Introduction to the course and motivation of the topic

Lecture 1

CHM 439
Quantum Chemistry

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Lecture Plan

- A (brief) historical motivation
- Introduction the course
- Particles *vs.* Waves: Some simulations

Introduction to the Course

- Assignments (almost weekly) 10%
- Quizzes -2 10%
- Mid-semester examination 30%
- End-semester examination 50%

Textbooks

1. Quantum Chemistry, Ira Levine
2. Molecular Quantum Mechanics, P. W. Atkins and Friedman.
3. Quantum Mechanics: Concepts and Applications, N. Zettili

Historical Motivation

Status of Physics in the 19th century (Classical mechanics ruled)

- Dynamics of material systems through motion of point particles (Newton's equations, Lagragian mechanics, etc. (**r**, **p**, t).
- Energy/disturbance propagation (without net displacement of matter) described through wave motion.
- 1801: Light was demonstrated to be a wave (Thomas Young's double-slit exit.)
- 1859: G. Kirchoff introduced the blackbody concept introduced to explain thermal emission and its primary dependence on temperature.
- 1860-1890: Boltzmann and Maxwell developed statistical mechanics; the former also later proposed the existence of discrete energy states.
- 1885: Balmer discovered a numerical relationship between visible spectral lines of hydrogen, the Balmer series. Generalised by Rydberg (1888) to get his formula.

Historical Motivation

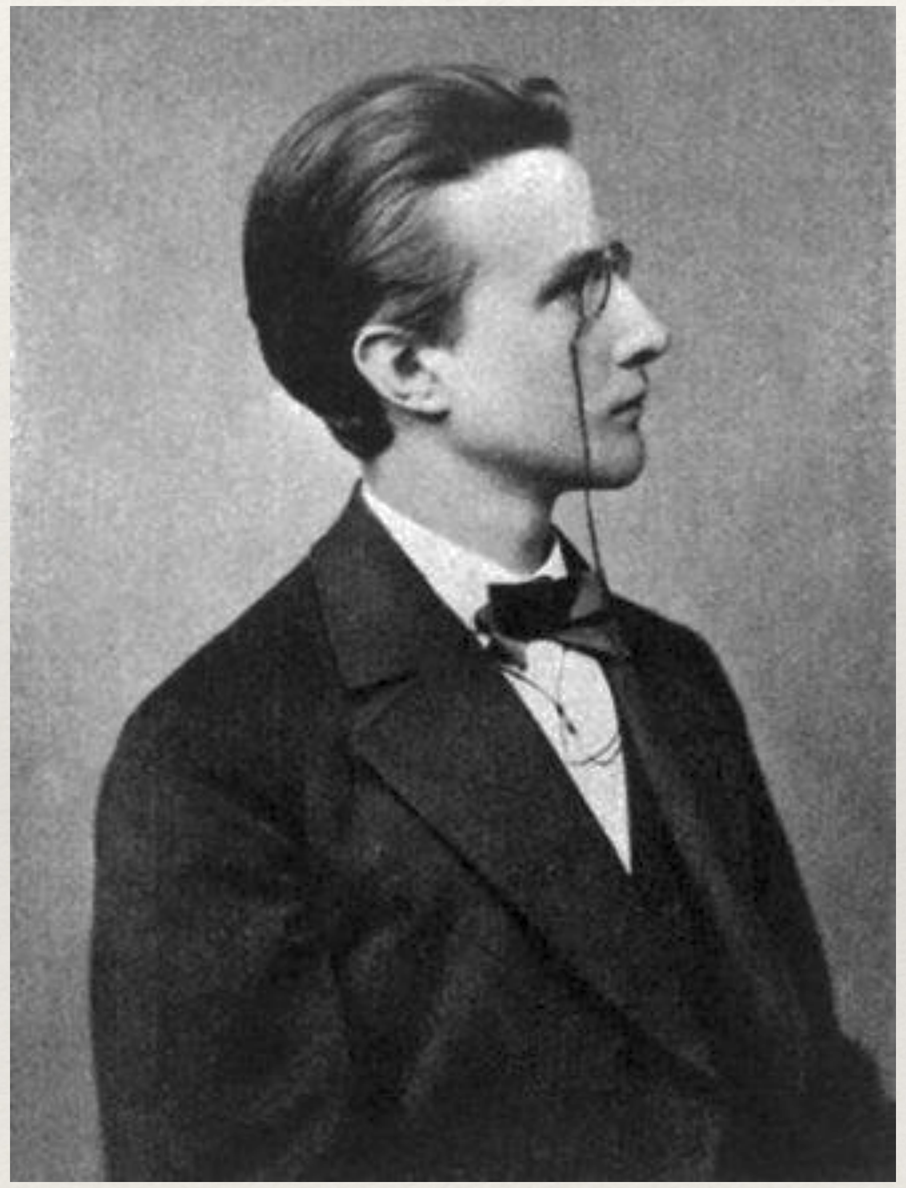
Status of Physics in the 19th century (Classical mechanics ruled) ***ctd*****…**

- 1885: Hertz discovered the photoelectric effect by shining light on metal surfaces and measuring energies of the charges emitted.
- 1888: Hertz demonstrates that light is made of electromagnetic waves as predicted by Maxwell.
- 1896-1897: Pieter Zeeman discovers the splitting of atomic emission lines under a magnetic field.
- 1897: J. J. Thompson discovers the electron.

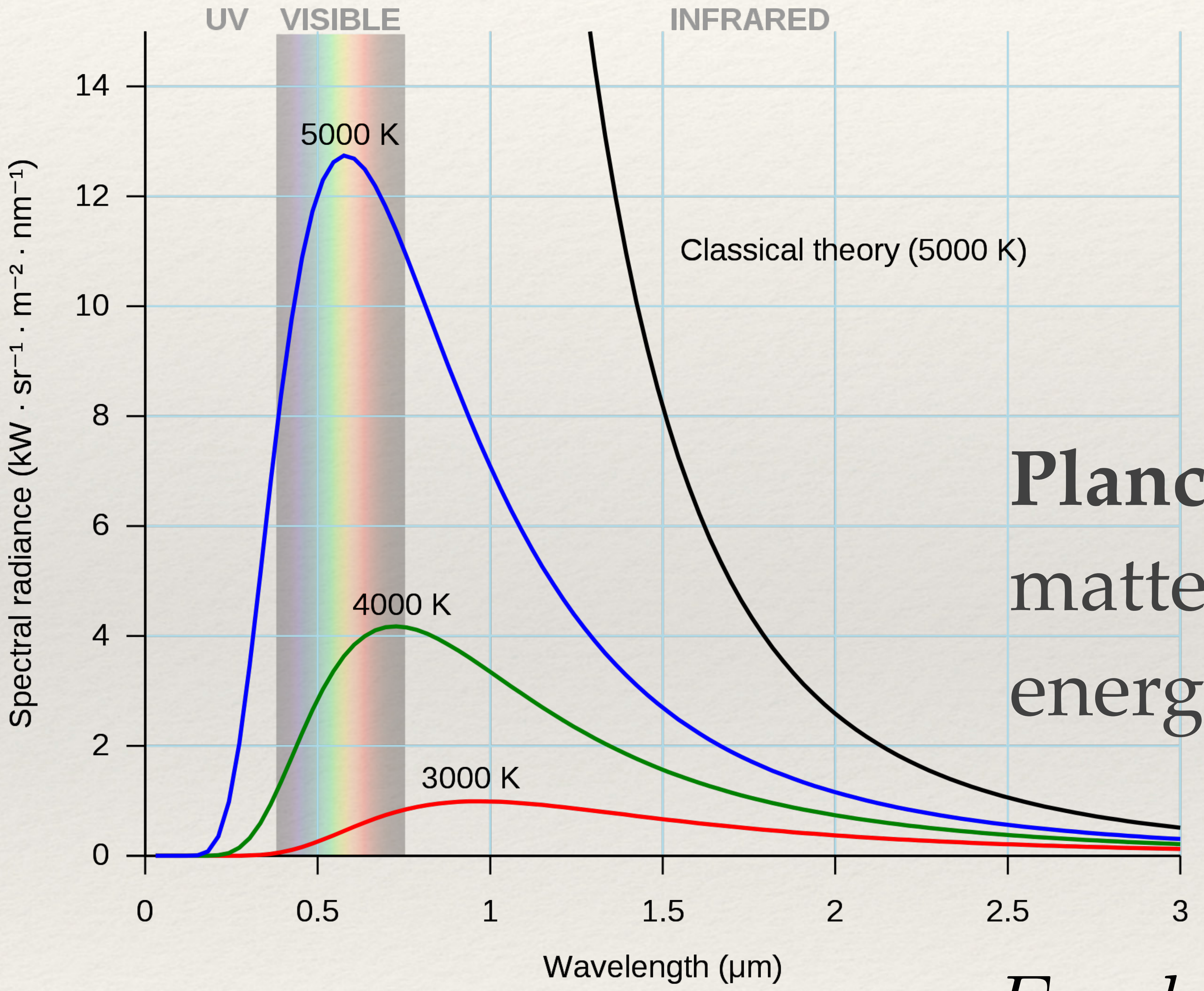
A bunch of discoveries that birthed the field of nuclear physics were made between 1895-1903 by Becquerel, Roentgen, Marie Curie, and Rutherford. The structure of the "atom" was then pursued.

Historical Motivation: A Quantum Leap

1900 Classical theories were unable to explain the nature of the blackbody spectrum.



Max Planck



Energy stored per unit wavelength

Rayleigh-Jeans Law

$$u(\lambda, T) = \frac{8\pi k_B T}{\lambda^4}$$

UV catastrophe!!

Planck: Energy exchanged between light and the matter of the blackbody was only in packets with energy proportional to the frequency of light.

$$E = h\nu$$

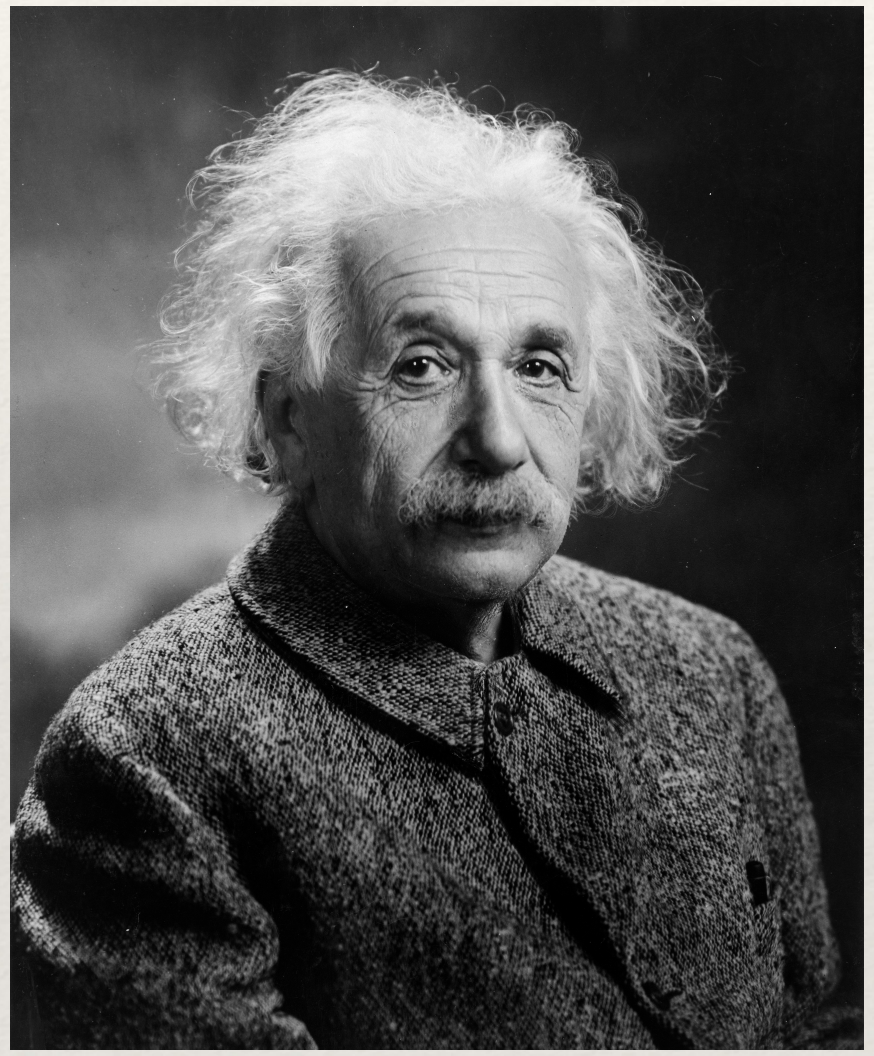
$$h = 6.631 \times 10^{-34} Js$$

Planck's Law

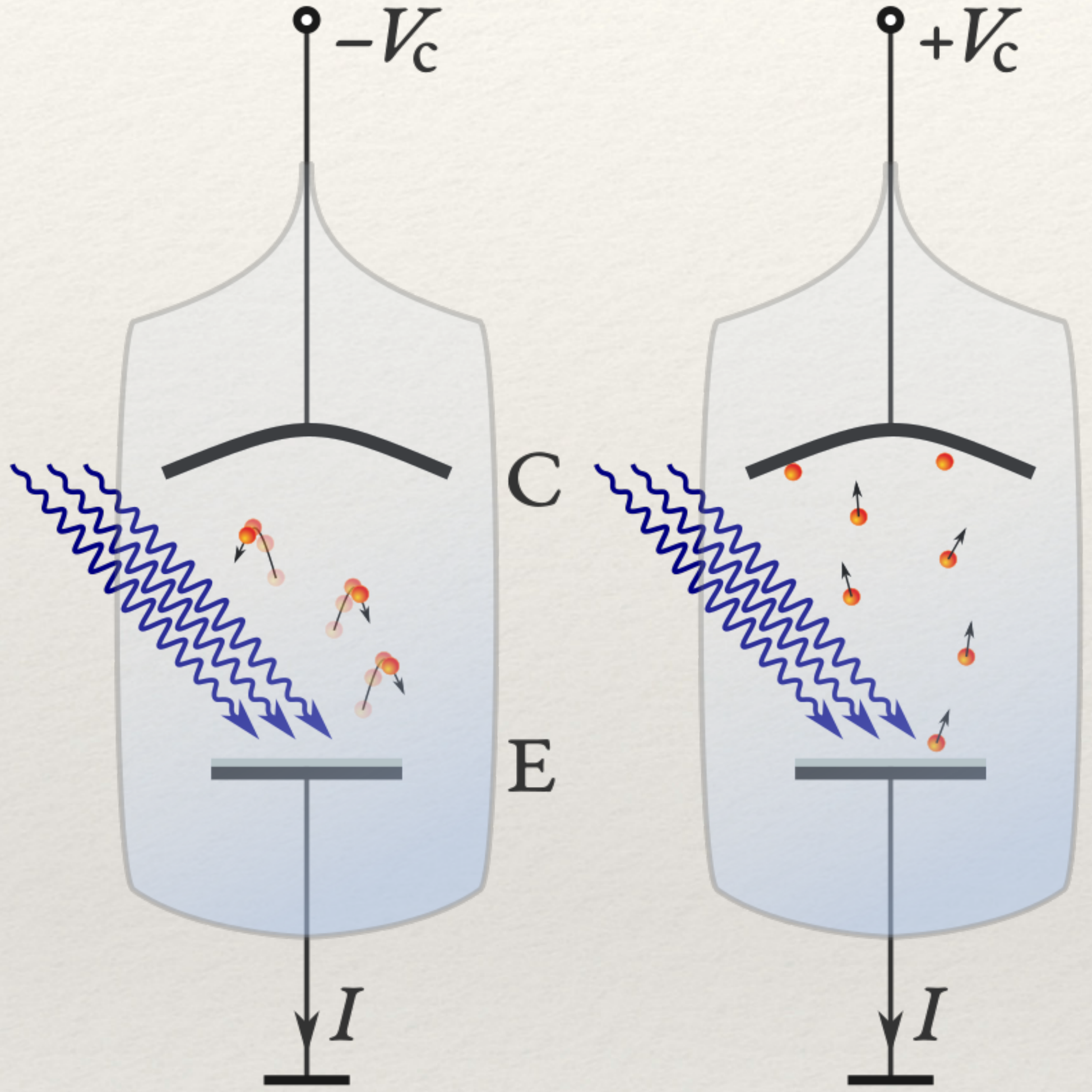
$$\boxed{u(\lambda, T) = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}}$$

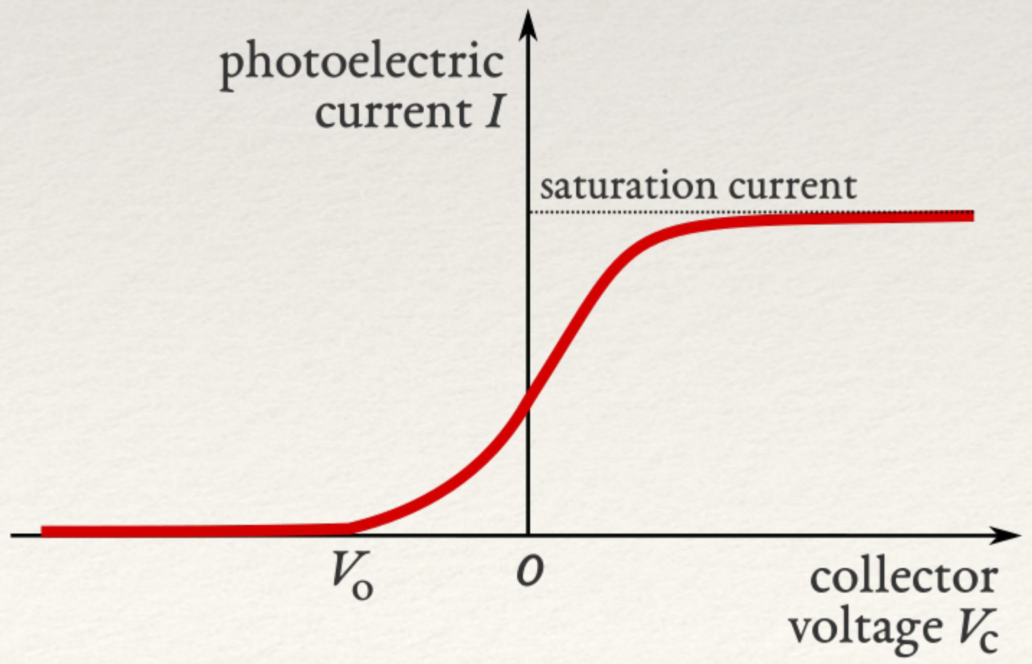
Historical Motivation: Light as a particle

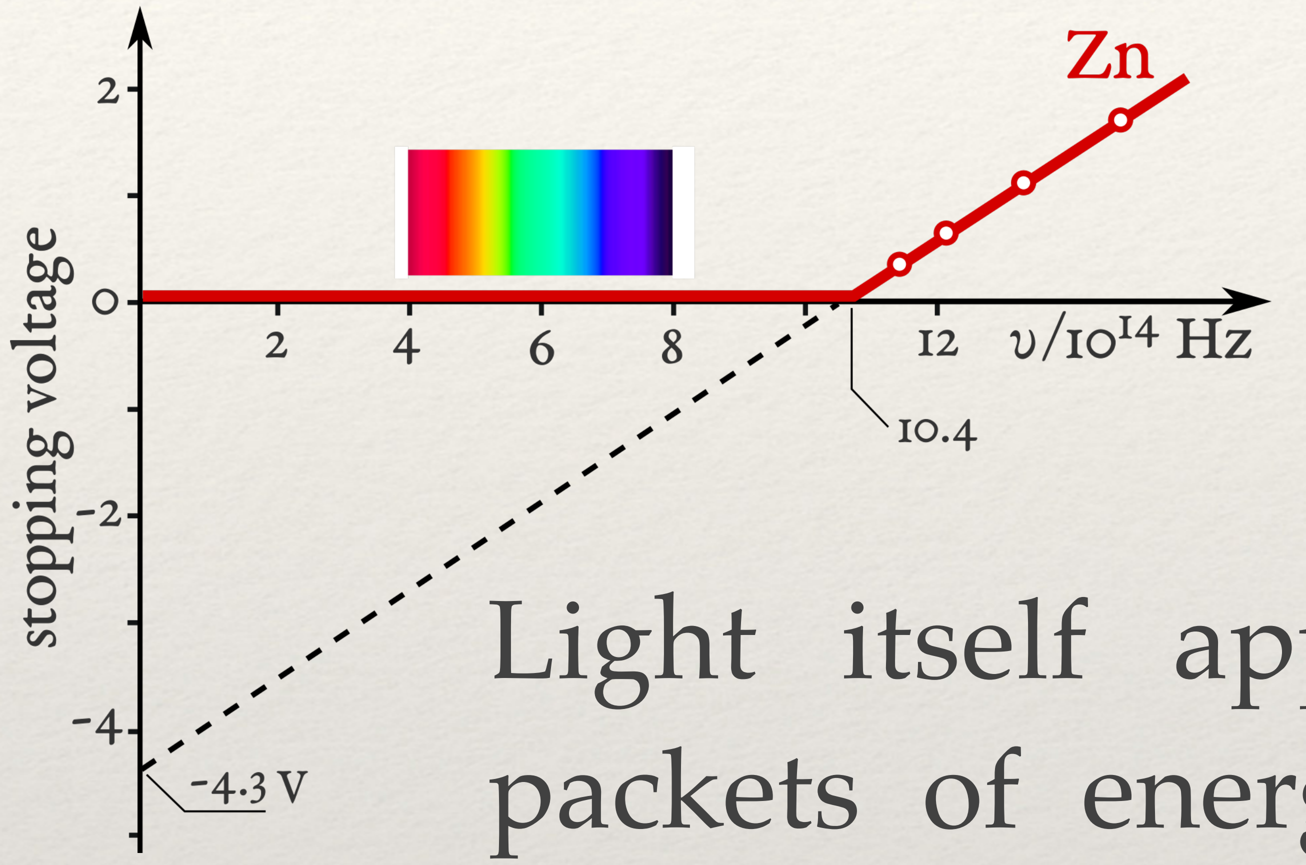
1905 Explained the photoelectric effect observed by Hertz using Planck's idea

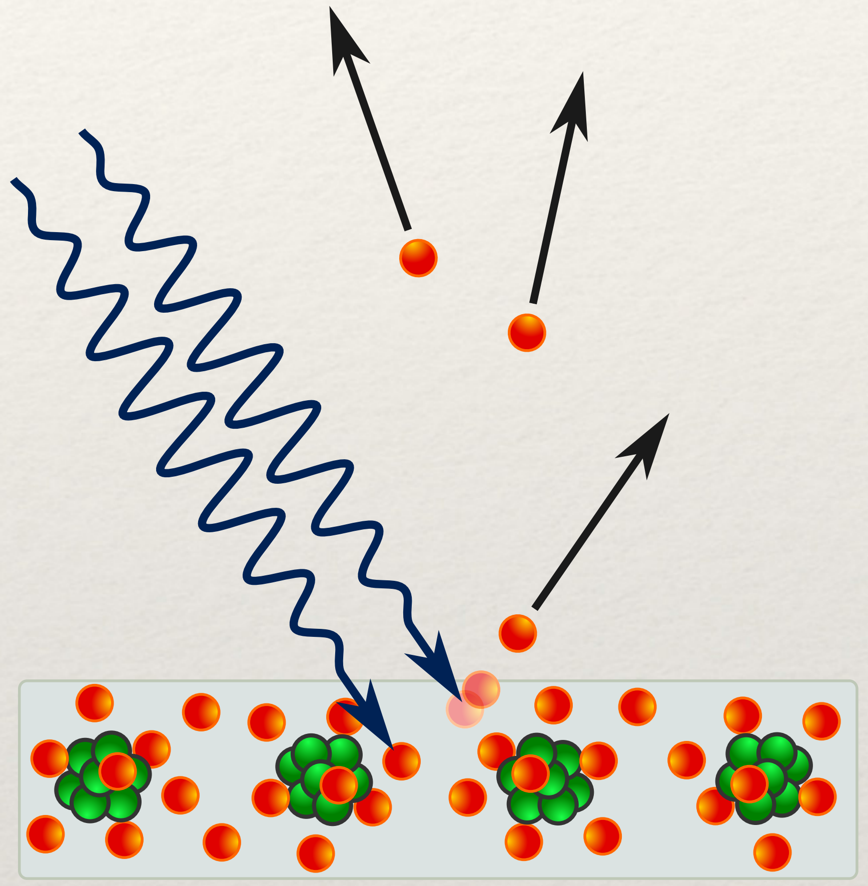


A. Einstein









Light itself appears as packets of energy when interacting with matter.

$$\boxed{h\nu = \Phi + \frac{1}{2}mv^2}$$

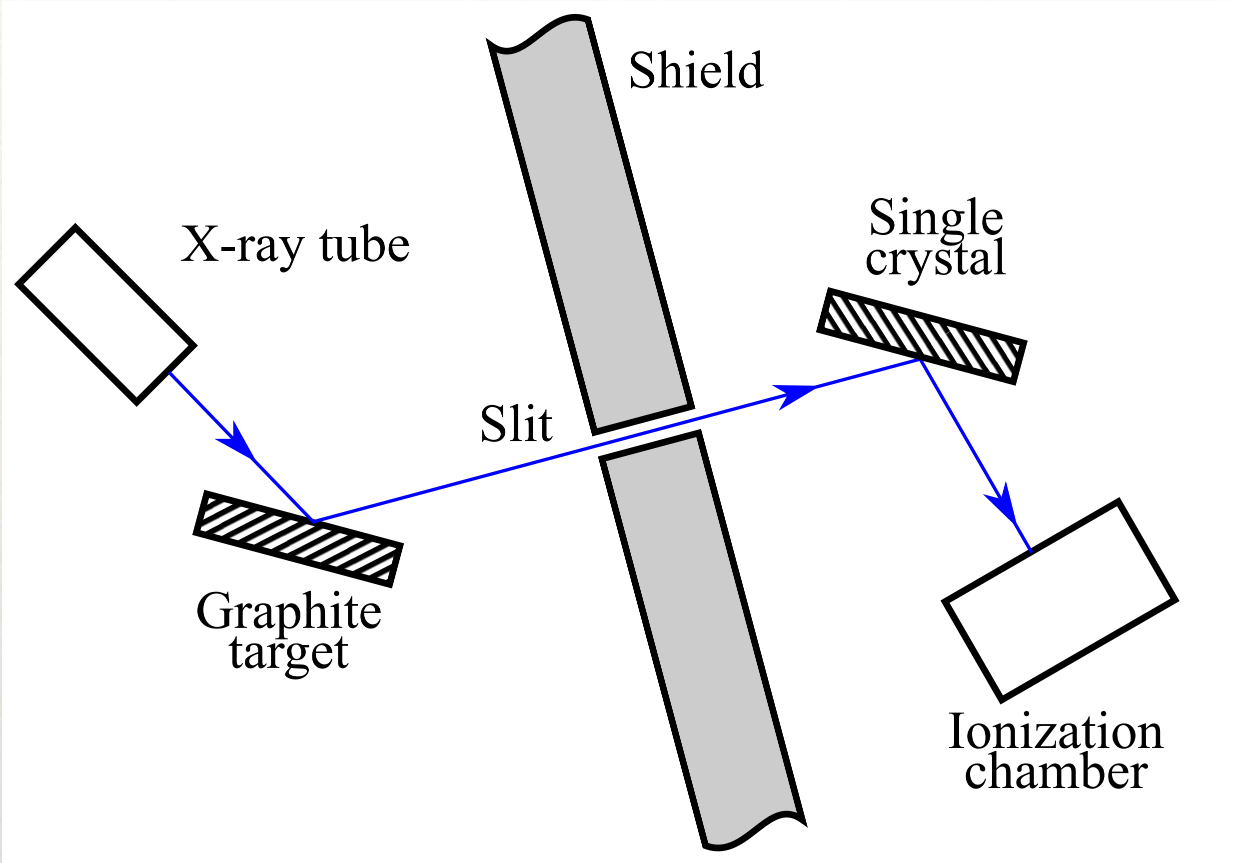
Particles are packets of energy and momentum.
Did Einstein identify light as particles here?

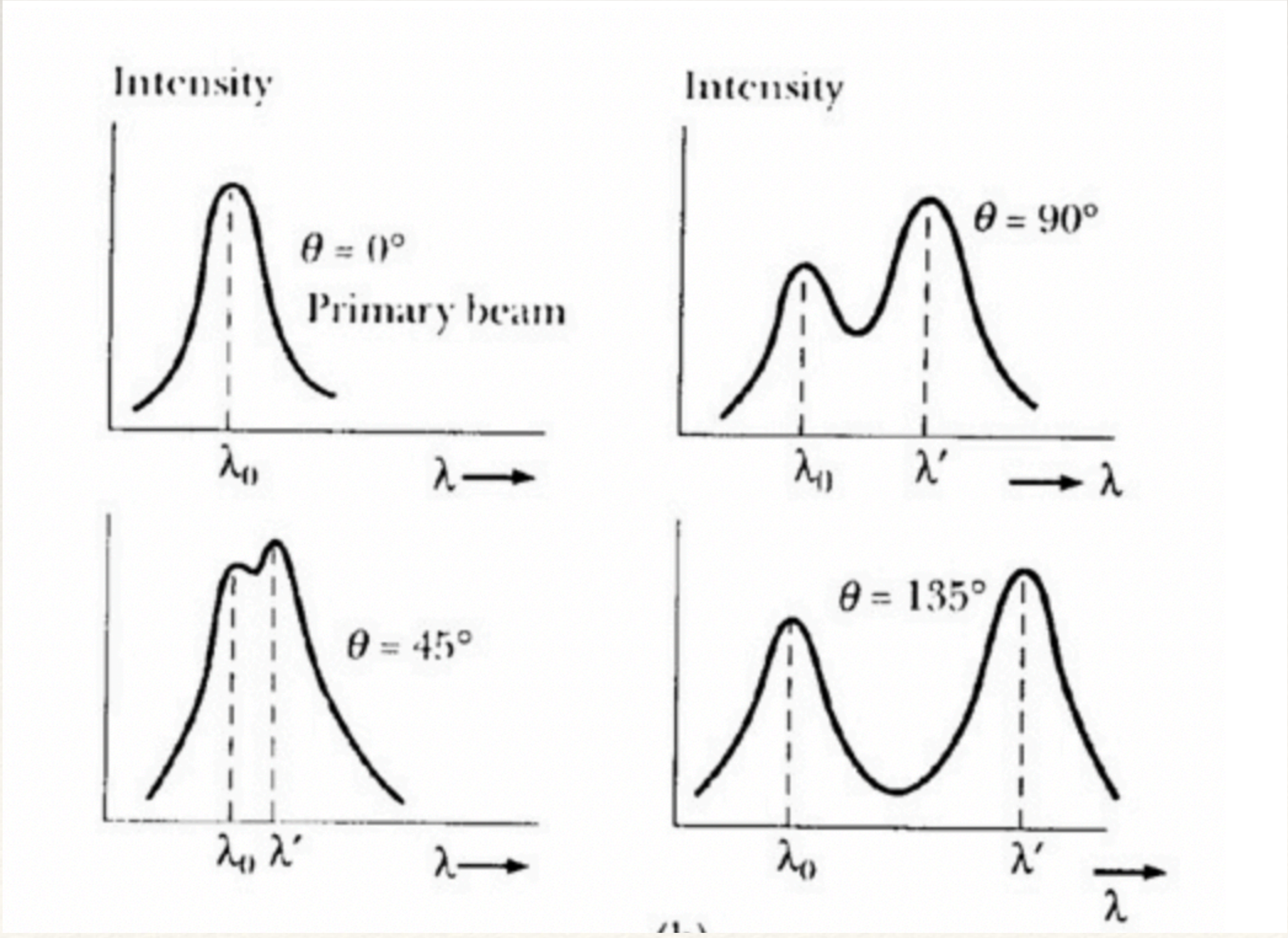
Historical Motivation: Light as a particle

1923

Explained the wavelength shifts during scattering of X-rays

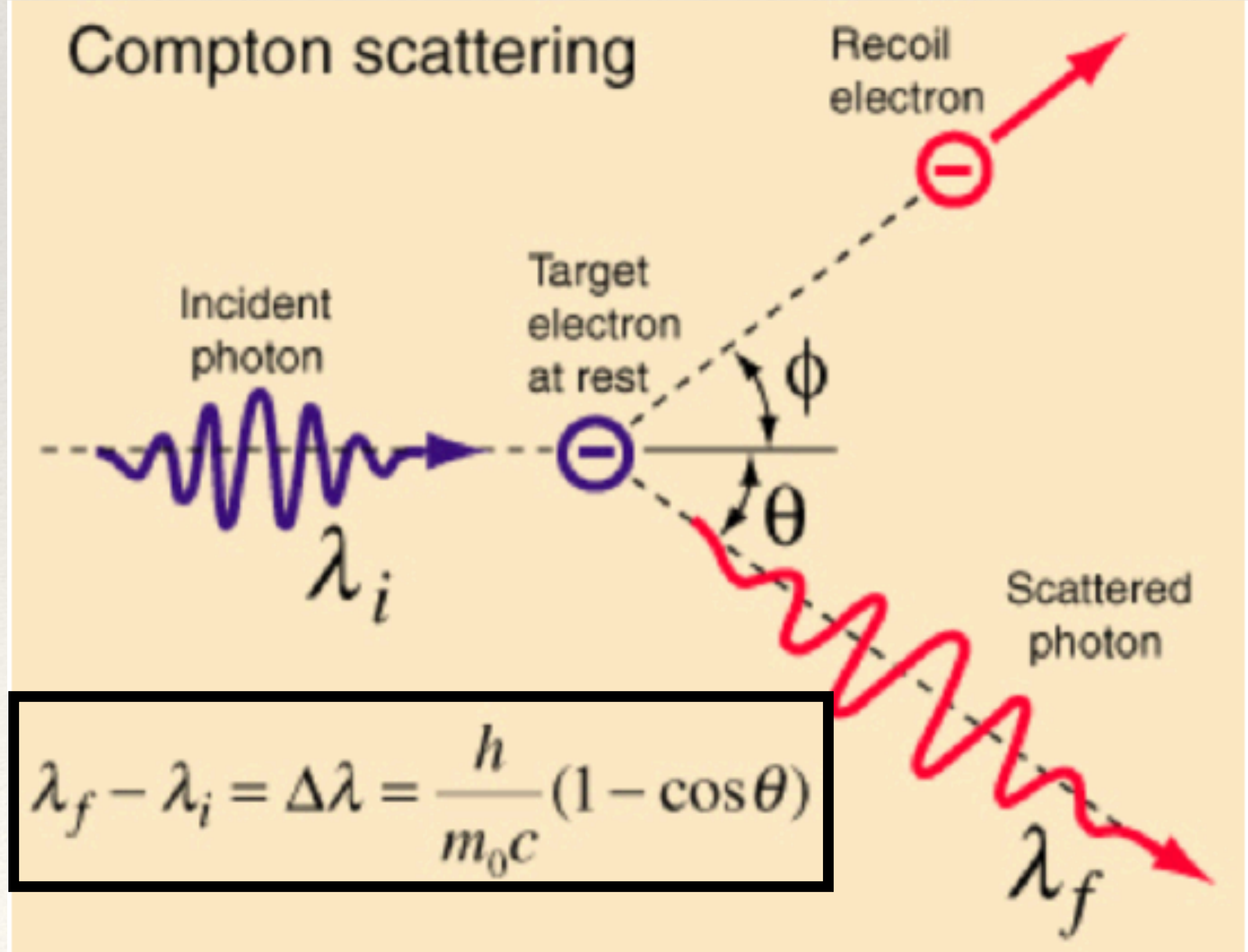
A. H. Compton



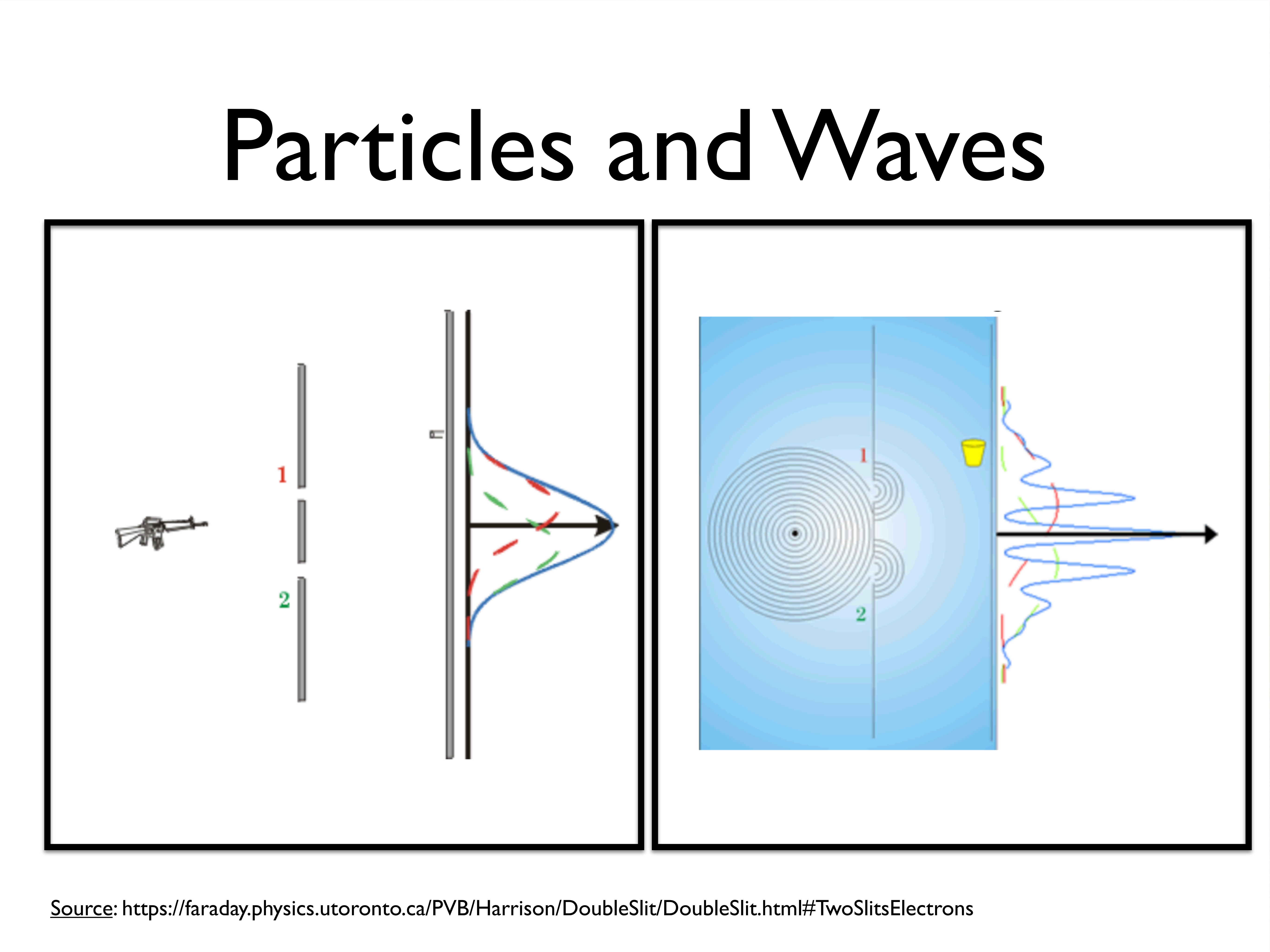


He showed that the only way to explain this was to assume the light particles also have momenta and along with fixed energy.

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



So is light a wave or a particle???



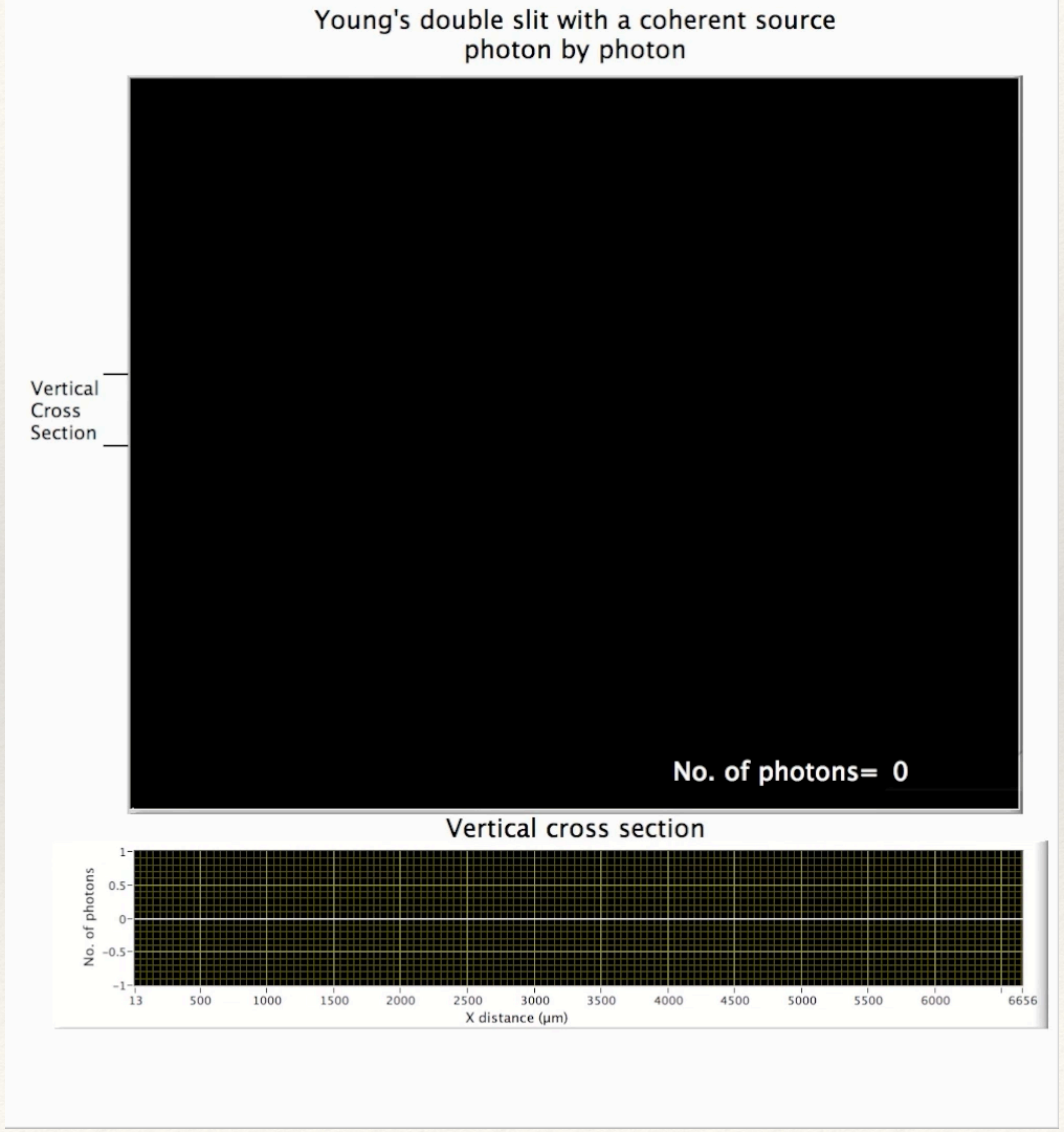
How should waves behave through a double-slit?

https://www.falstad.com/ripple/

So is light a wave or a particle???

How do photons behave through a double-slit?

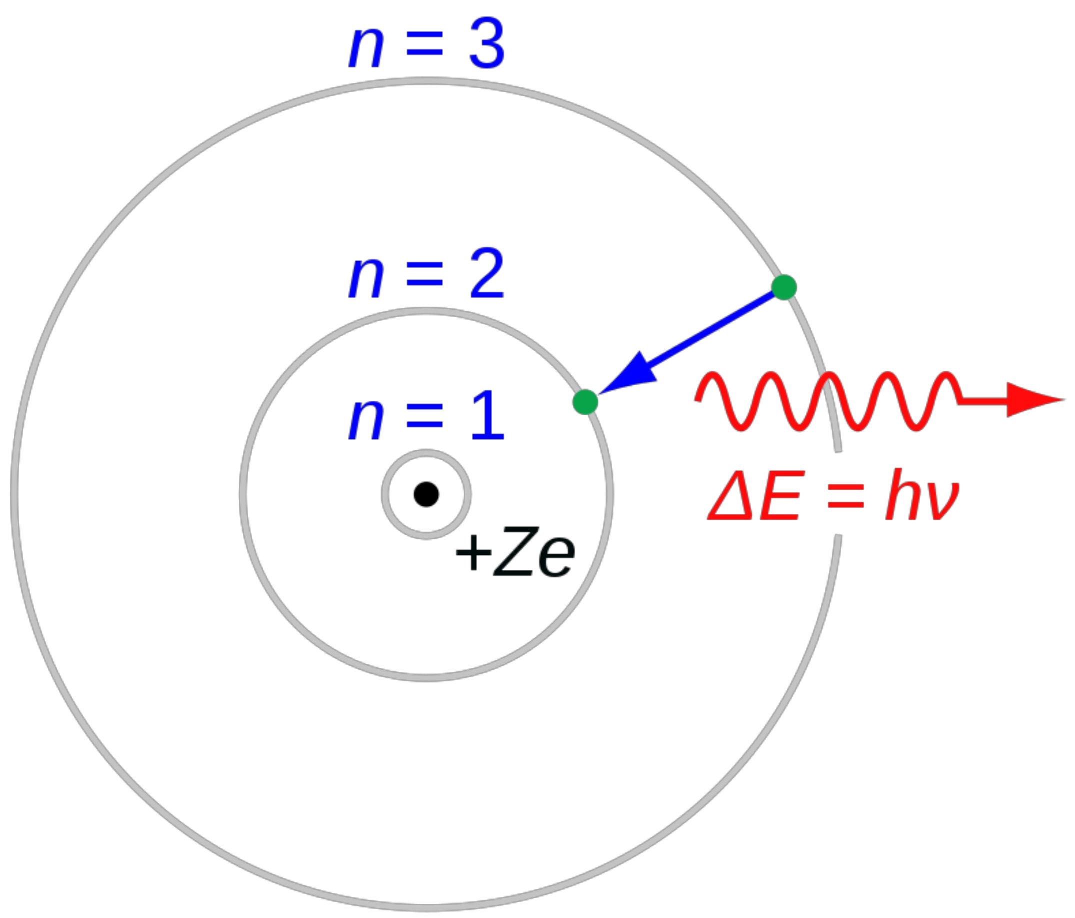
Am. J. Phys. 84, 671–677 (2016)



Atomic Structure

Bohr proposed a model for the H atom to explain the Ritz combination law

Neils Bohr



$$\bar{\nu}_{ab} = R_H \left(\frac{1}{n_a^2} - \frac{1}{n_b^2} \right)$$

$$E_n = -\frac{m}{2\hbar^2} \left(\frac{Ze^2}{4\pi\epsilon_0} \right)^2 \frac{1}{n^2}$$

Atomic Structure

1914 Franck-Hertz show the shell structure of the atoms and energy quantization
1921 Stern-Gerlach show electron has an intrinsic angular momentum (spin)

1923 Louis de Broglie hypothesis
Matter waves

$$\nu = \frac{E}{h}$$

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

1923-27 G.P.Thomson and Davisson-Germer experiments show electron's wave nature

Interestingly, J.J.Thomson discovered the electron in 1897 (as a particle!!). Father and son both won Nobel prizes for their respective discoveries.

Is matter a wave or a particle?

Another nice demonstration of how the wave-particle duality of quantum mechanics works:

Not completely correct!

- Non-quantum objects will for two lumps as
- Upon observation, electron going through one slit will still show interference!

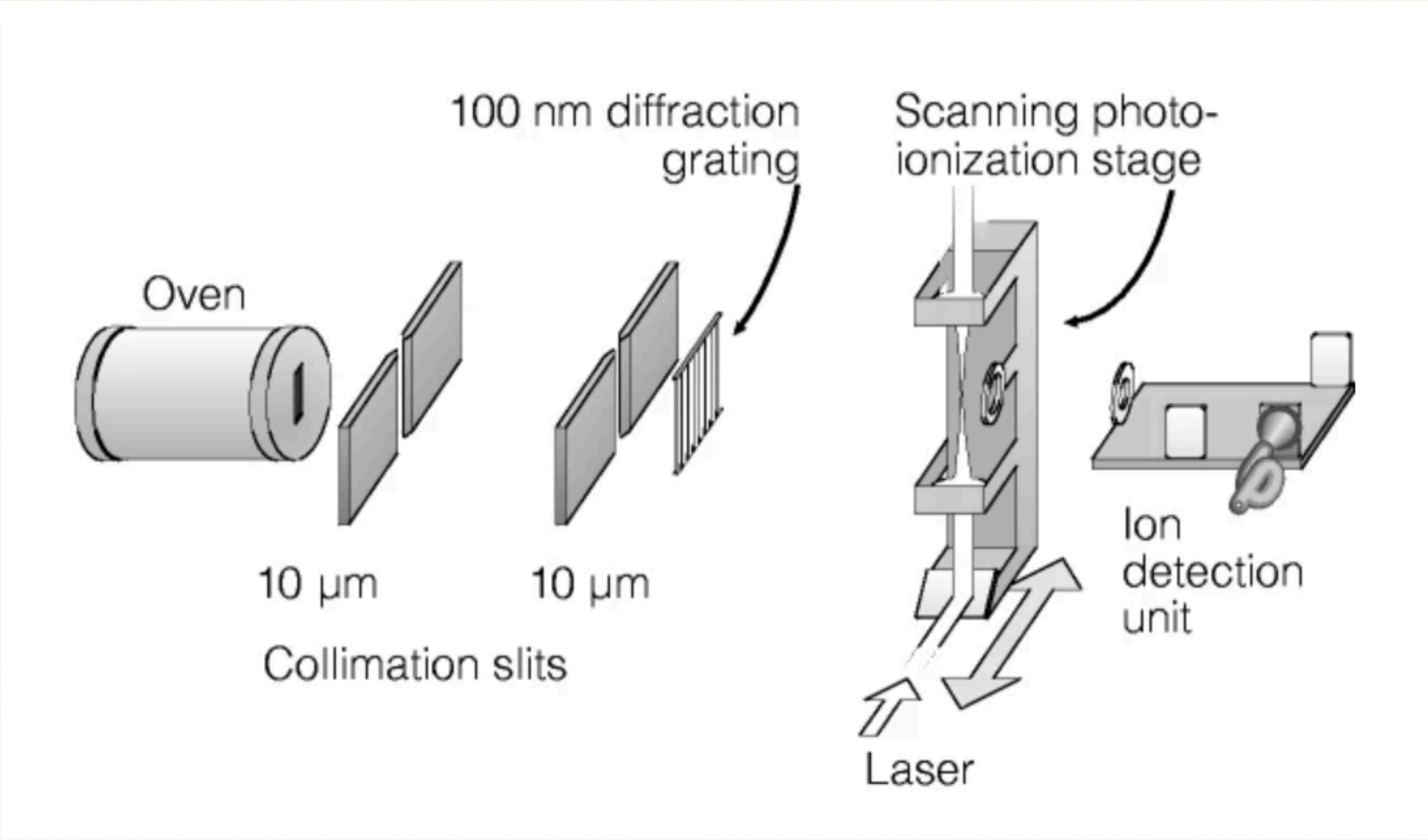
Summary of the double-slit experiment with electrons

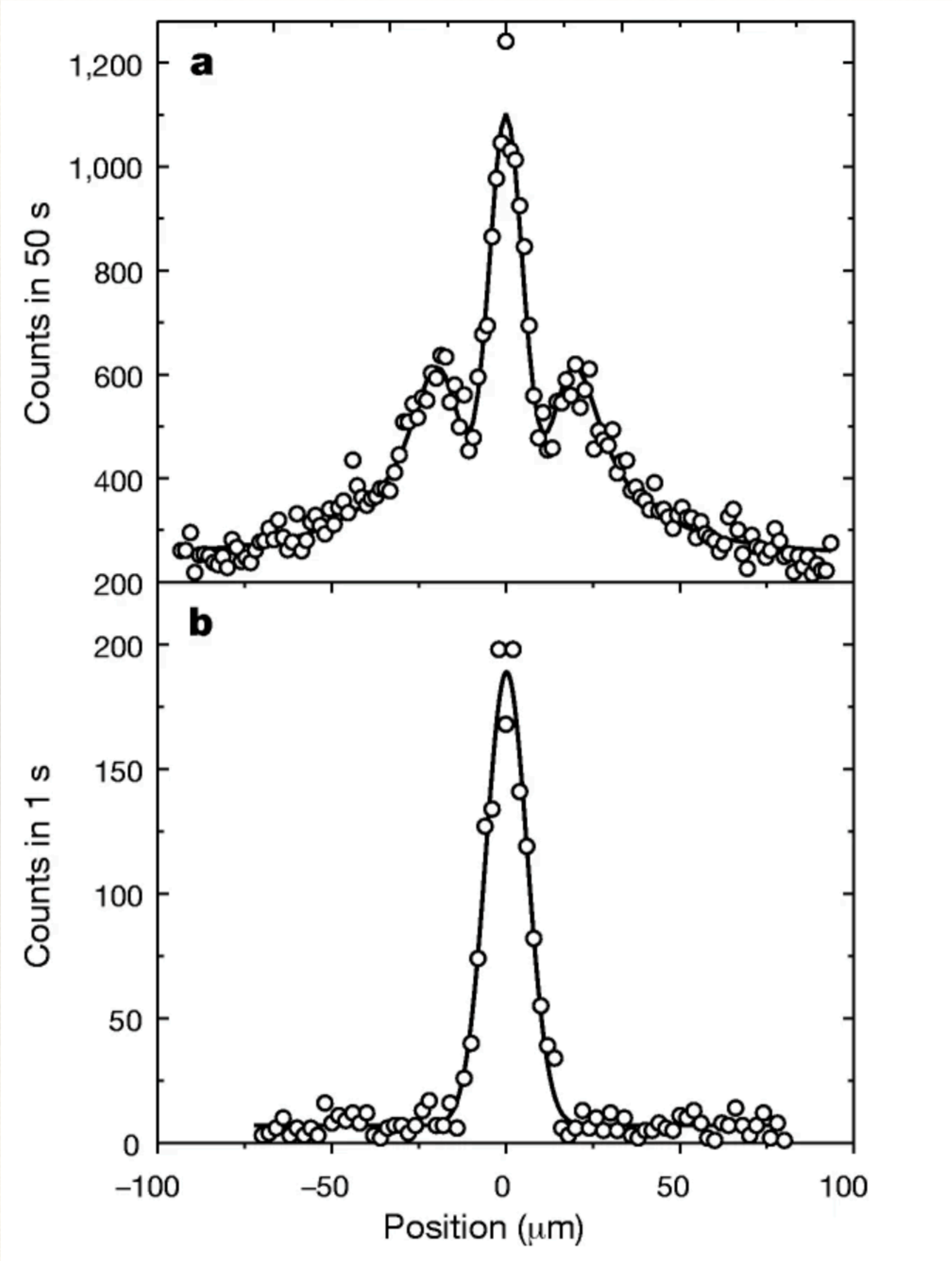
- Interference pattern observed at the detector when both slits are open.
- Closing either slit results in "particle-like" distribution at the detector (predominantly one bump).*
- Slowing down the rate of electrons (one electron at a time) still gives the interference pattern.
- If we try to observe which slit the particle goes through we get back the "particle-like" distribution.
- The fate of each electron cannot be predicted but the final interference patten is exactly reproducible (for the same source and same slits).

N.B. Here, "particle-like" actually refers to a single-slit interference pattern!

Interference of matter waves for larger particles

Interference in C_{60} molecules (*Nature* **401**, 680, 1999)

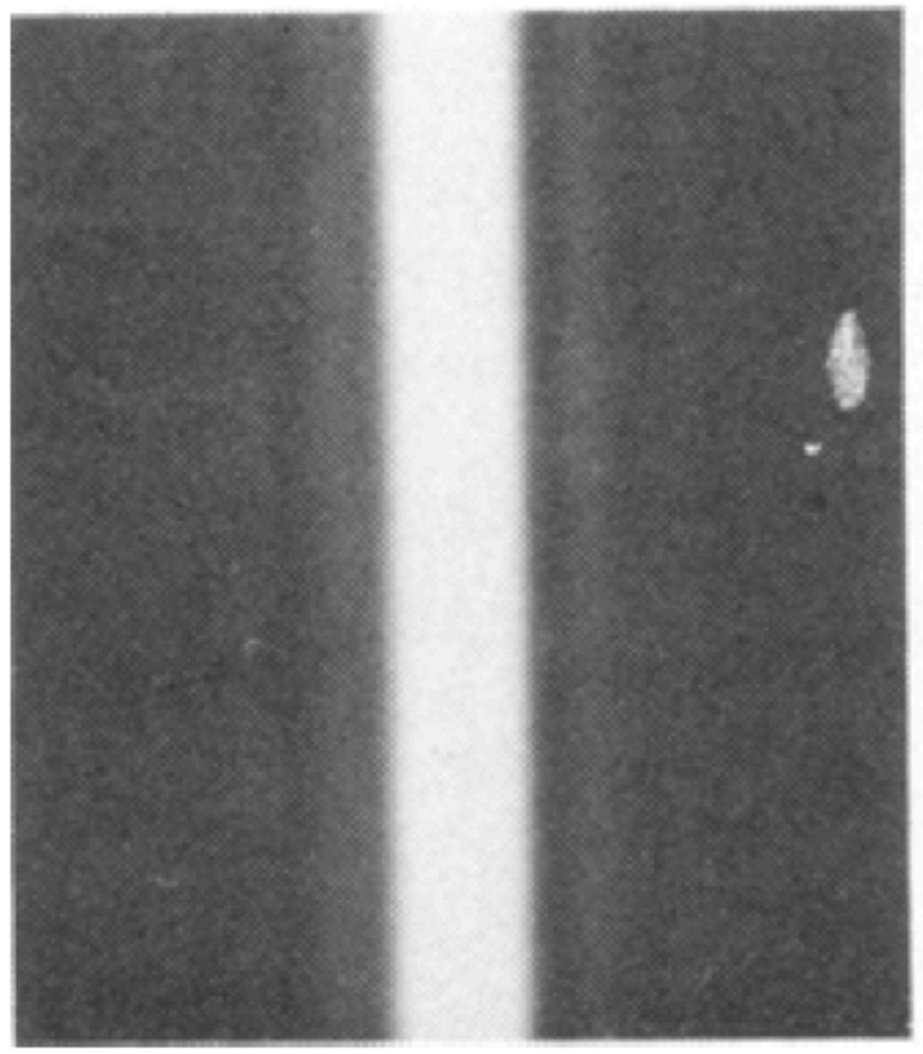




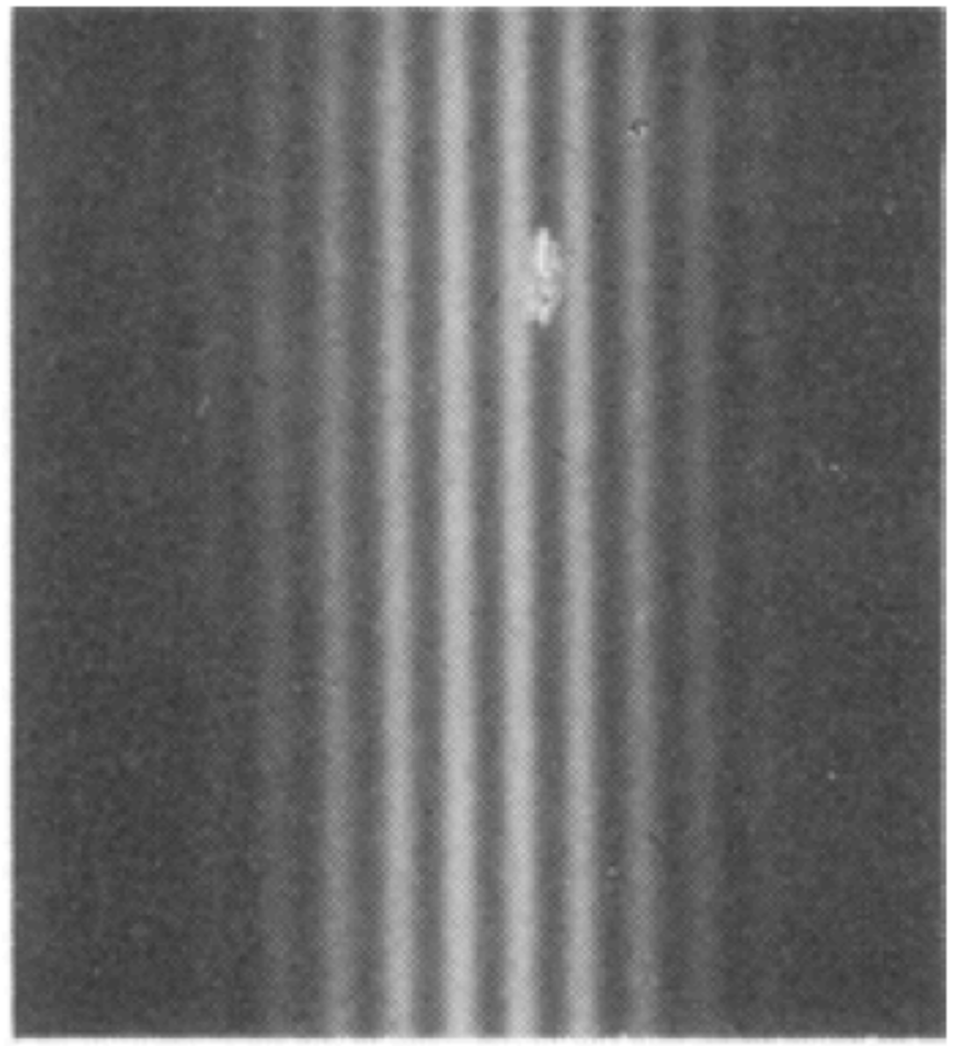
Without grating
(Single slit)

Interference of matter waves for larger particles

Electron diffraction through multiple slits (*Am. J. Phys.* **42**, 4, 1974)



Single slit



Two slits

Acknowledgements

Wikipedia commons
Google images
YouTube
The textbooks of the course.