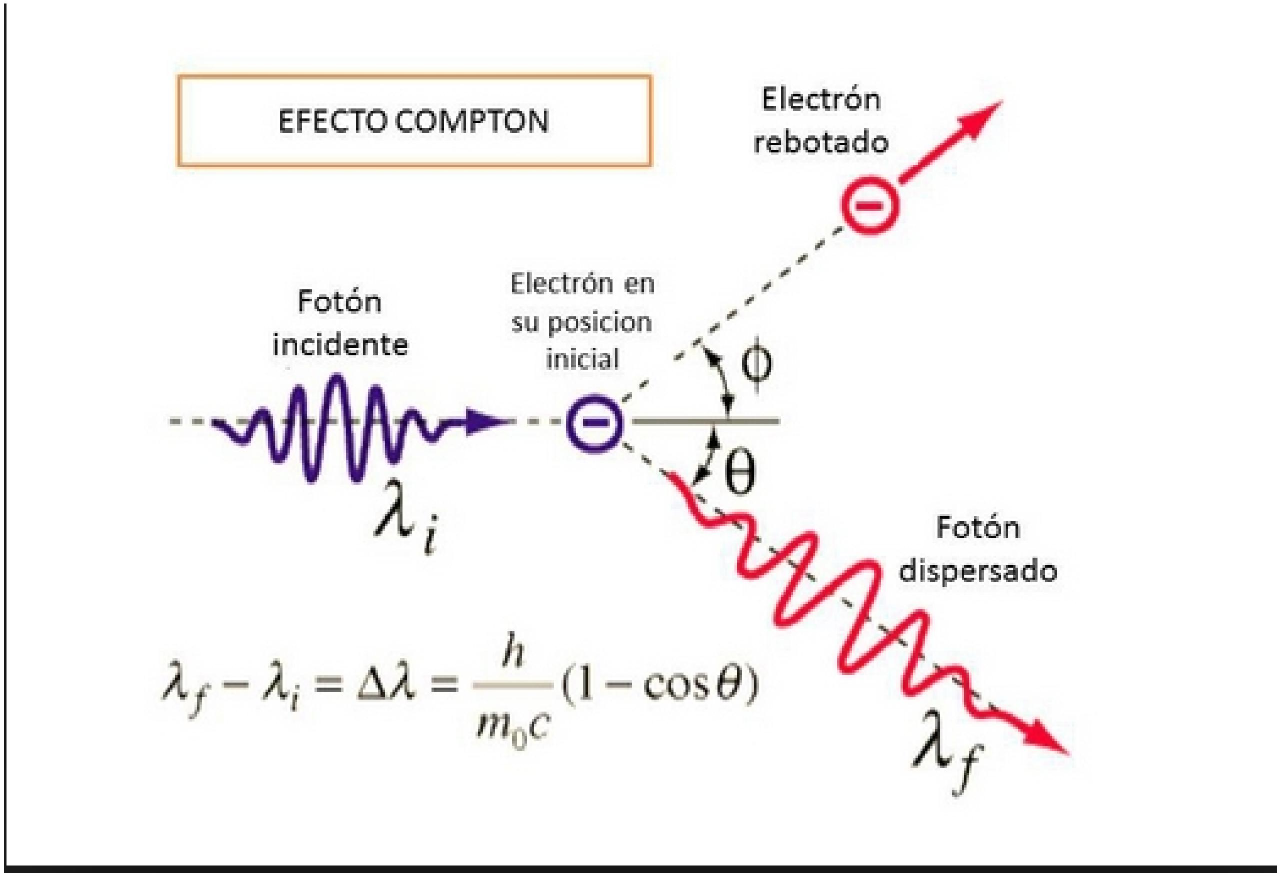


Experiência da dupla fenda

A luz é onda!!

E, se a luz fosse constituída de partículas?

Efeito Compton (1892-1962, Nobel Física 1927)



Radiação do Corpo Negro

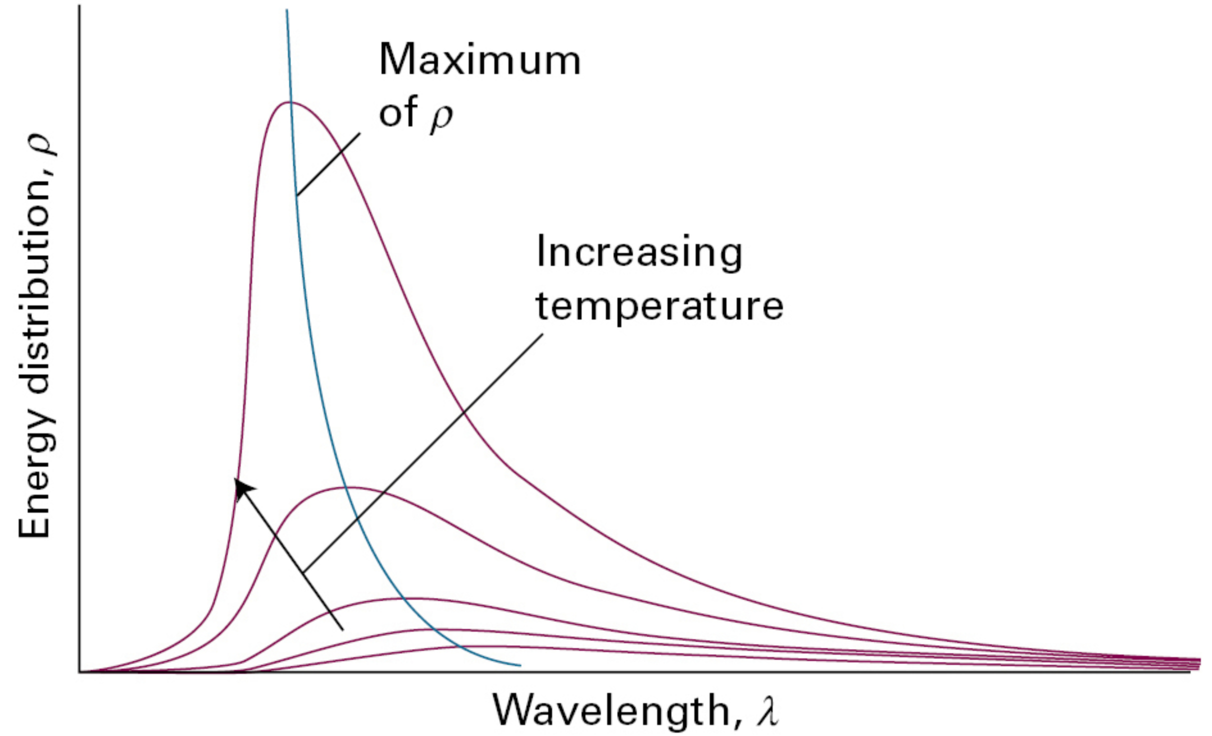


Figure 7A.1 The energy distribution in a black-body cavity at several temperatures. Note how the spectral density of states increases in the region of shorter wavelength as the temperature is raised, and how the peak shifts to shorter wavelengths.

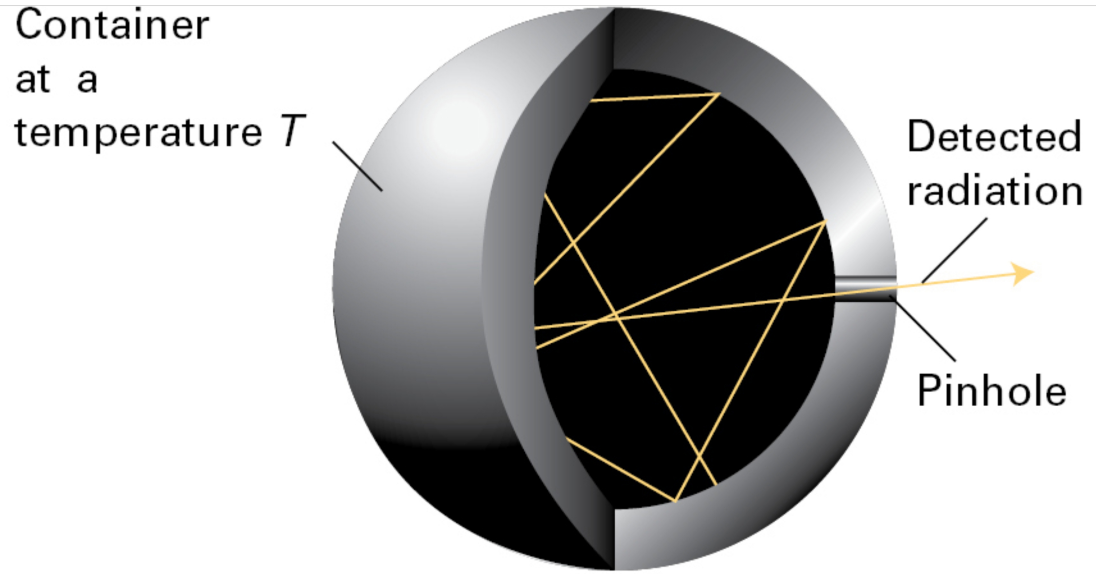


Figure 7A.2 An experimental representation of a black body is a pinhole in an otherwise closed container. The radiation is reflected many times within the container and comes to thermal equilibrium with the walls. Radiation leaking out through the pinhole is characteristic of the radiation within the container.

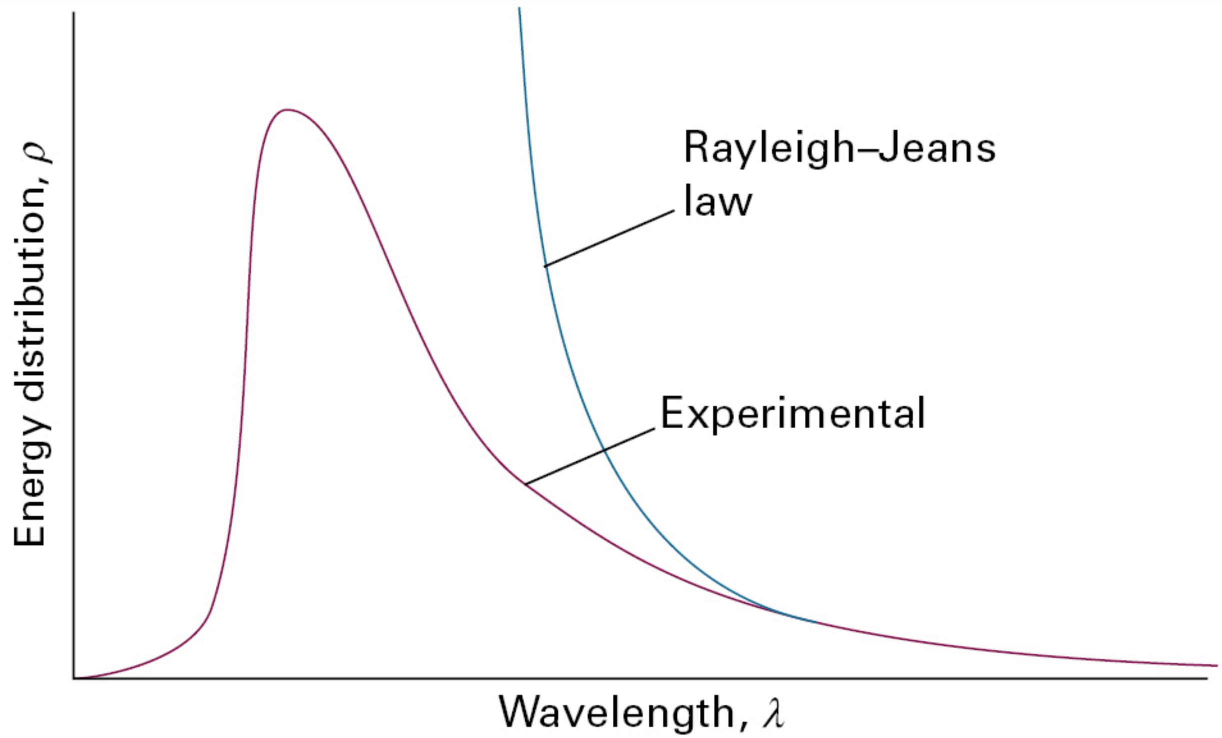


Figure 7A.4 The Rayleigh–Jeans law (eqn 7A.4) predicts an infinite spectral density of states at short wavelengths. This approach to infinity is called the ultraviolet catastrophe.

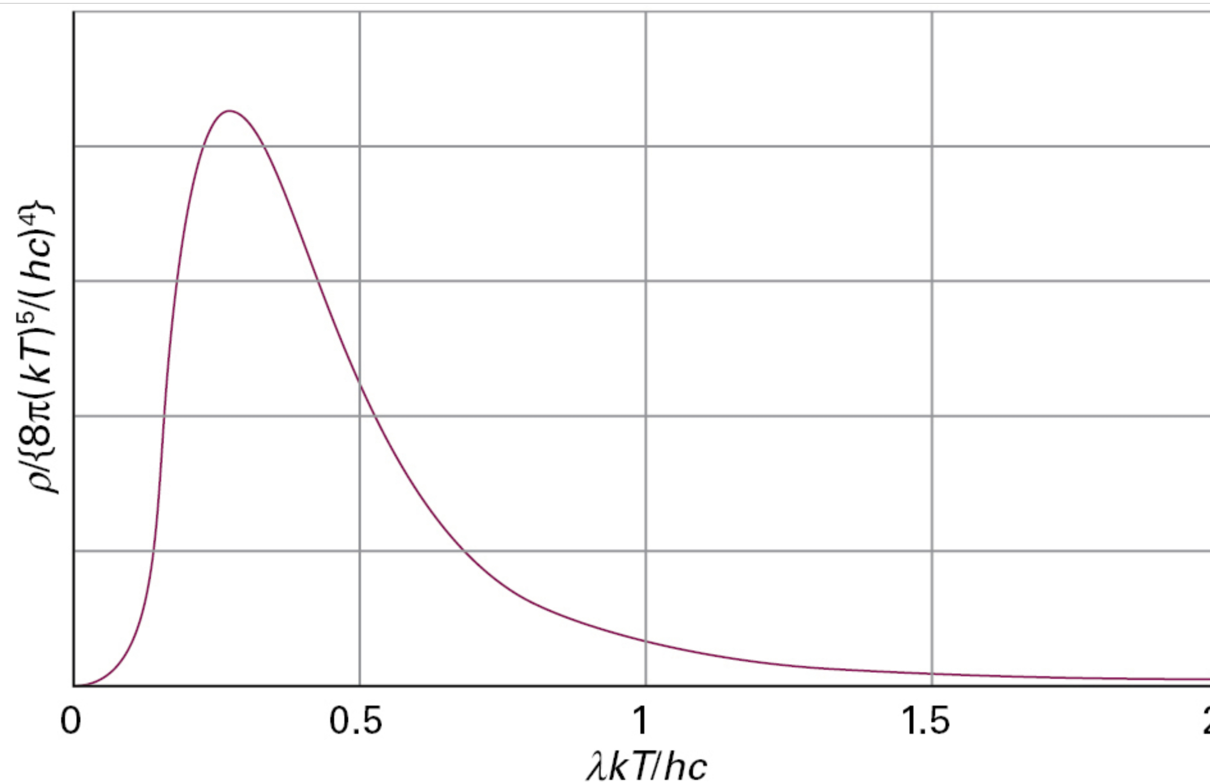


Figure 7A.5 The Planck distribution (eqn 7A.6) accounts very well for the experimentally determined distribution of black-body radiation. Planck's quantization hypothesis essentially quenches the contributions of high frequency, short wavelength oscillators. The distribution coincides with the Rayleigh–Jeans distribution at long wavelengths.

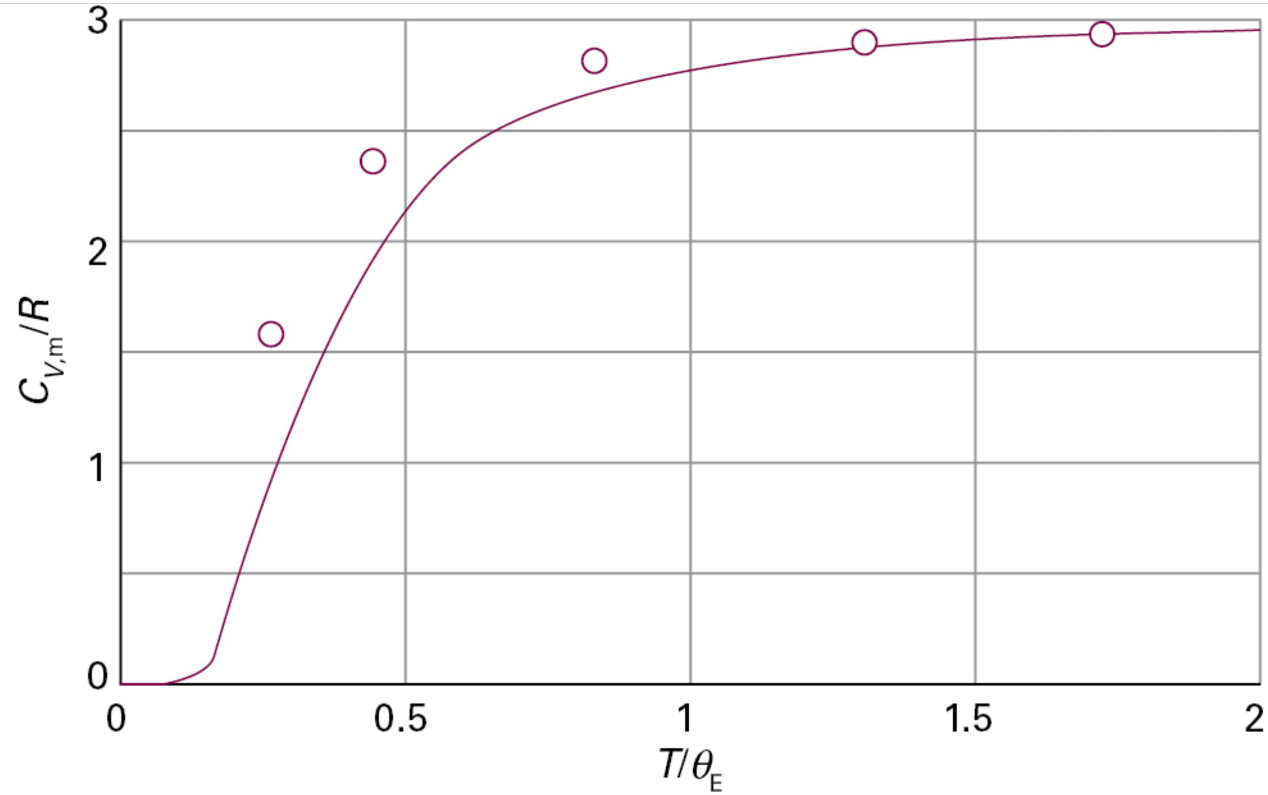


Figure 7A.6 Experimental low-temperature molar heat capacities and the temperature dependence predicted on the basis of Einstein's theory. His equation (eqn 7A.10) accounts for the dependence fairly well, but is everywhere too low.

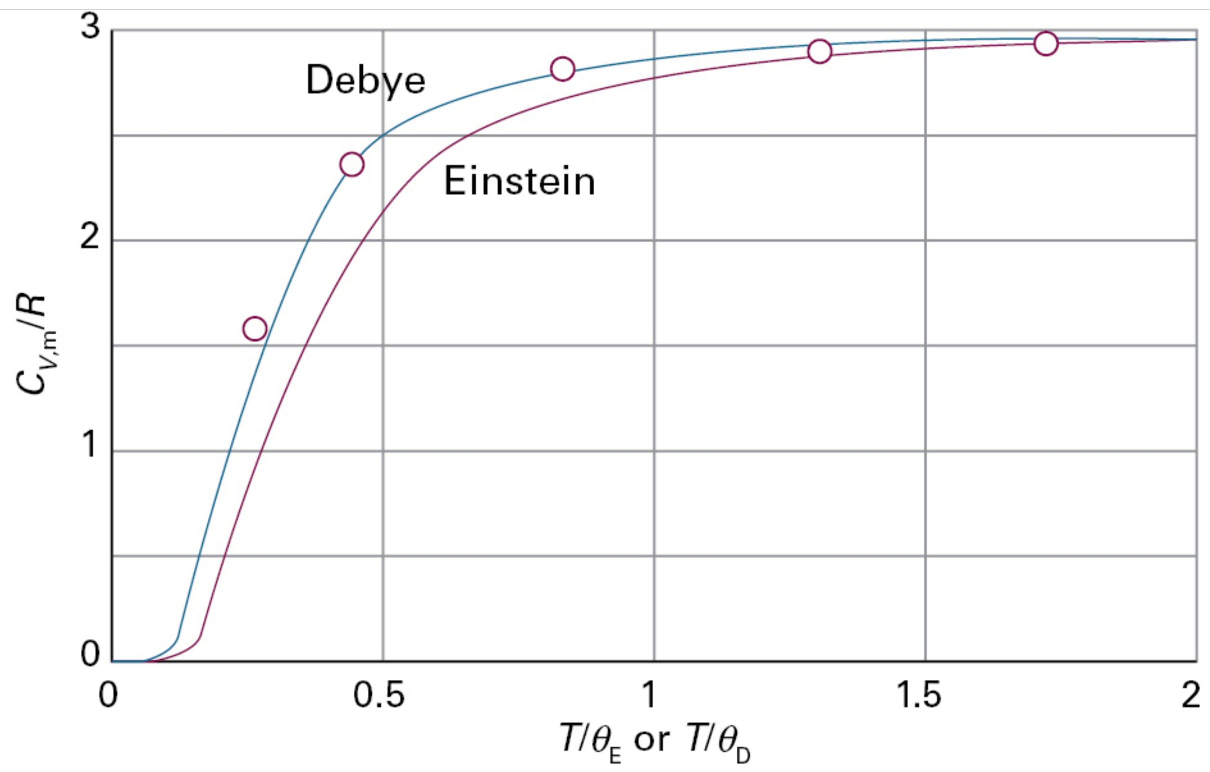


Figure 7A.7 Debye's modification of Einstein's calculation (eqn 7A.11) gives very good agreement with experiment. For copper, $T/\theta_D = 2$ corresponds to about 170 K, so the detection of deviations from Dulong and Petit's law had to await advances in low-temperature physics.

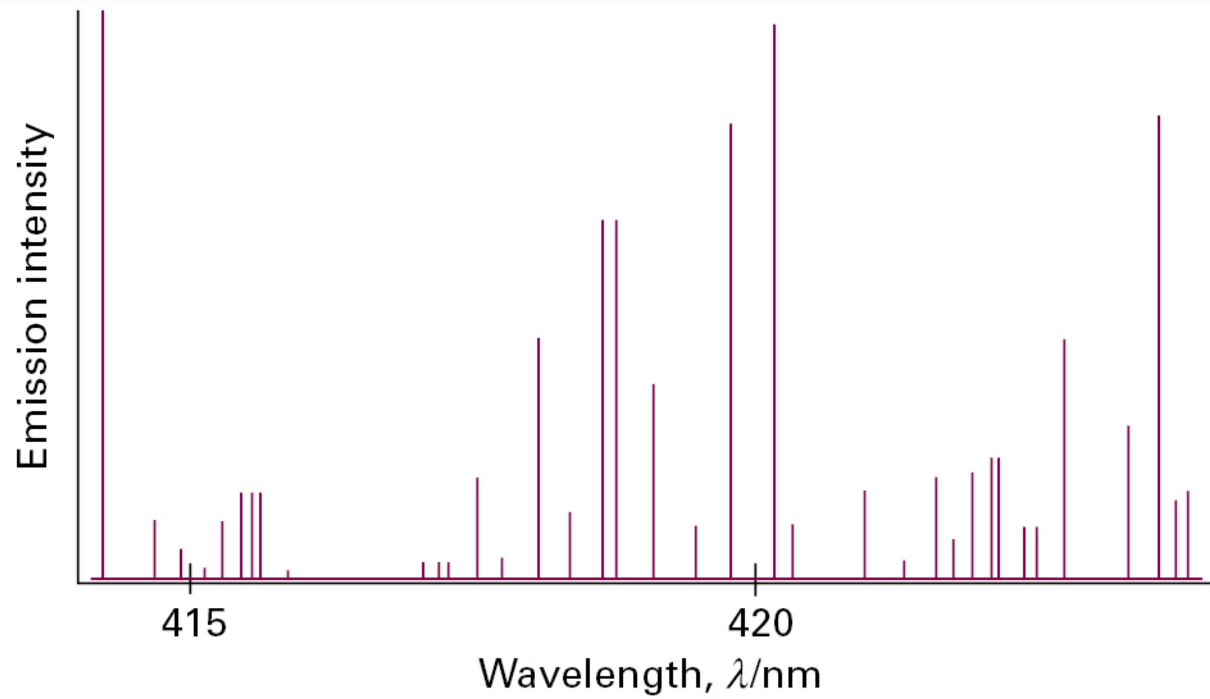


Figure 7A.8 A region of the spectrum of radiation emitted by excited iron atoms consists of radiation at a series of discrete wavelengths (or frequencies).

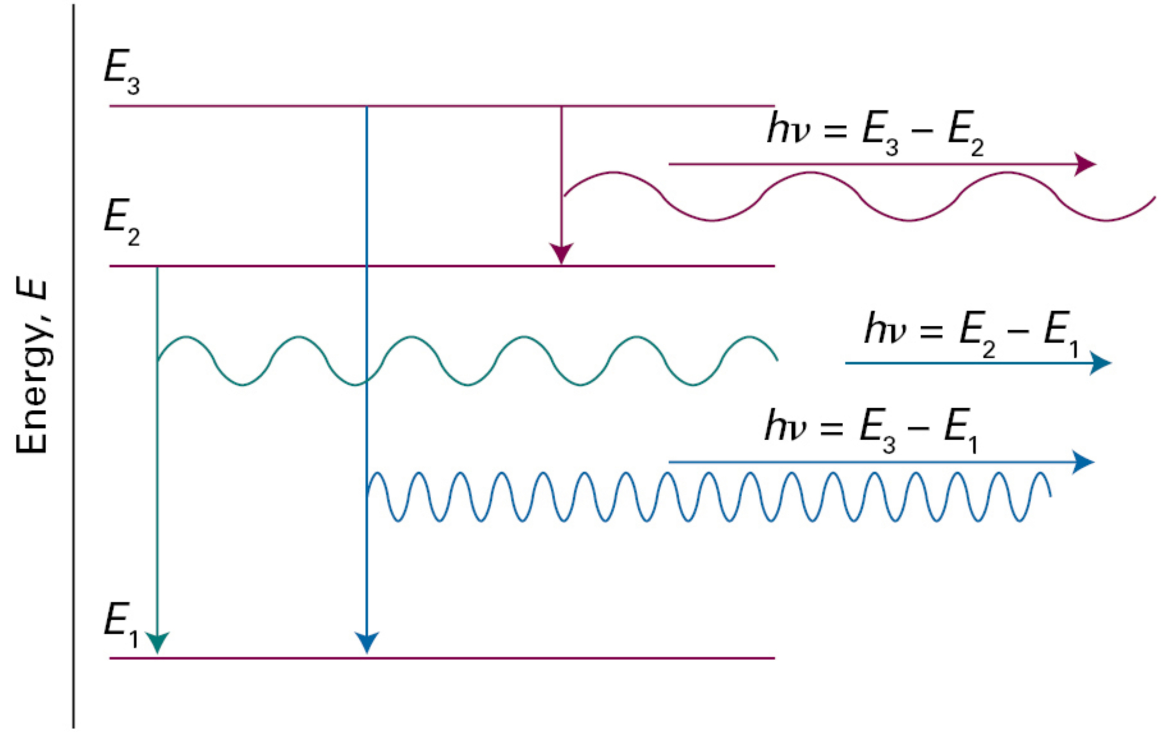
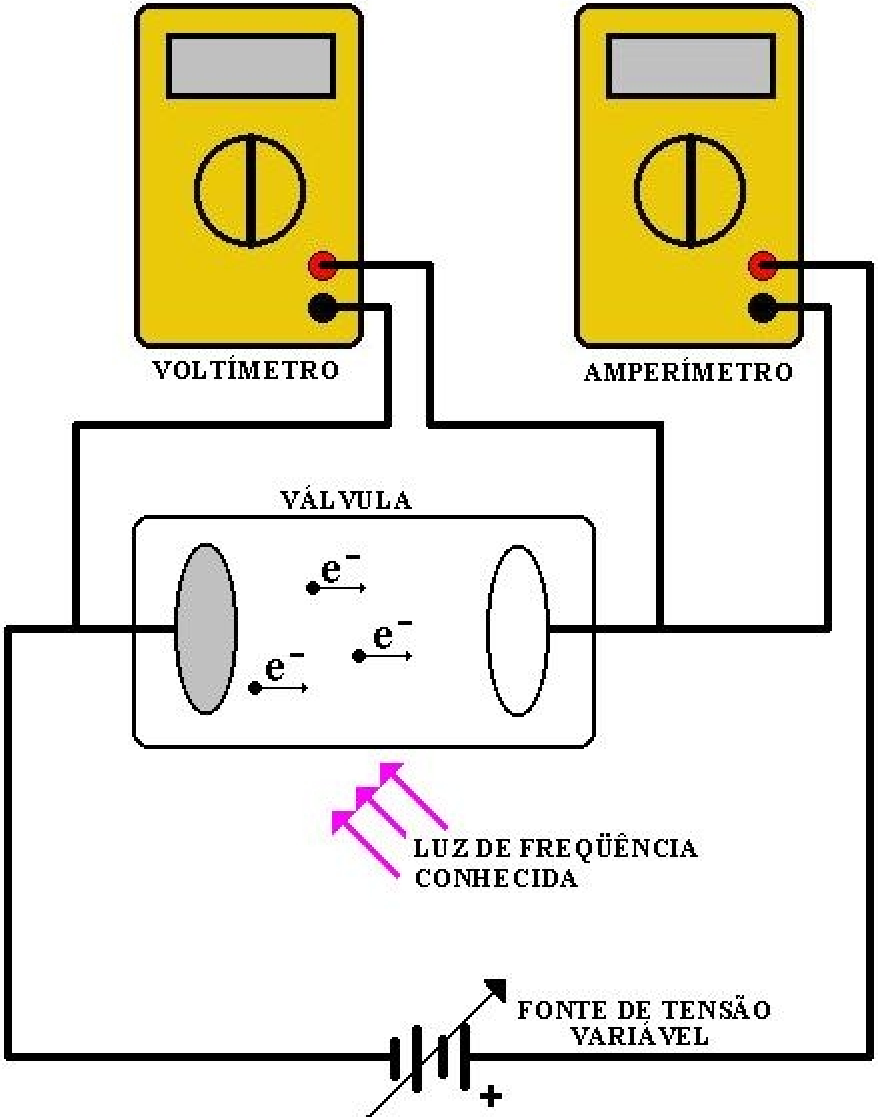


Figure 7A.10 Spectroscopic transitions, such as those shown above, can be accounted for if we assume that a molecule emits electromagnetic radiation as it changes between discrete energy levels. Note that high-frequency radiation is emitted when the energy change is large.

Efeito Fotoelétrico
(Einstein)



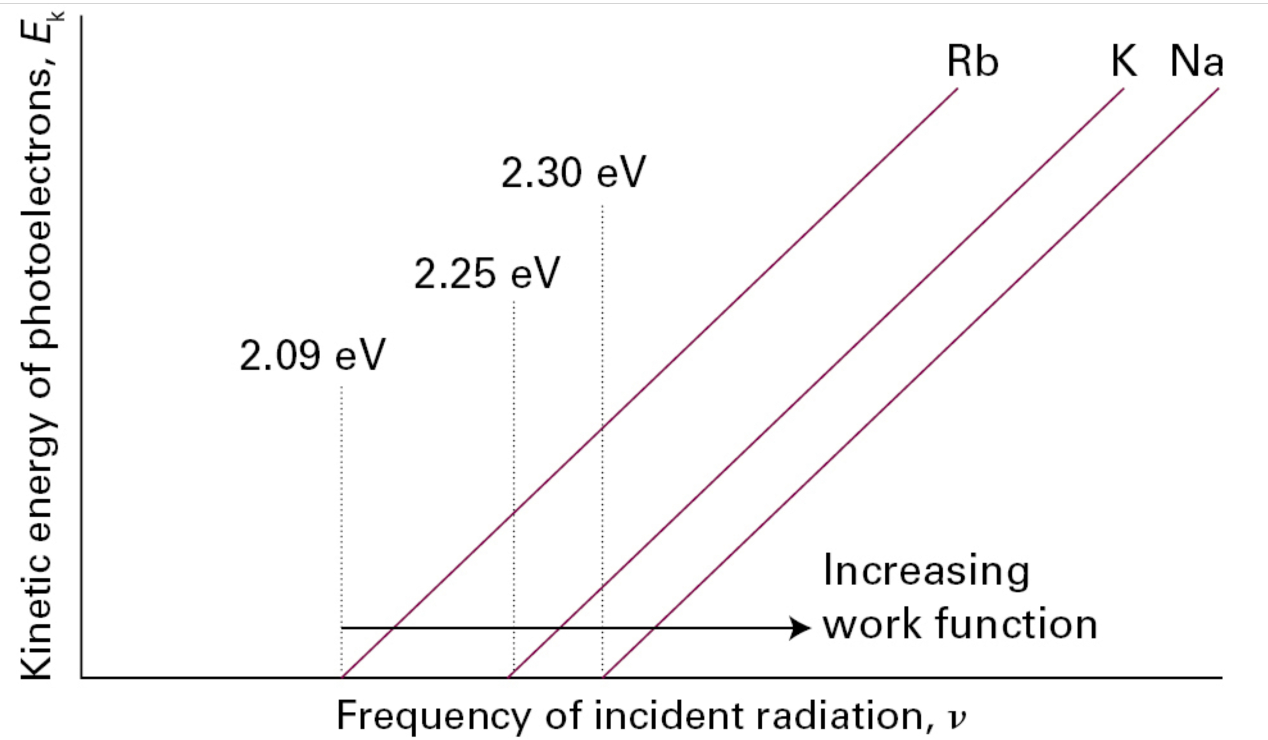


Figure 7A.11 In the photoelectric effect, it is found that no electrons are ejected when the incident radiation has a frequency below a value characteristic of the metal, and, above that value, the kinetic energy of the photoelectrons varies linearly with the frequency of the incident radiation.

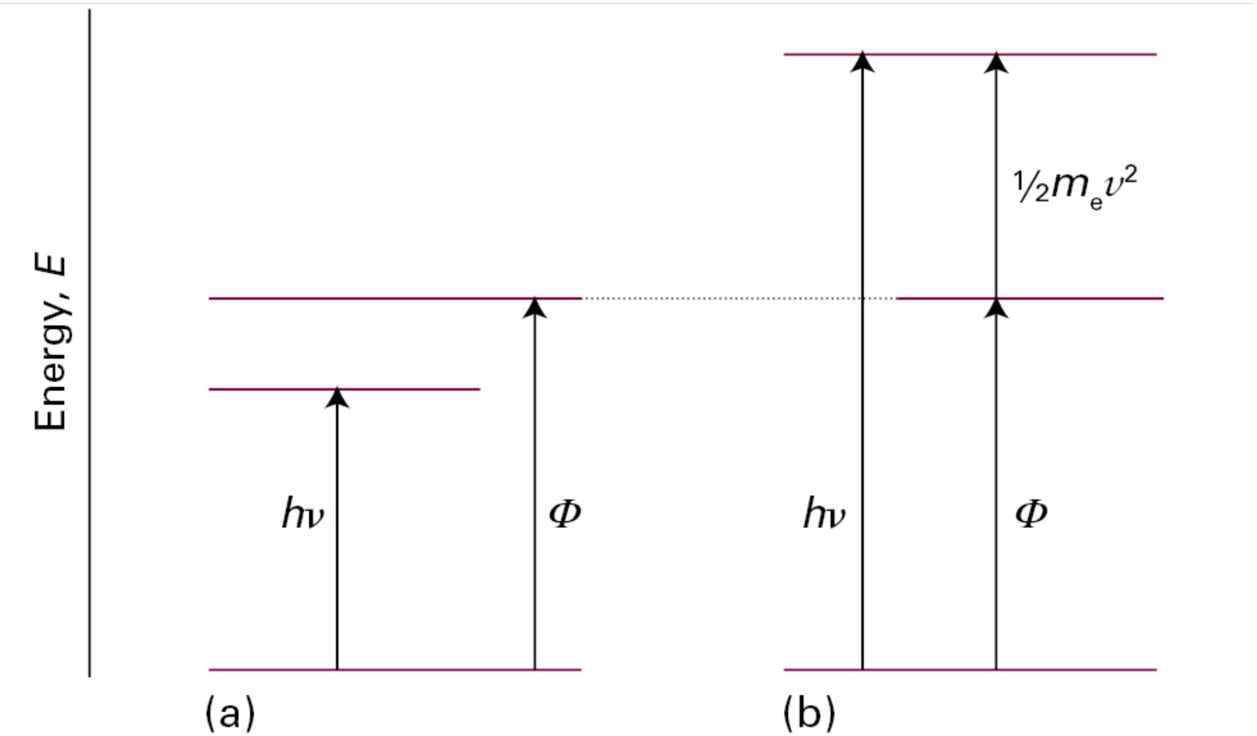


Figure 7A.12 The photoelectric effect can be explained if it is supposed that the incident radiation is composed of photons that have energy proportional to the frequency of the radiation. (a) The energy of the photon is insufficient to drive an electron out of the metal. (b) The energy of the photon is more than enough to eject an electron, and the excess energy is carried away as the kinetic energy of the photoelectron.

Davisson e G. P. Thomson
(Nobel 1937)

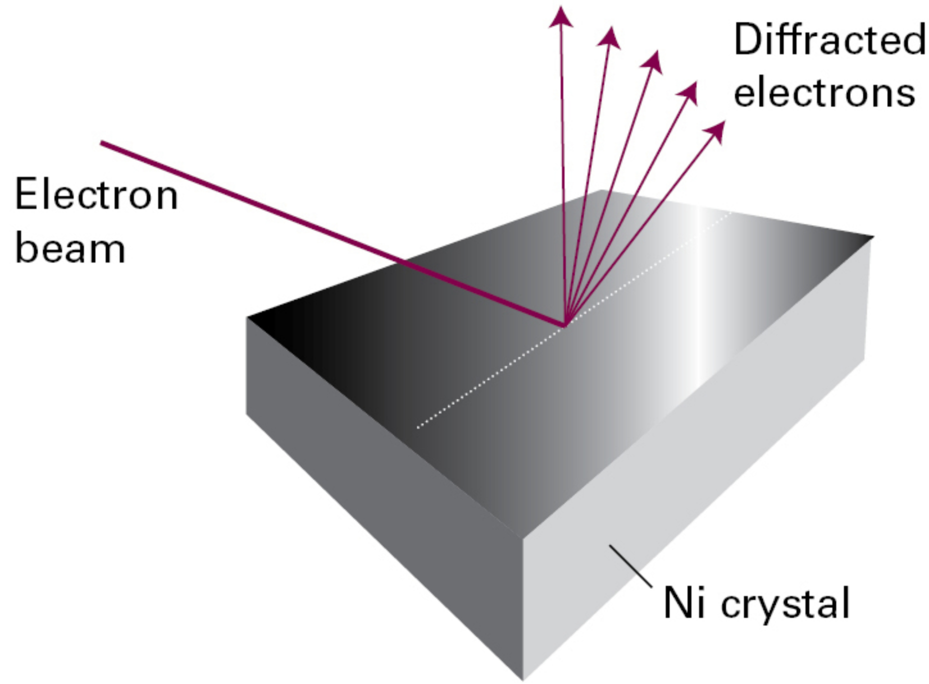


Figure 7A.13 The Davisson–Germer experiment. The scattering of an electron beam from a nickel crystal shows a variation of intensity characteristic of a diffraction experiment in which waves interfere constructively and destructively in different directions.

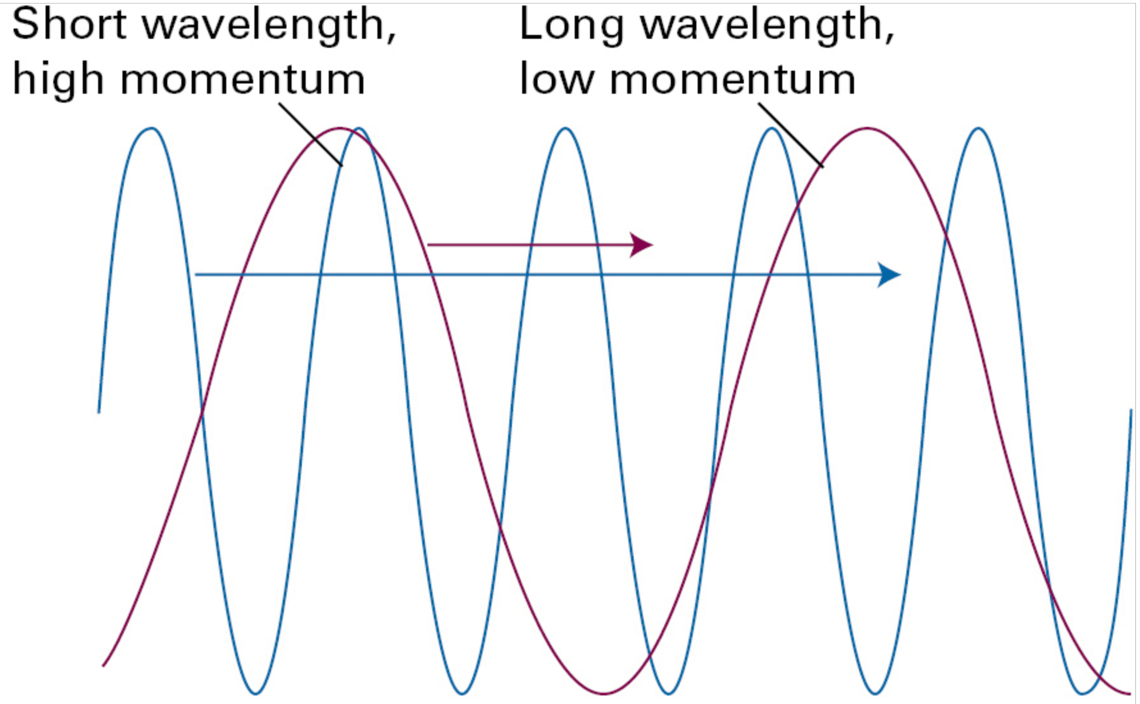


Figure 7A.14 An illustration of the de Broglie relation between momentum and wavelength. The wave is associated with a particle. A particle with high momentum corresponds to a wave with a short wavelength, and vice versa.