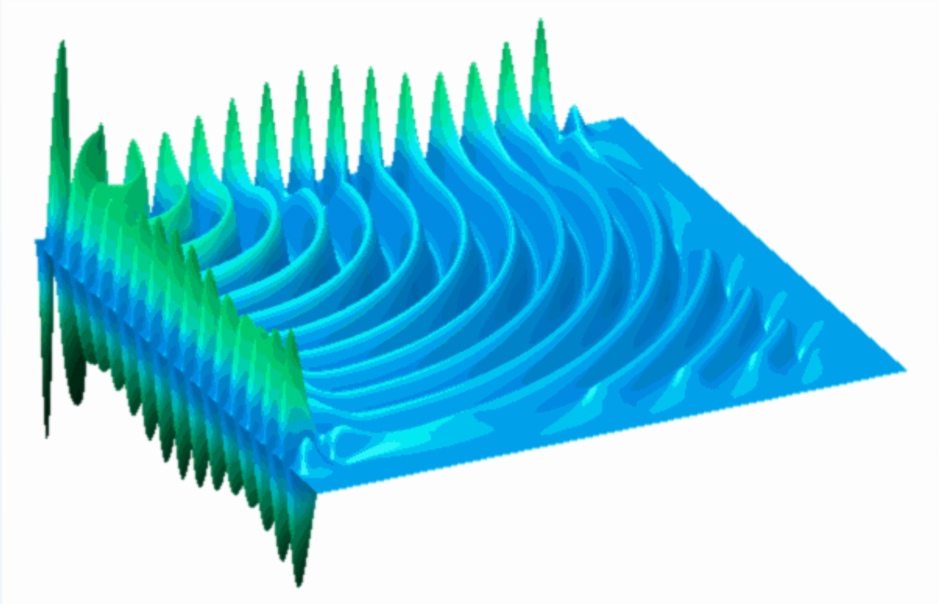
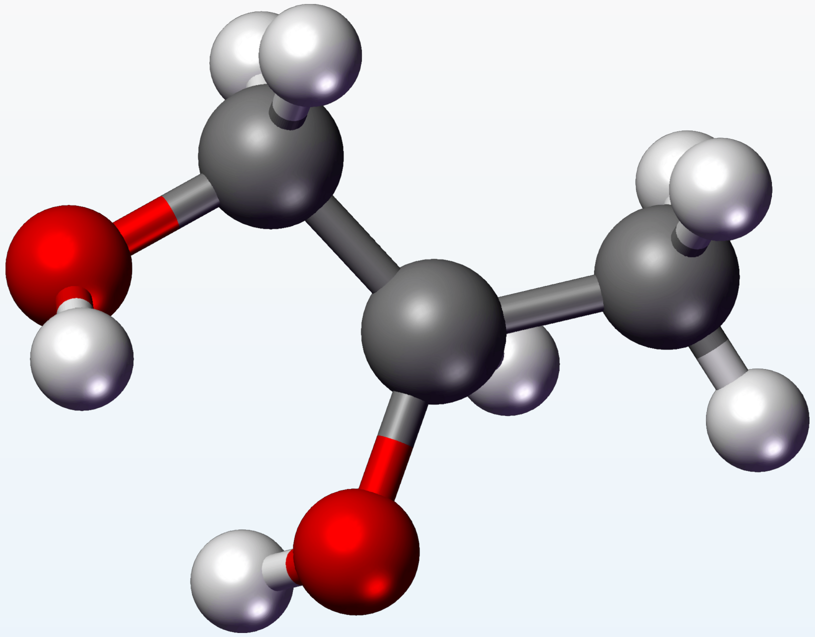




Van Quantum tot Molecuul (X_420545)

academic year 2016-2017

Vrije Universiteit Amsterdam
Faculteit Exacte Wetenschappen
BSc Programma Medische Natuurwetenschappen

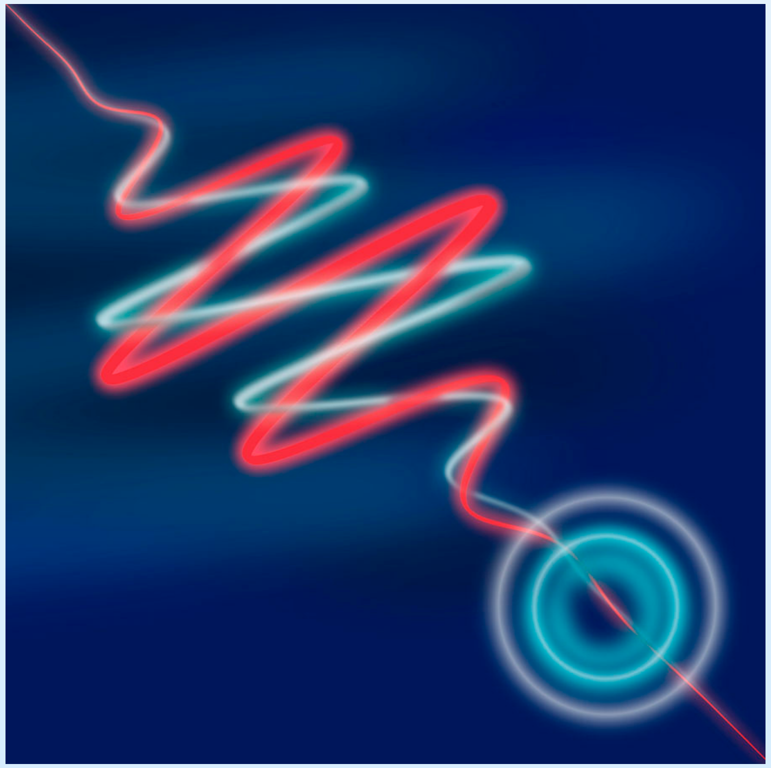
HC1

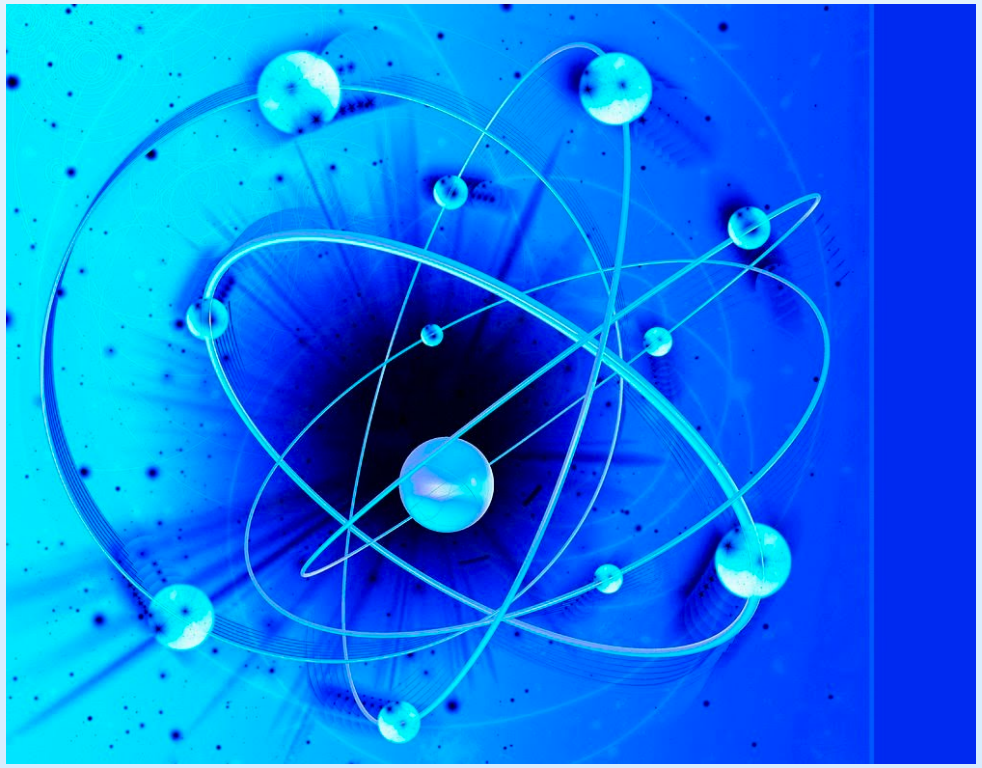
Learning Goals HC1

- ☑ To review the experimental results that lead to the **development of quantum theory**

- ☑ To understand that both matter particles and light have associated a **dual wave/particle description**

- ☑ To motivate that quantum theory is necessary to describe the **structure and properties of particles, atoms and molecules**





Why quantum theory?

By the **end of the XIXth century**, it seemed that known physical theories were enough to describe the **wide majority of known physical phenomena:**

☑ Electromagnetic theory (Maxwell, Ampere, Faraday,…)

☑ Classical mechanics, including gravity orbital motion (Galileo, Newton, Lagrange, ..)

☑ Thermodynamics and statistical mechanics (Boltzman, Maxwell, Gibbs, Thomson, …)

☑ Optics (Newton, Young, Fresnel, …)

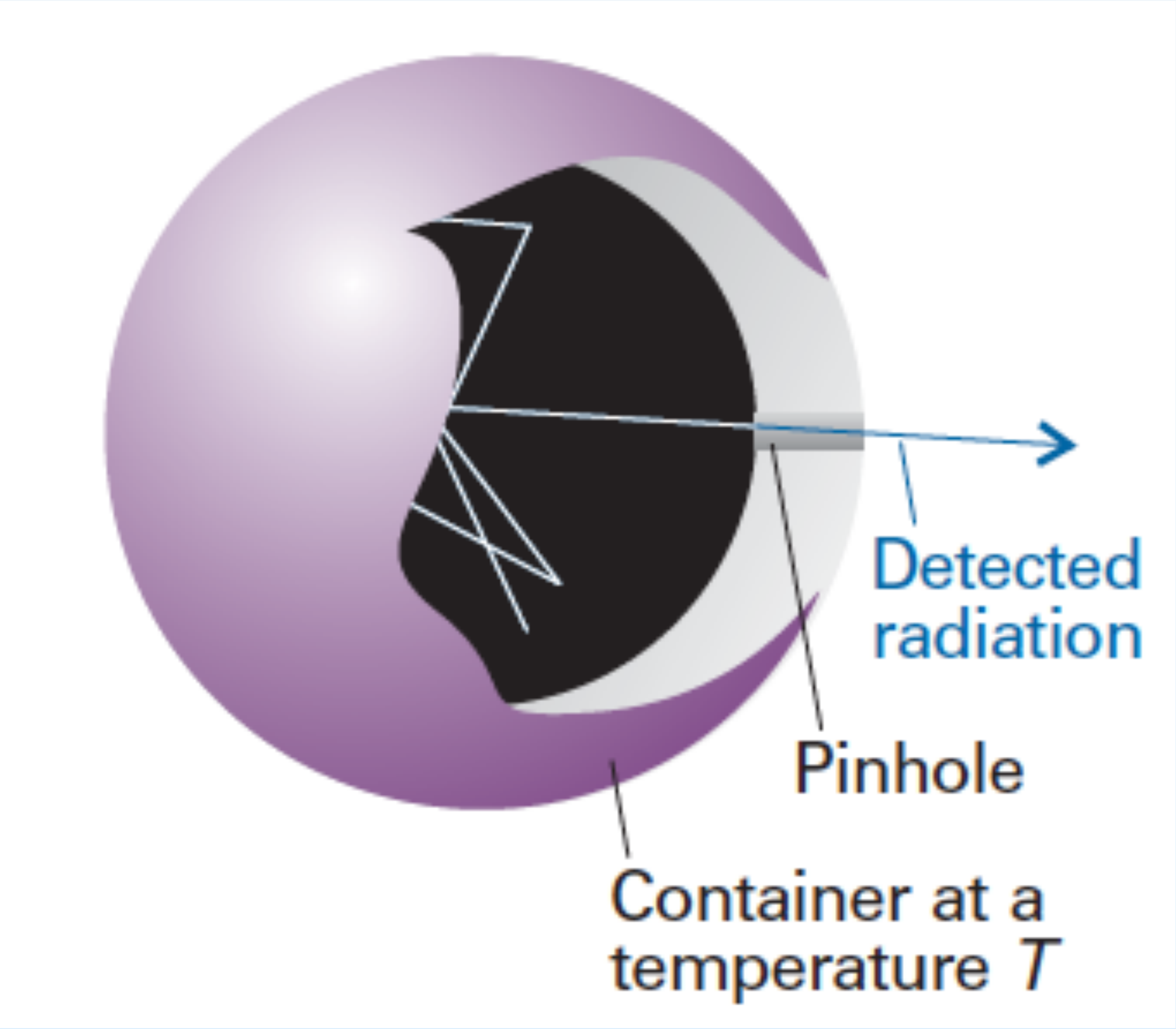
"… it seems probable that most of the grand underlying principles have already been firmly established … An eminent physicist remarked that the future truths of physical science are to be looked for in the ***sixth place of decimals****"*, Albert Michelson, 1894

The end of physics? While some phenomena still resisted explanation, it was commonly thought that sorting them was just a matter of time.

"the devil is in the details", unattributed

The black-body spectrum

One of these *little details* was the description of electromagnetic radiation emitted by a *black body,* an idealised body that **absorbs all incident radiation** (hence is *black*)



An idealised representation of a black body is a container at temperature T with a pinhole as only aperture, so that **radiation emitting the container is in thermal equilibrium with it** (since it has scattered N>>1 times with its walls)

The black-body spectrum

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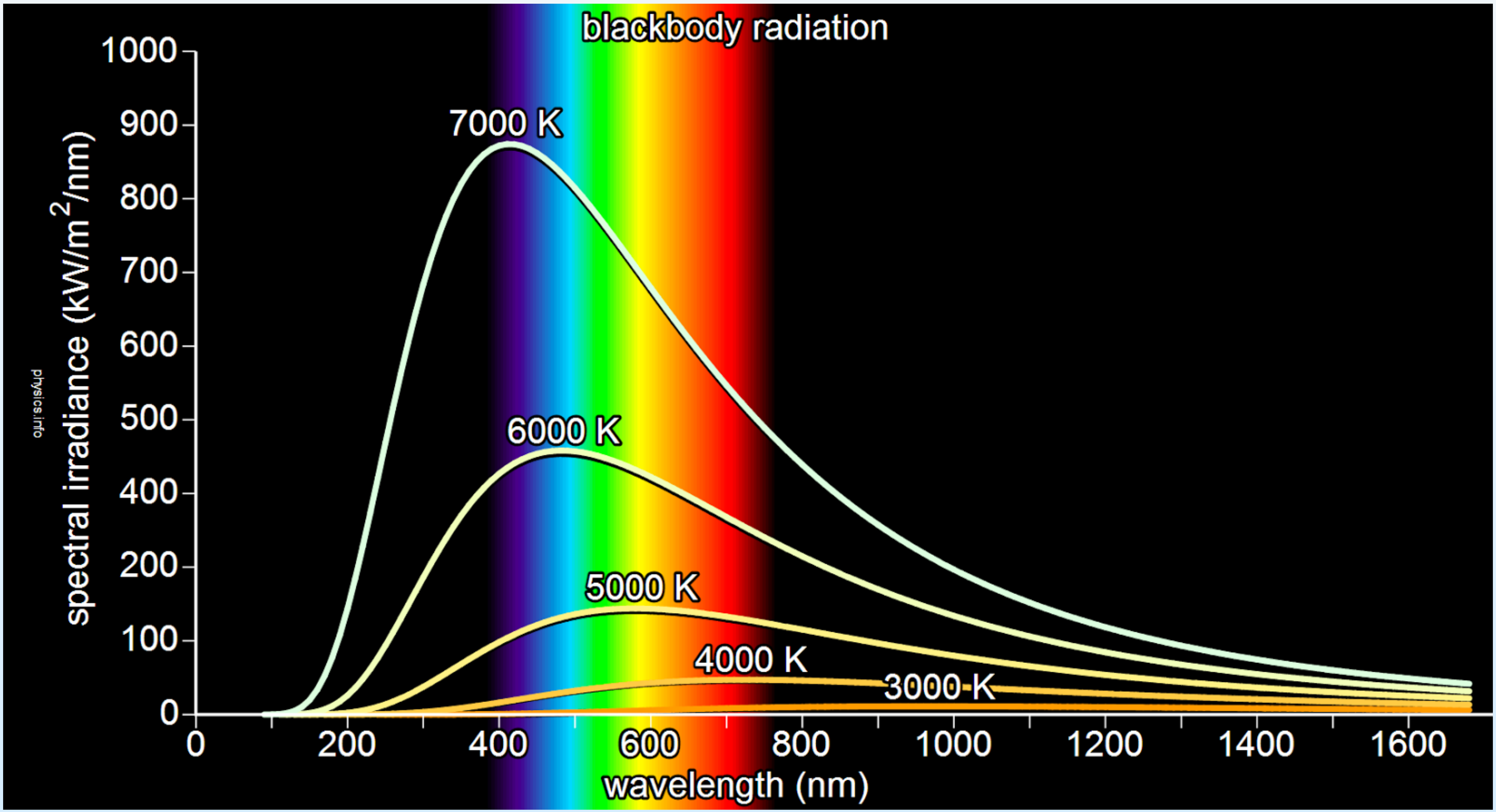

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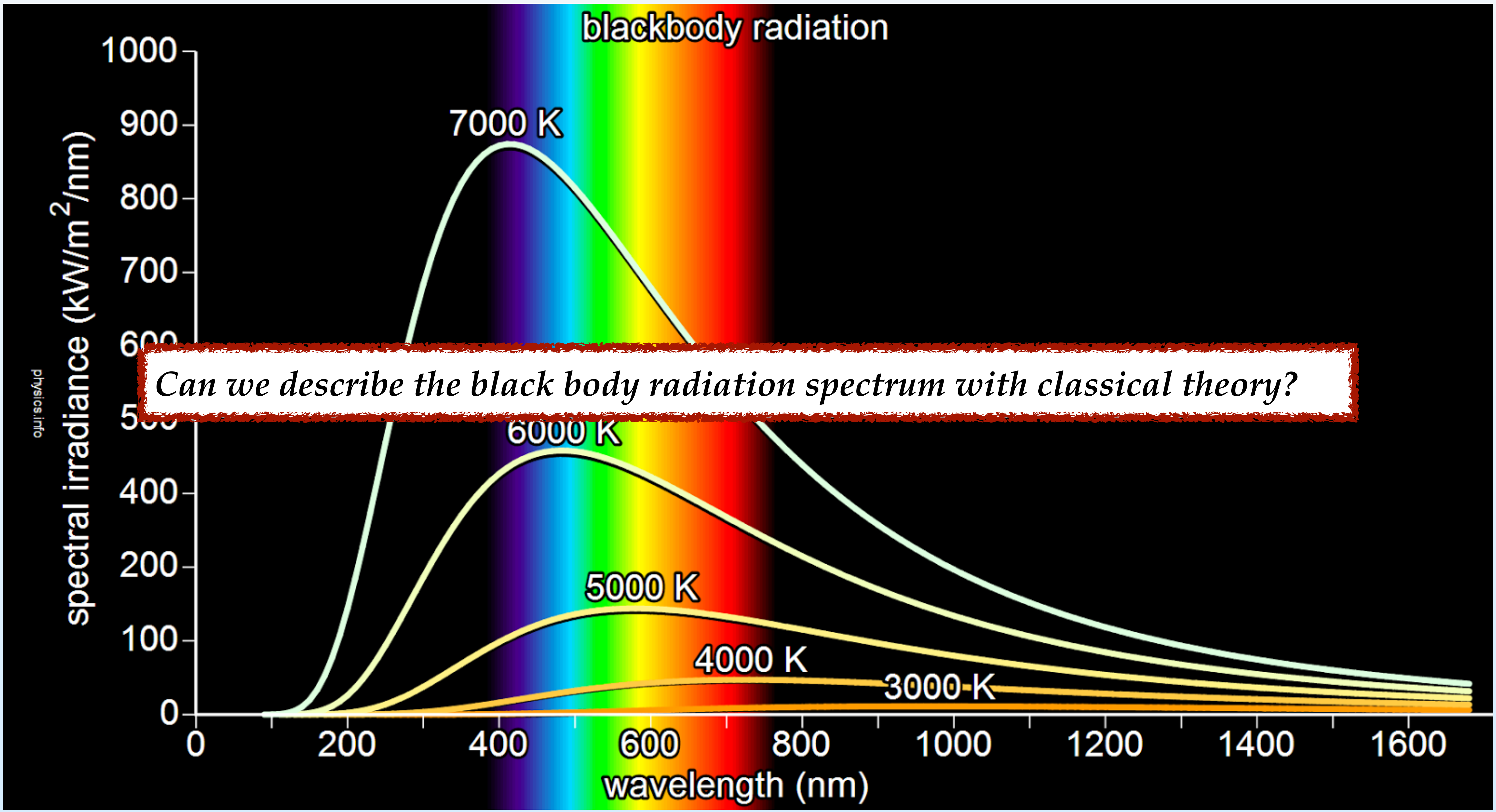


Can we describe the black body radiation spectrum with classical theory?

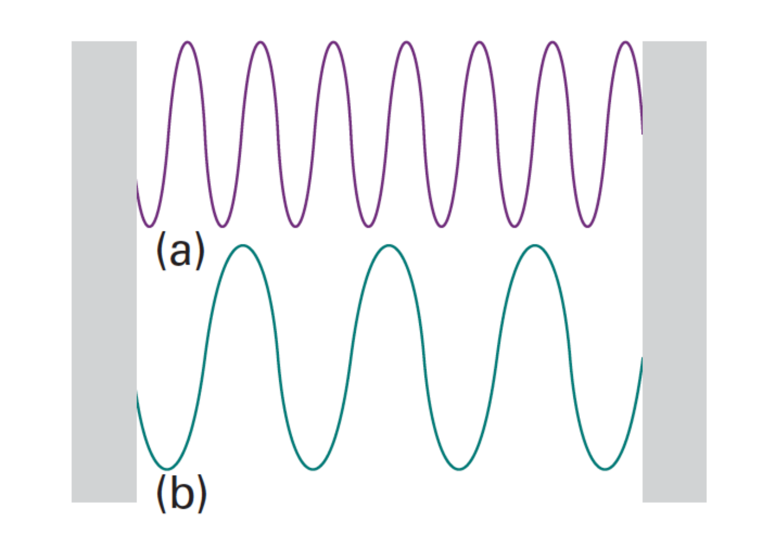
The black-body spectrum

The energy distribution as a function of the radiation wavelength is proportional to the **density of states** ρ that can be populated at this wavelength

$$d\mathcal{E} = \rho d\lambda$$

Classically, electromagnetic waves can be modelled as a **collection of oscillators** where **all possible frequencies are allowed**.

$$E = A\cos(\omega t - kx)\ ,\omega = 2\pi\nu\,, k = \frac{2\pi}{\lambda}$$



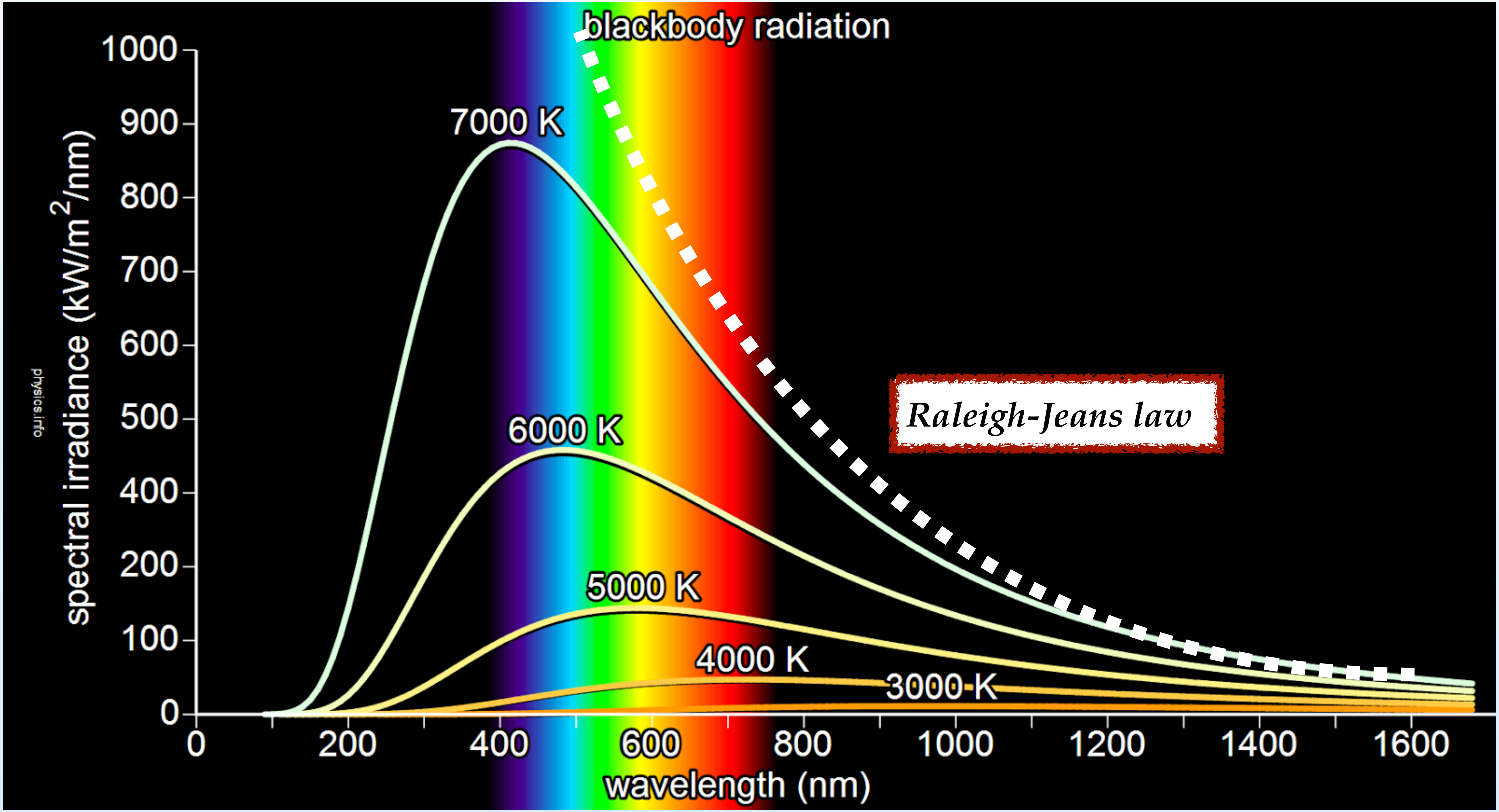
Using the equipartition theorem, one finds the **Rayleigh-Jeans law** for the density of states, with decreases with the radiation **λ**

$$\rho = \frac{8\pi kT}{\lambda^4}$$

How well classical theory describes data?

The ultraviolet catastrophe

The **Rayleigh-Jeans law** describes well the data at high λ (small E) but fails spectacularly at small λ (large E): this is the **ultraviolet catastrophe**, in classical physics the total energy radiated by a black body should be **infinite!**



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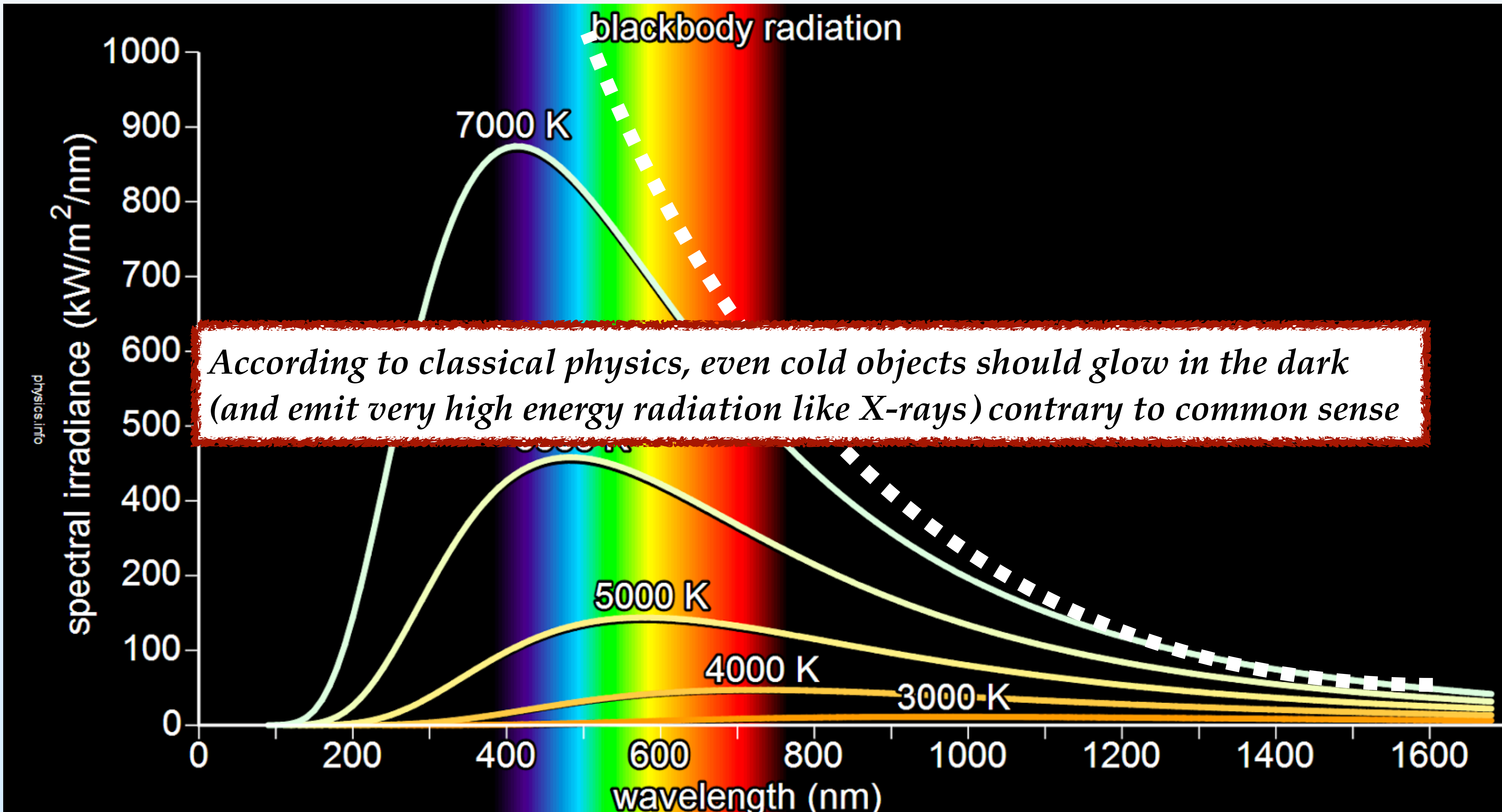


Planck's "quantum" hypothesis

Max Plank found that the black-body spectrum could be described if one made the **hypothesis** that electromagnetic waves cannot take any possible energies, but rather that their energies are **quantized,** *i.e.,* they are multiples of a basic **quantum of energy**

$$E = nh\nu = nh\frac{c}{\lambda}$$

with ***n*** an integer number

where the proportionality constant ***h*** is known as **Planck's constant**

With this assumption, the density of states turns out to be instead

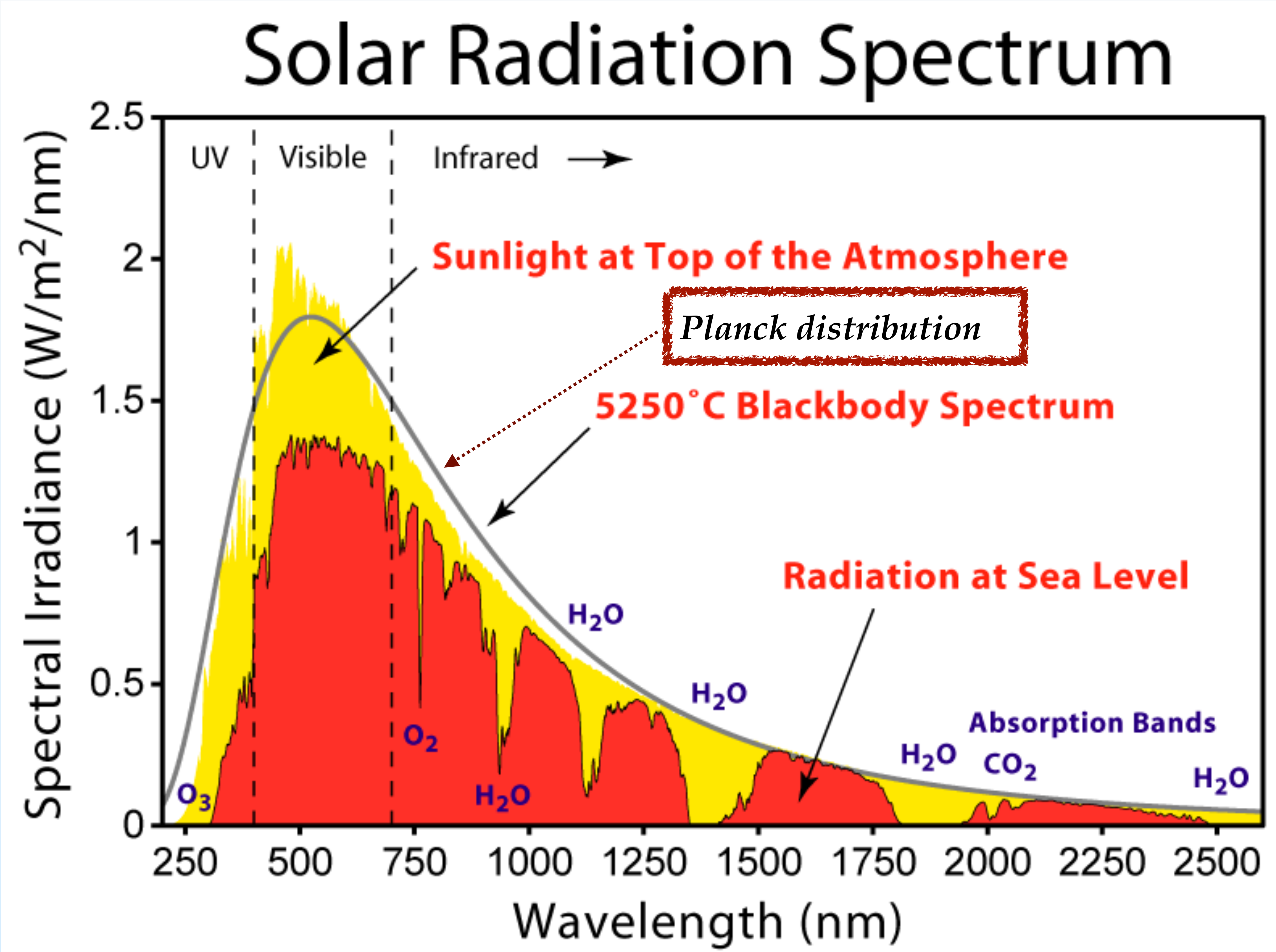
$$\rho = \frac{8\pi hc}{\lambda^5 (e^{hc/\lambda kT} - 1)}$$

which is known as the **Planck distribution**, nicely reproducing the experimental data

Planck's constant, one of the fundamental constants of Nature, is fitted from data:

$$h = 6.6 \cdot 10^{-34} J \cdot s$$

The Sun as a black body



Planck's distribution

An important feature of the Planck distribution is that it has the **correct limiting behaviour,** in particular for large wavelengths it reproduces **the Rayleigh-Jeans law**

$$\rho = \frac{8\pi hc}{\lambda^5(e^{hc/\lambda kT} - 1)}$$

as can be seen by using the Taylor expansion of the exponential in the **$\lambda \to \infty$ limit**

$$e^{hc/\lambda kT} - 1 = \left(1 + \frac{hc}{\lambda kT} + \cdots\right) - 1 \approx \frac{hc}{\lambda kT}$$

In the Planck distribution, the **$\lambda \to 0$ (E $\to \infty$) limit** is now well behaved

$$\rho = \frac{8\pi hc}{\lambda^5\left(e^{hc/\lambda kT} - 1\right)} \simeq \frac{8\pi hc}{\lambda^5} e^{-hc/\lambda kT} \to 0$$

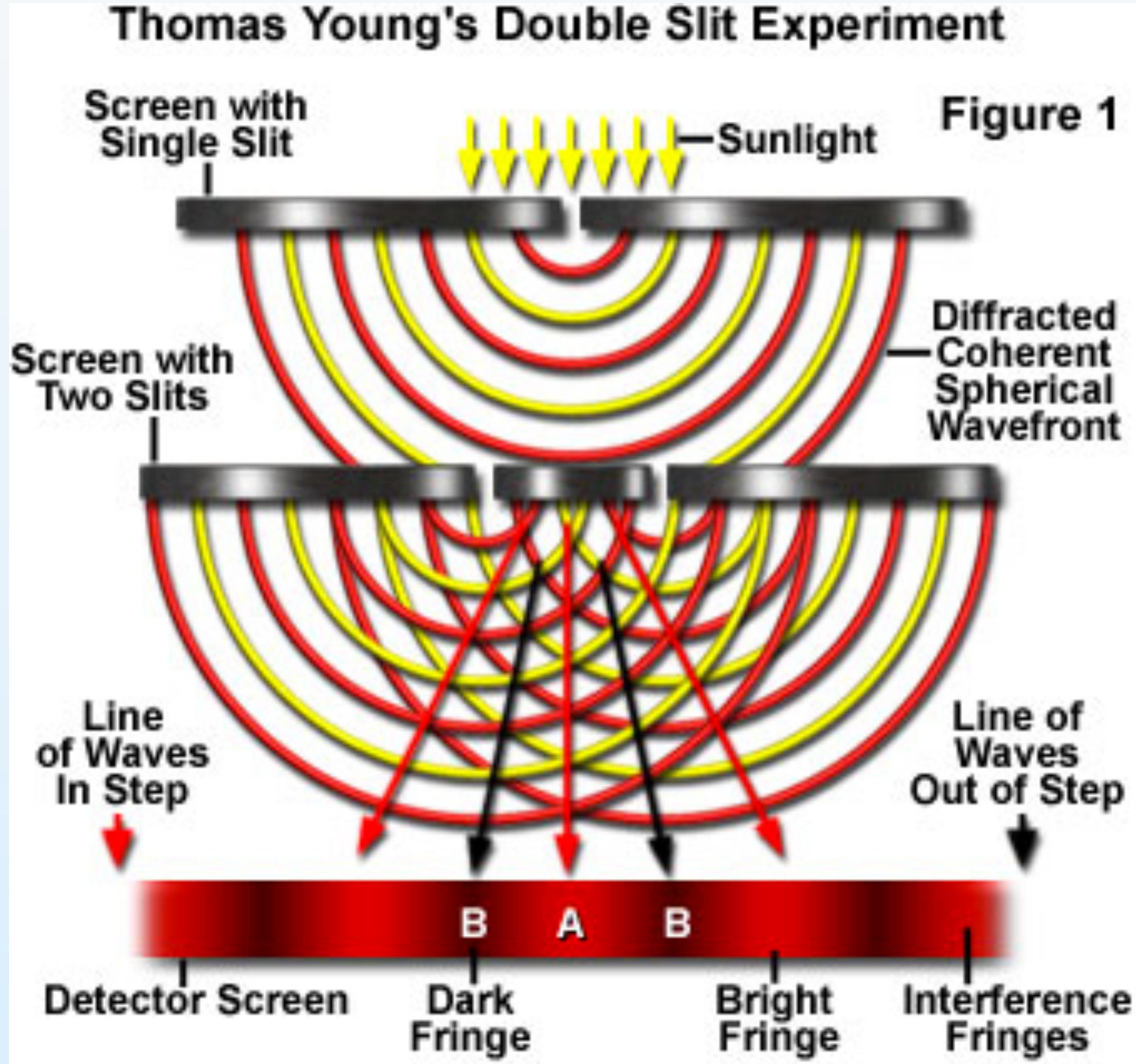
because the high-ν oscillators will only be excited if the **black-body walls can provide an energy (at least) hν**, which is **increasingly unlikely** for a fixed temperature

Wave-particle duality

In Maxwell's electromagnetism, light is described by an **electromagnetic wave**

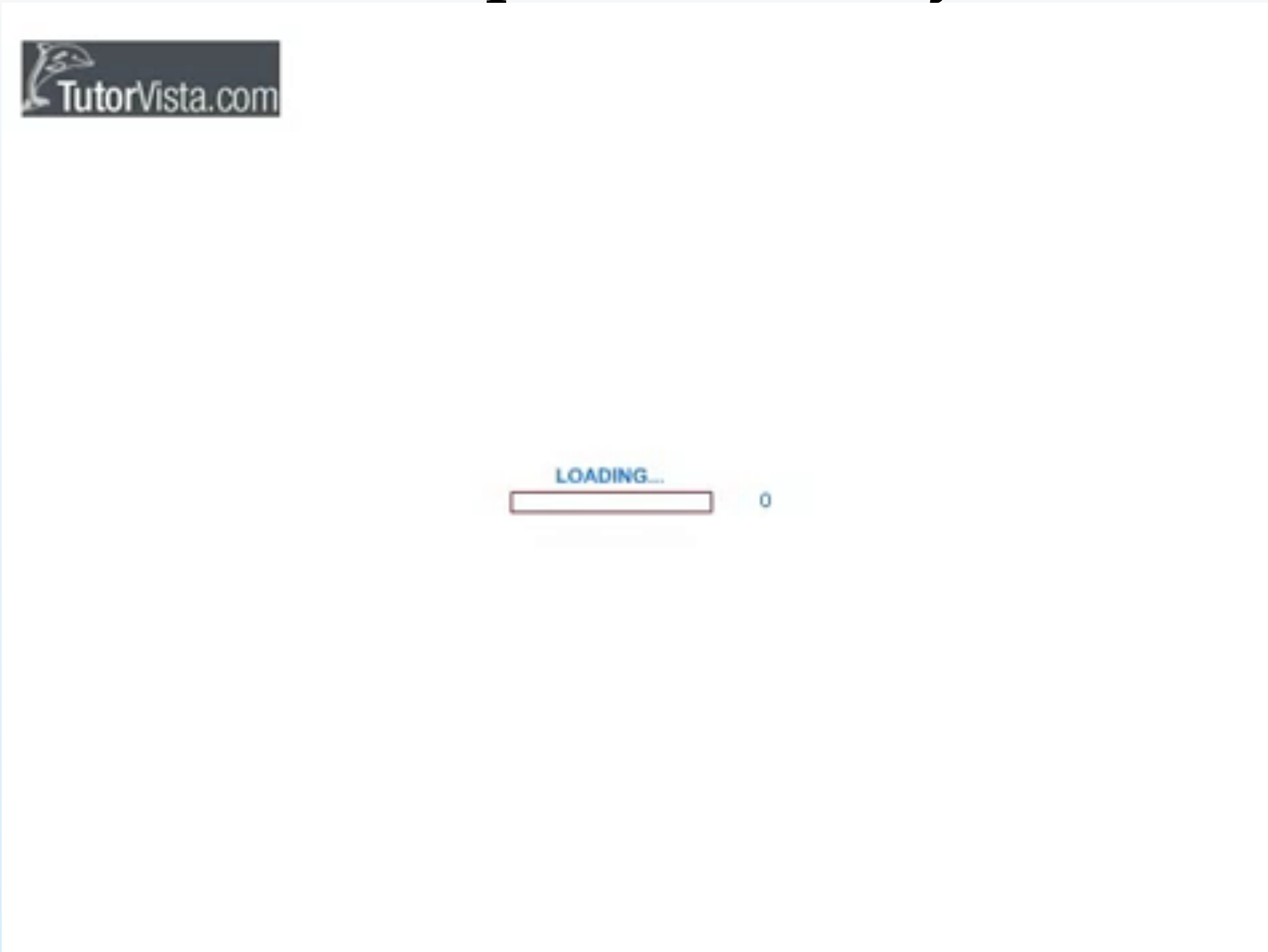
Indeed, light behaves an obvious **wave-like behaviour** (interference, diffraction), as shown for example in **Young's double slit experiment**

The appearance of **interference fringes** is a tell-tale sign of wave-like phenomena



$$E = A\cos(\omega t - kx)\;,\omega = 2\pi\nu\,,k = \frac{2\pi}{\lambda}$$

Wave-particle duality



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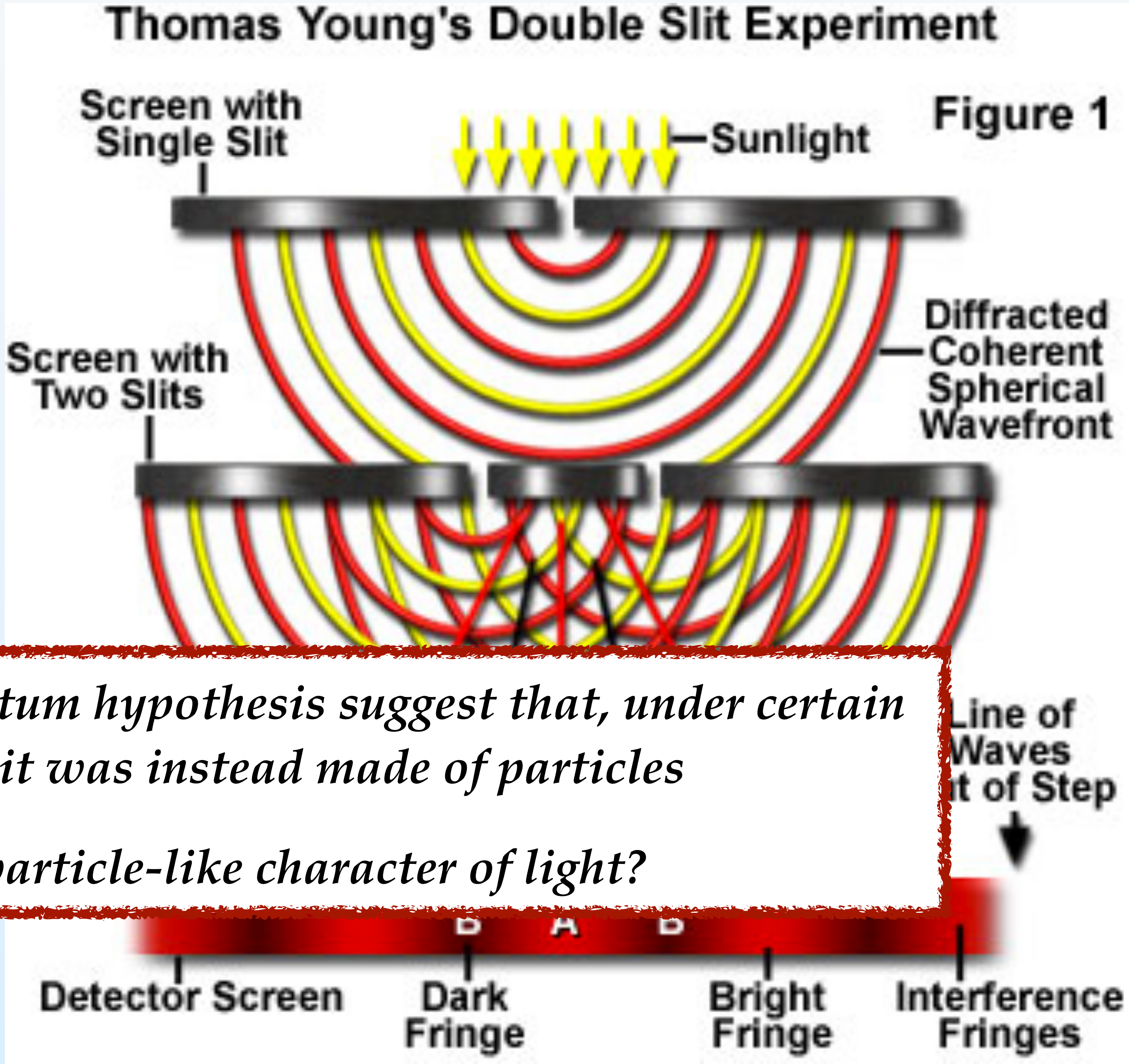


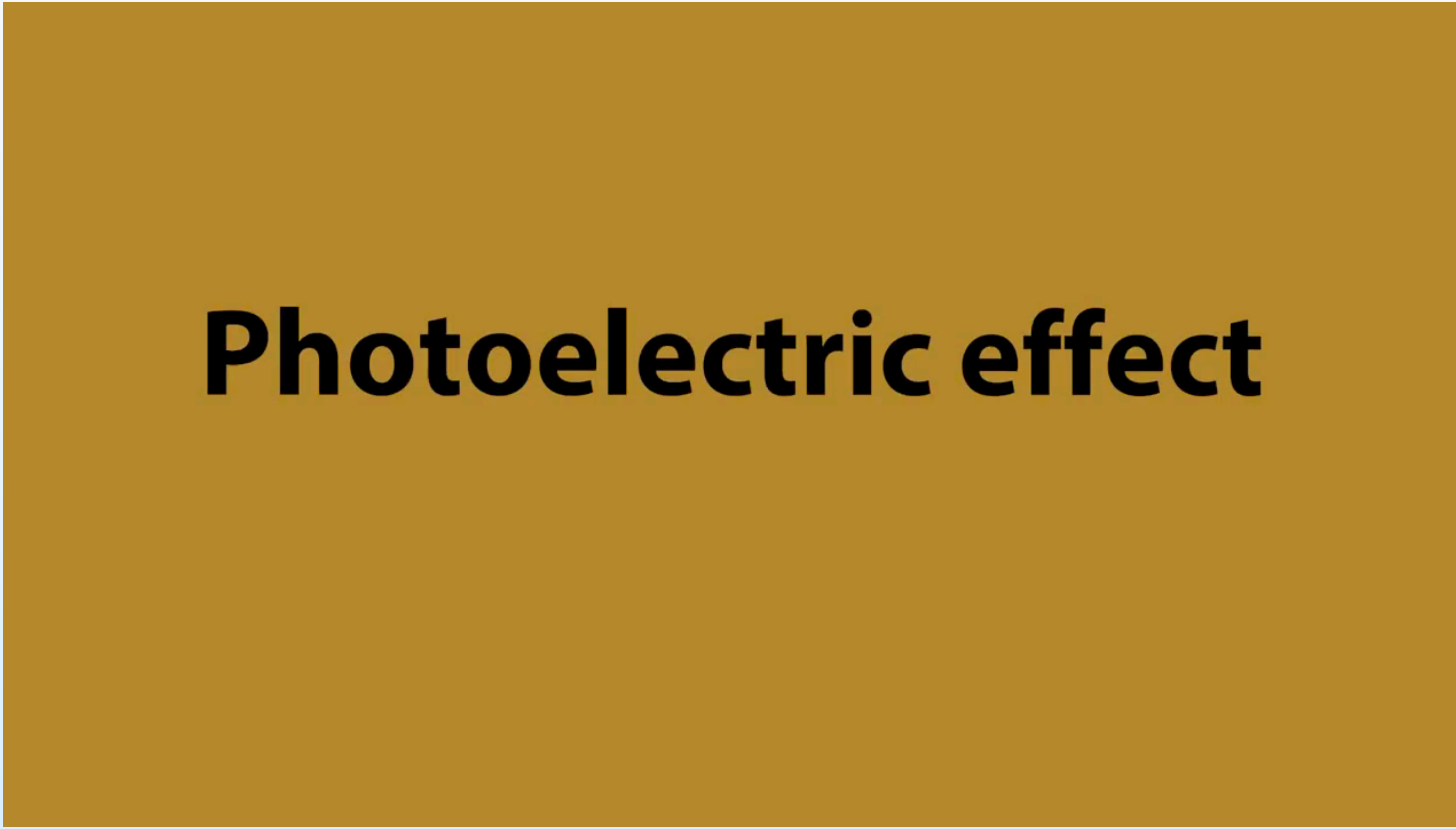
The
fri
like

On the other hand, Planck's quantum hypothesis suggest that, under certain conditions, light can behave as if it was instead made of particles

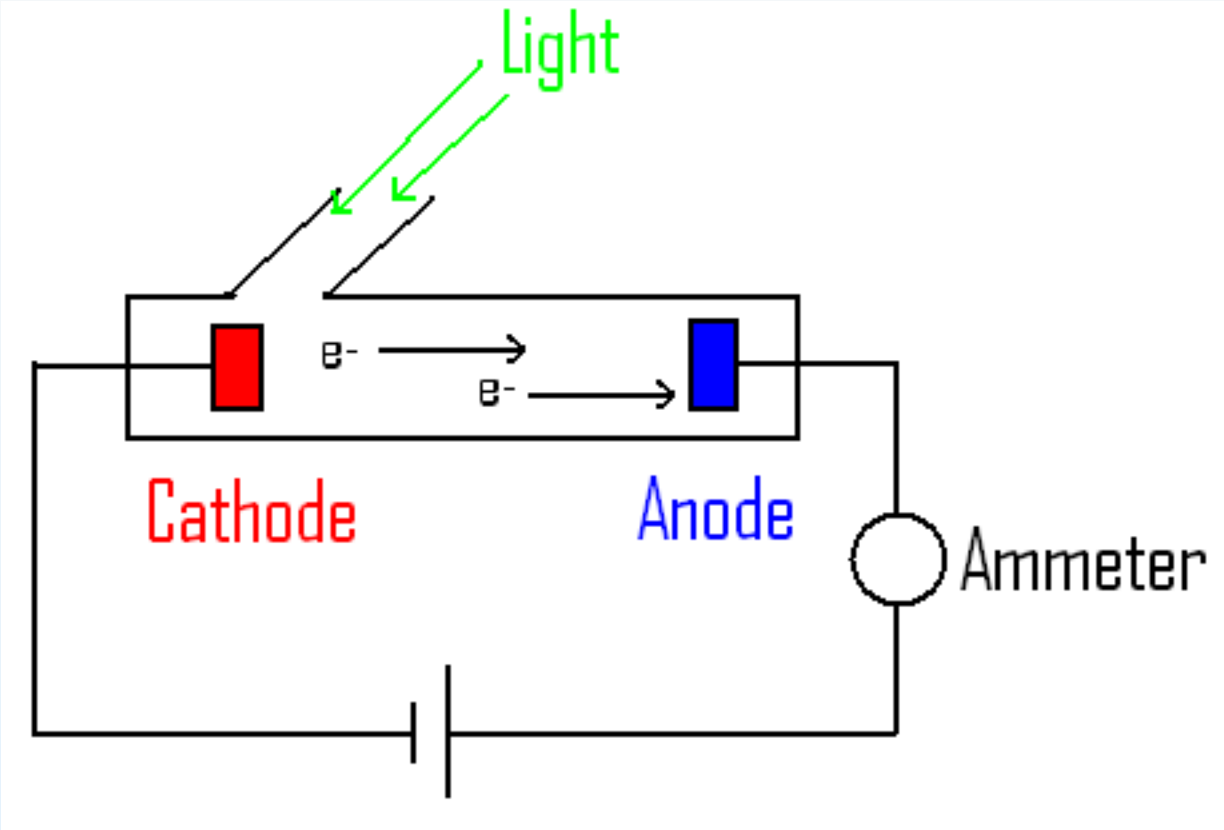
How can we verify this possible particle-like character of light?

$$E = A\cos\left(\omega t - kx\right) \,,\omega = 2\pi\nu\,, k = \frac{2\pi}{\lambda}$$

The photoelectric effect



The photoelectric effect

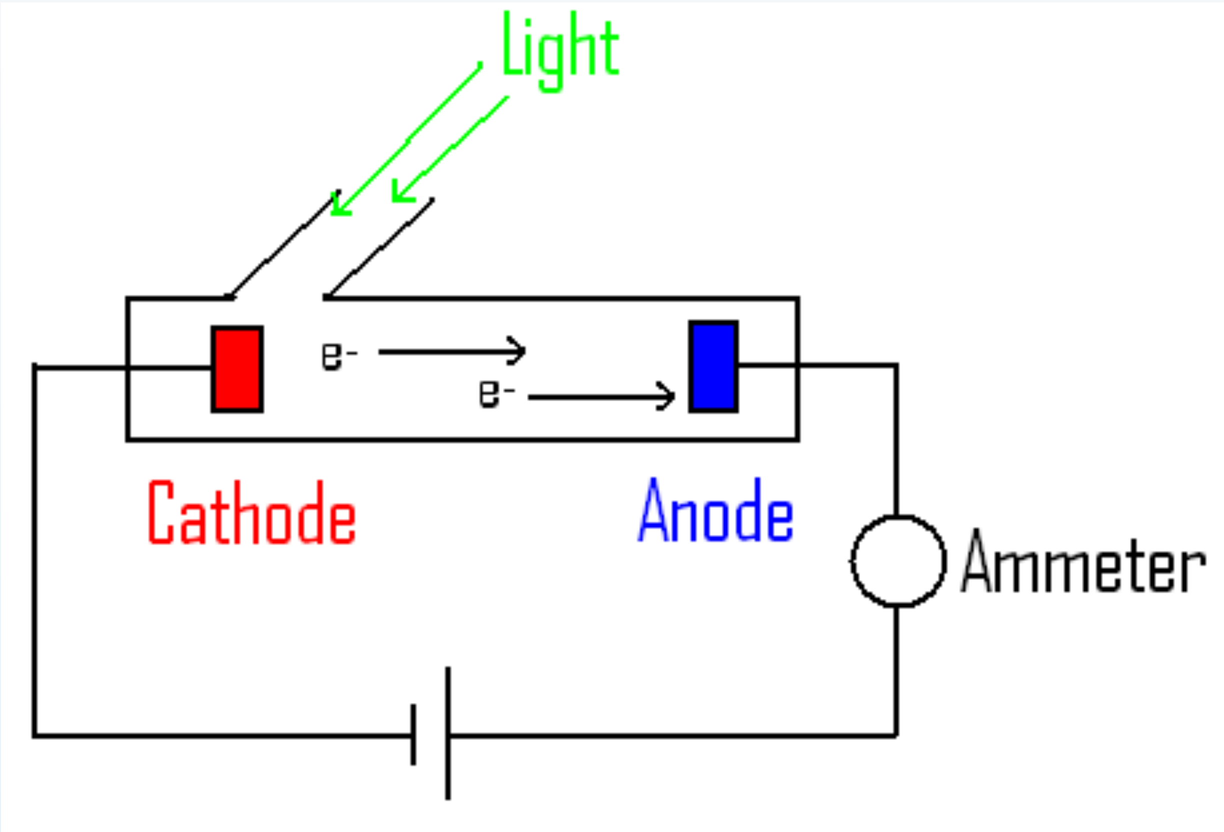


- Incident light on a **metallic surface** (cathode) induces **electron emission**, which are collected by the anode leading to a **electric current in the circuit**

- In **classical physics**, incident light is described by a **plane EM wave**: provided that **light has enough intensity**, it should be possible to induce **electron emission regardless of its frequency**

however ….

The photoelectric effect



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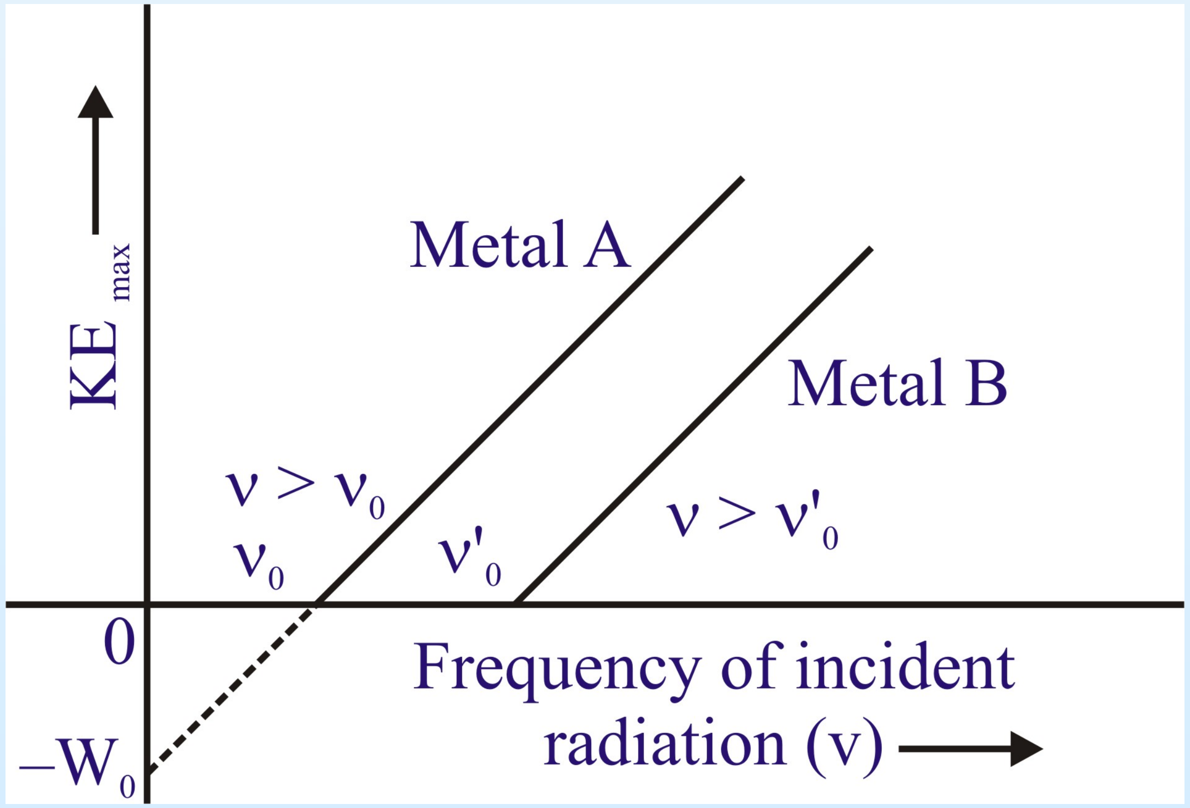
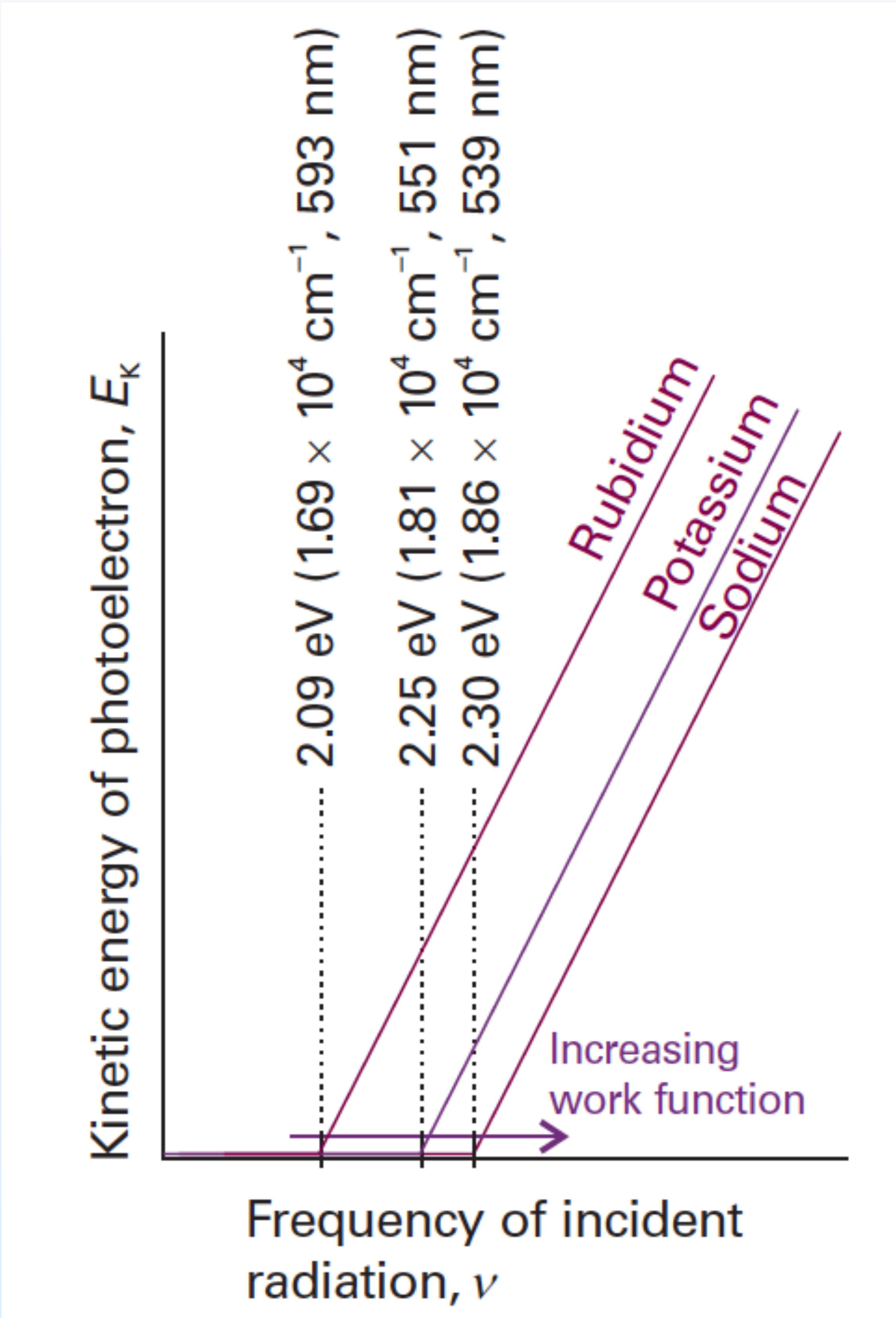


- **Experimentally**, it is found that, for a given material, only **light with frequencies above some threshold** is able to excite electrons, **irrespectively of its intensity**

- In addition, **the kinetic energy of the photoelectrons** increases linearly with the radiation frequency, but is **independent of the light intensity**

The photoelectric effect



- In 1905, Einstein explained the photoelectric effect with the assumption that **light is made of particle-like quanta (photons) with energy**

$$E(\nu) = h\nu$$

- This neatly explained the **experimental observations** about the photoelectric effect:

1) An electron interacts with **individual photons,** each requiring a **minimal amount of energy** (work function ϕ, material-specific) to eject the electron

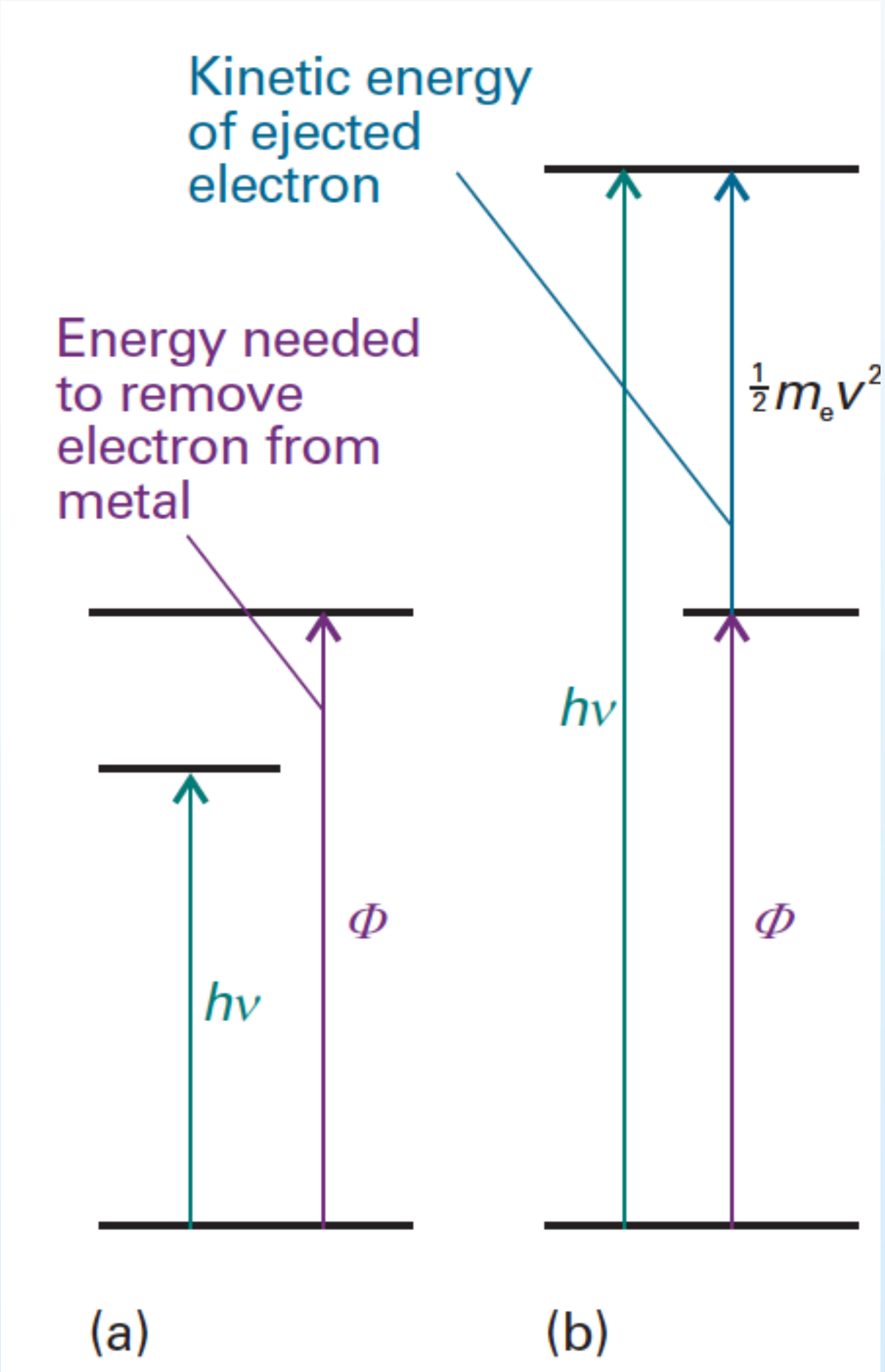
2) This sets a condition on the **minimal frequency of radiation** to exhibit the PE, **irrespective of intensity**

$$E(\nu) \geq \Phi \to \nu_{\min} = \Phi/h$$

3) From energy conservation, the **kinetic energy of the electrons will increase linearly** with the frequency ν

$$E_{\rm kin} = \frac{1}{2} m_e v_e^2 = E(\nu) - \Phi \to v_e = \sqrt{\frac{2(h\nu - \Phi)}{m_e}}$$

The photoelectric effect



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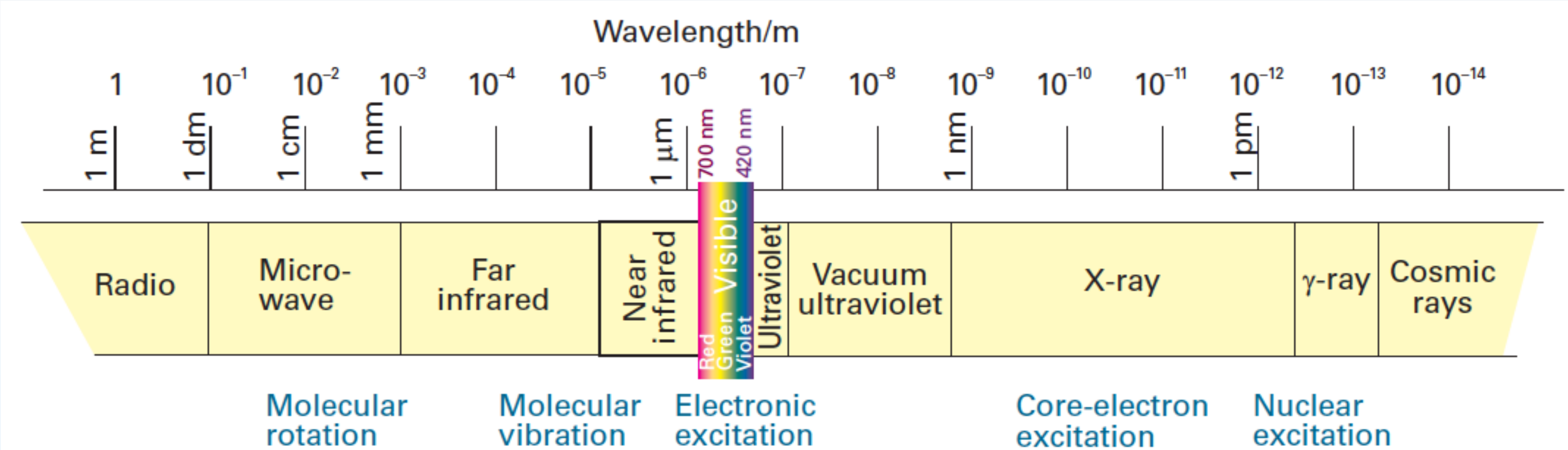
Light as a particle



This **particle-like nature of light** is exhibited for all frequencies, from radio waves (large wavelength, low energy) to X-rays (small wavelengths, high energy)

Einstein's hypothesis is one step further than Planck's, who only assumed the **quantisation of allowed energies for electromagnetic radiation** (without implying a particle-like nature of light)

So **light can behave either as a wave or as a particle**, depending on the conditions. This duality is an inherent property of quantum theory

The photoelectric effect has been verified even for extremely low light intensities, **consisting of only one photon at a time**

Wave-particle duality reloaded

The photoelectric effect shows that **light can exhibit matter-like behaviour**

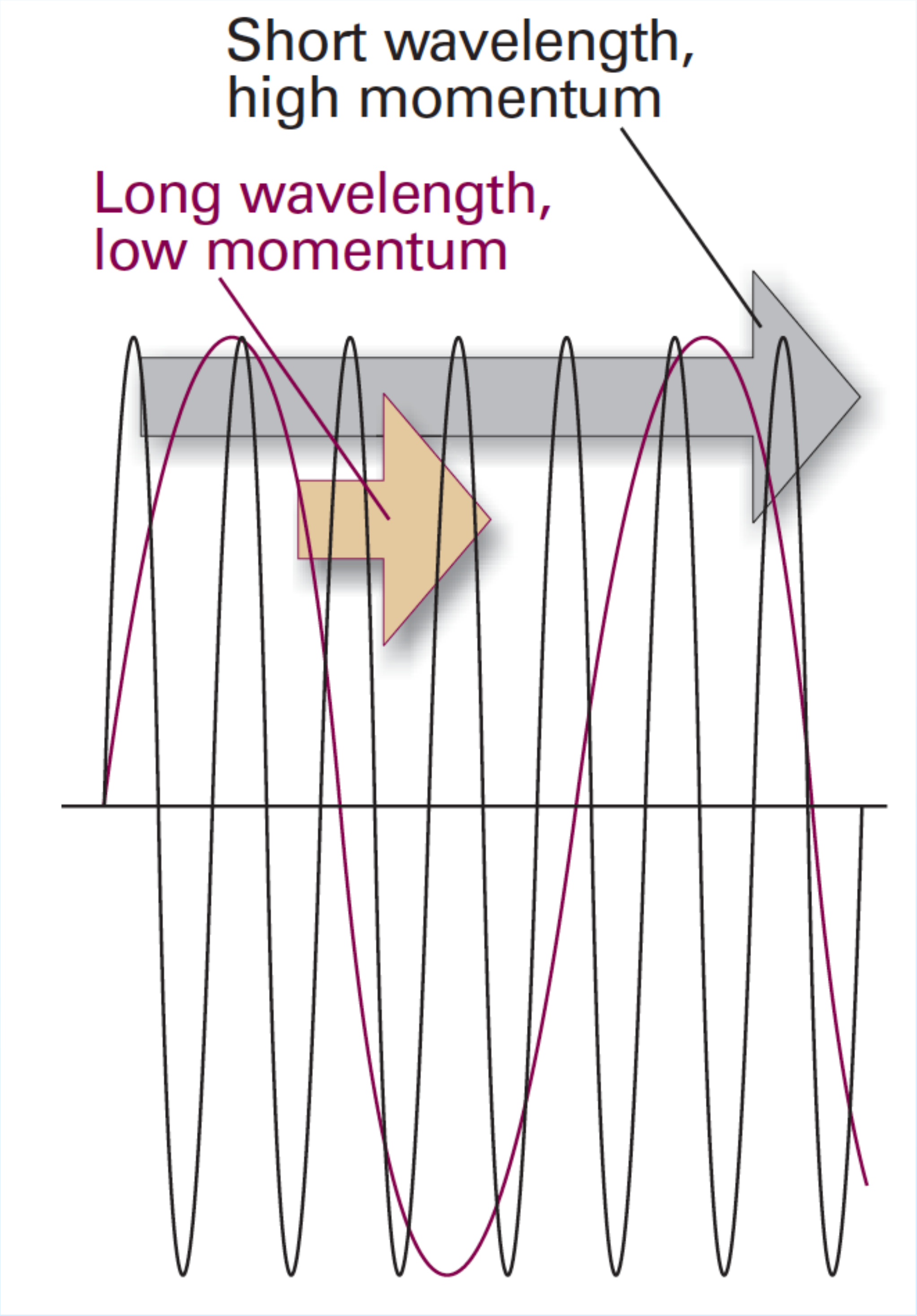
Remarkably, in some conditions, **matter particles can also exhibit wave-like behaviour**

In 1924, De Broglie suggested that any **matter particle** with momentum **p** should be assigned a **wavelength** inversely proportional to it (*De Broglie wavelength*)

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

and therefore should exhibit **wave-light behaviour at distances** $\lesssim \lambda$

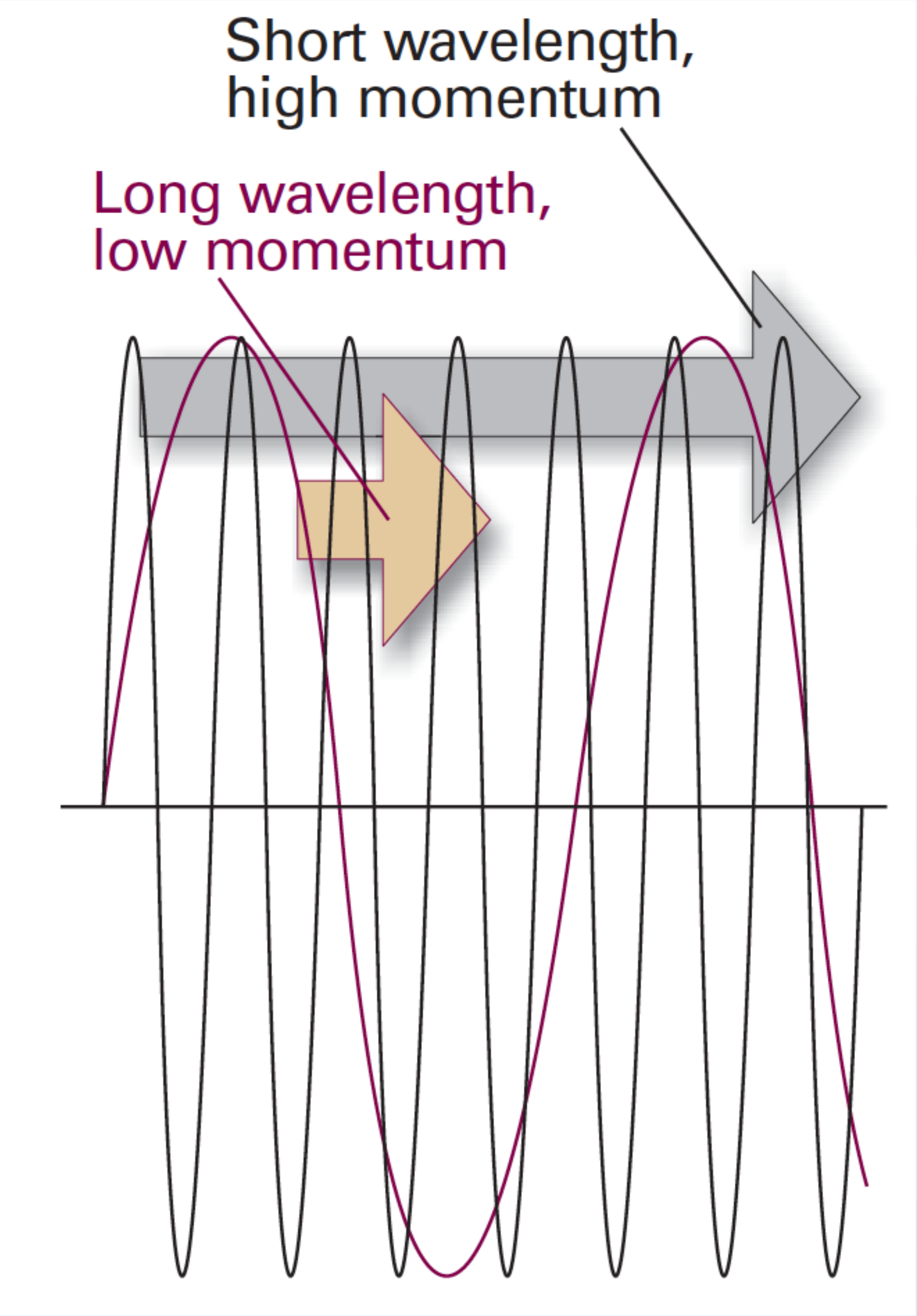
High-momentum particles have associated very short wavelengths and conversely



Wave-particle duality reloaded

A **car of mass 1000 kg moving at a velocity of 100 km/h** has the De Broglie wavelength of:

$$p = mv = 2.8 \cdot 10^4 \ \mathrm{kg\,m/s}\,, \lambda = \frac{h}{p} = 2 \cdot 10^{-38} \ \mathrm{m}$$



Wave-particle duality reloaded

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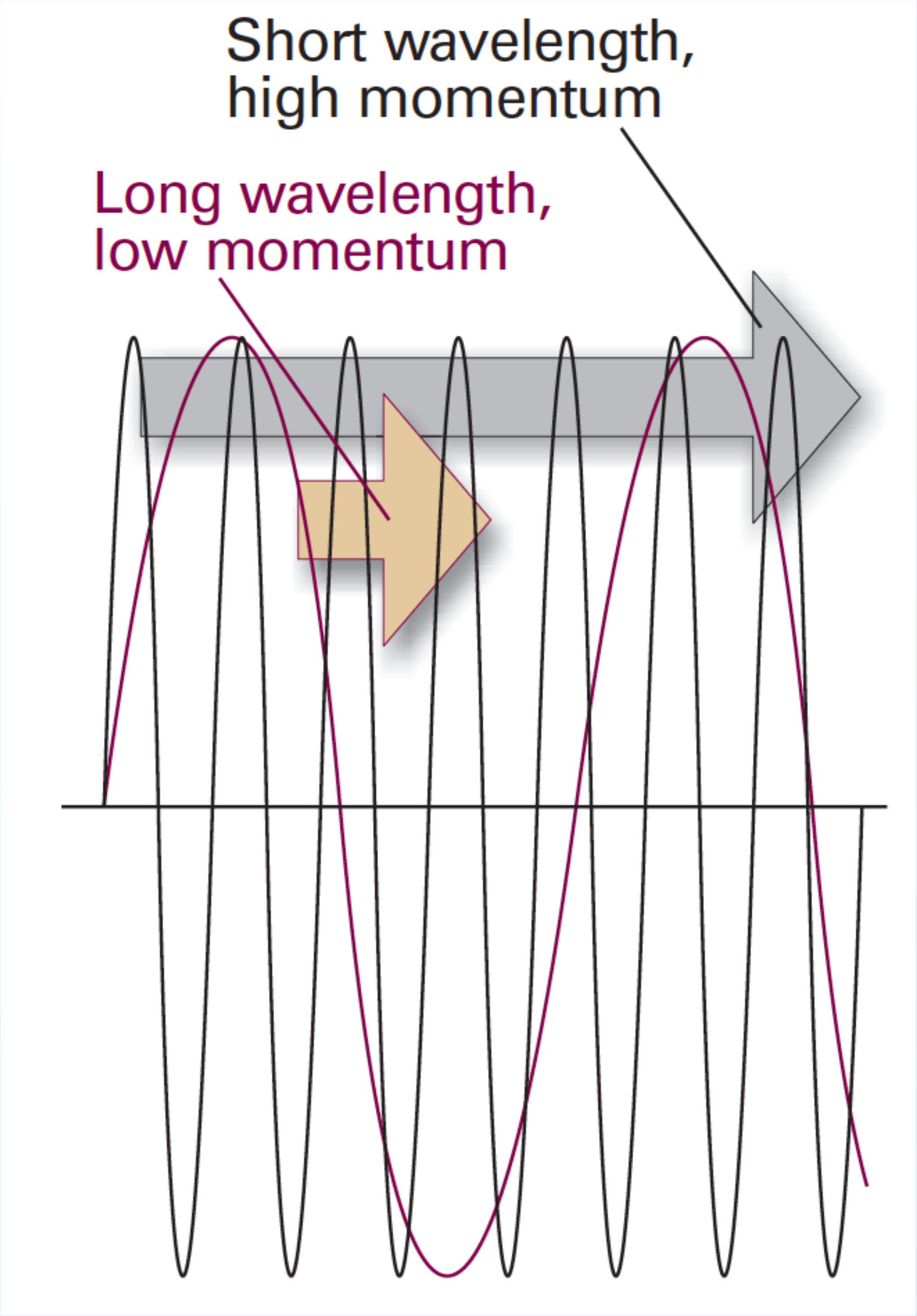
tiny distances, impossible to observe the quantum wave nature of a car



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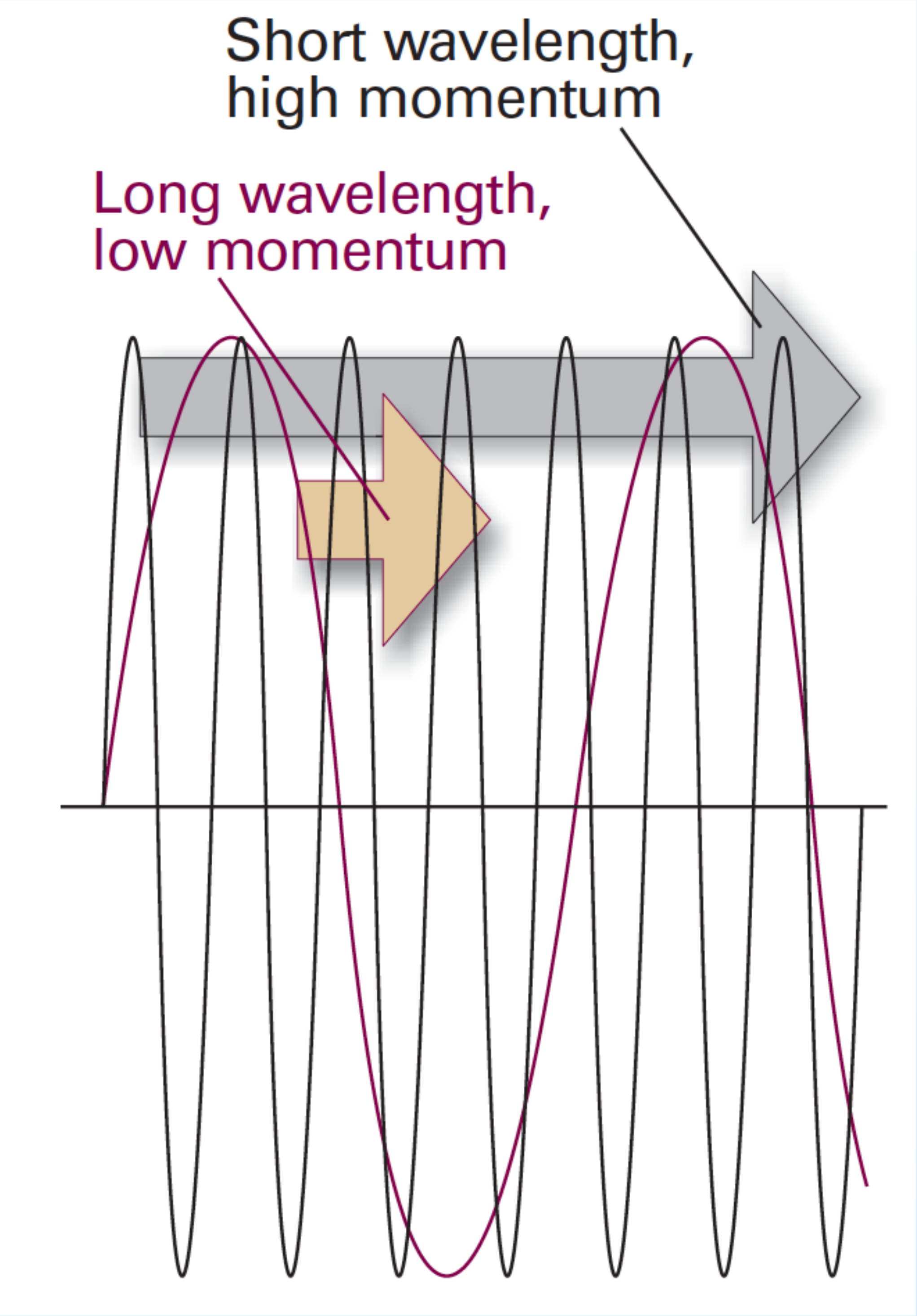
An **electron with energy of E=40 keV** has a De Broglie wavelength of around **$6{\times}10^{-12}$ m**



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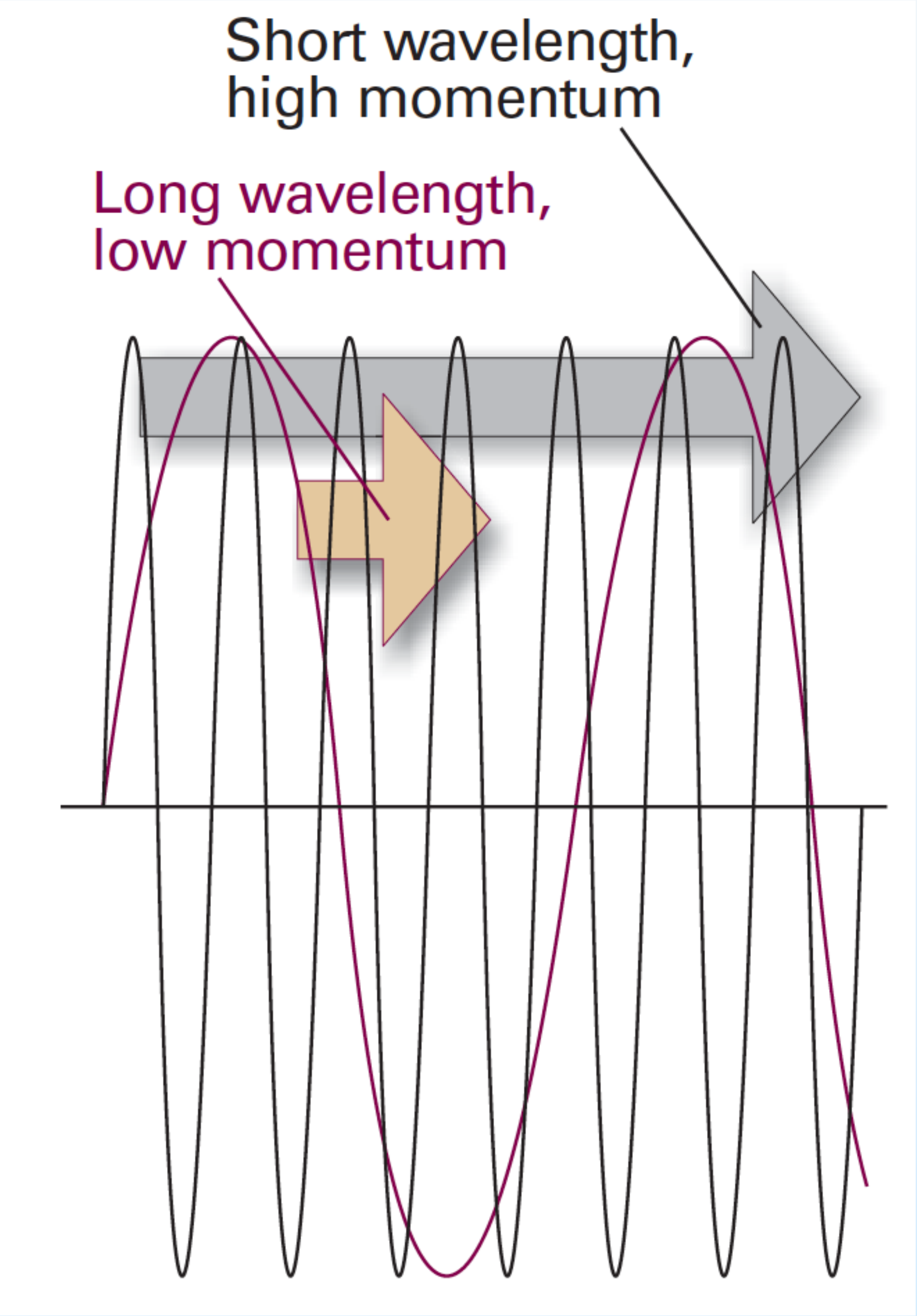
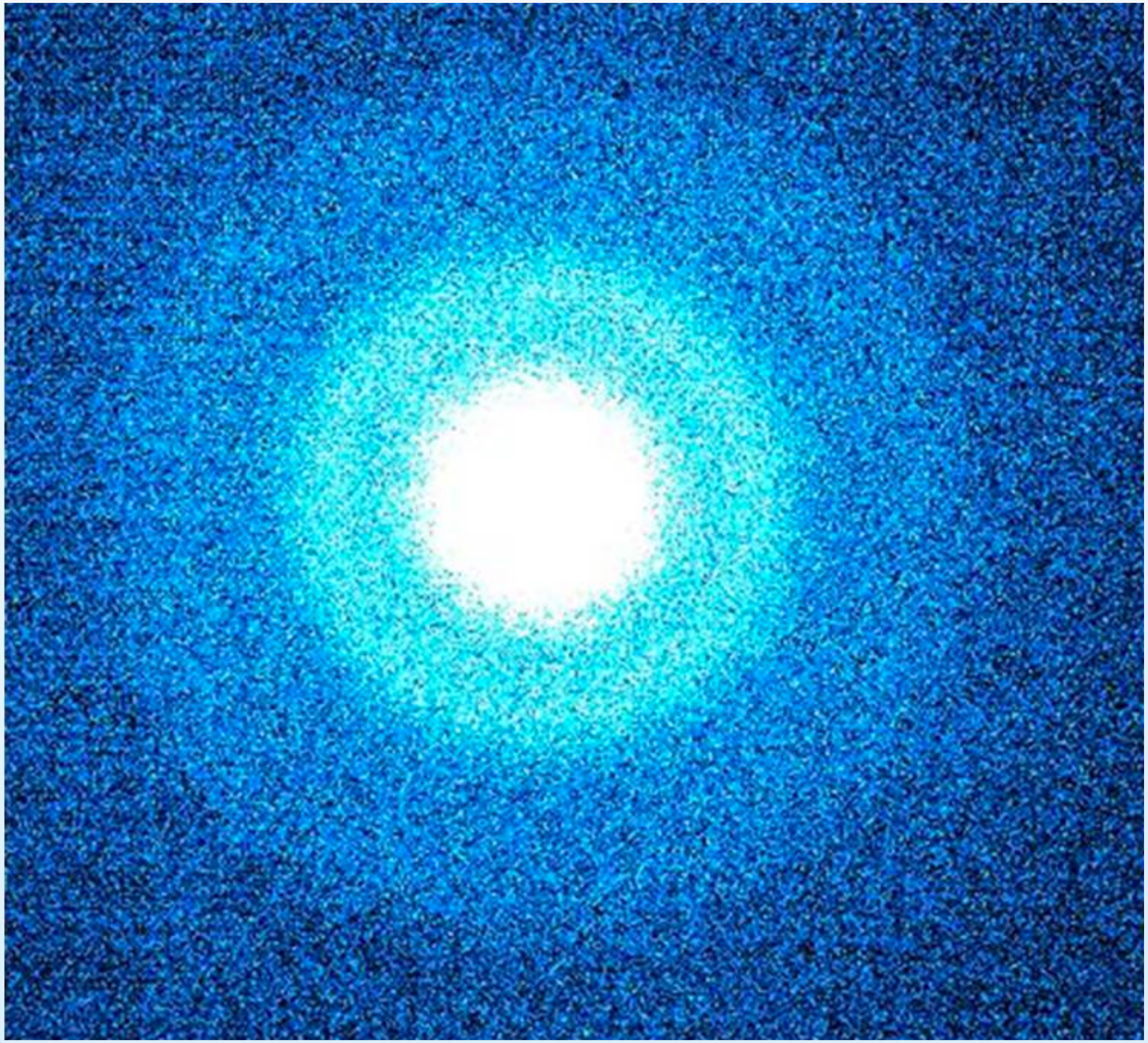
tiny distances, impossible to observe the quantum wave nature of a car

An **electron with energy of E=40 keV** has a De Broglie wavelength of around $\mathbf{6{\times}10^{-12}\ m}$

Its wave behaviour can thus be observed (*i.e.* diffraction on a crystalline solid)



Wave behaviour of electrons



Diffraction pattern of **electrons** that have traverse a crystalline solid

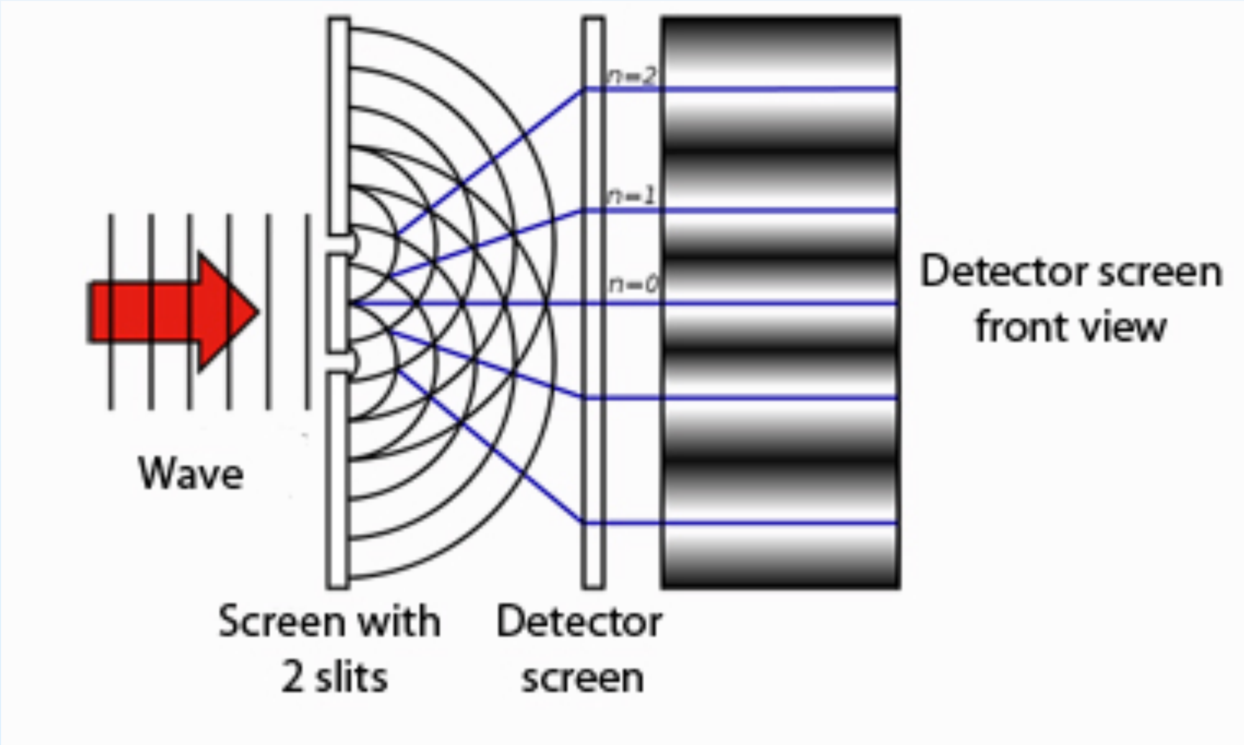
Their wave-like nature arises from i**nterferences within the crystal lattice**

The double slit experiment

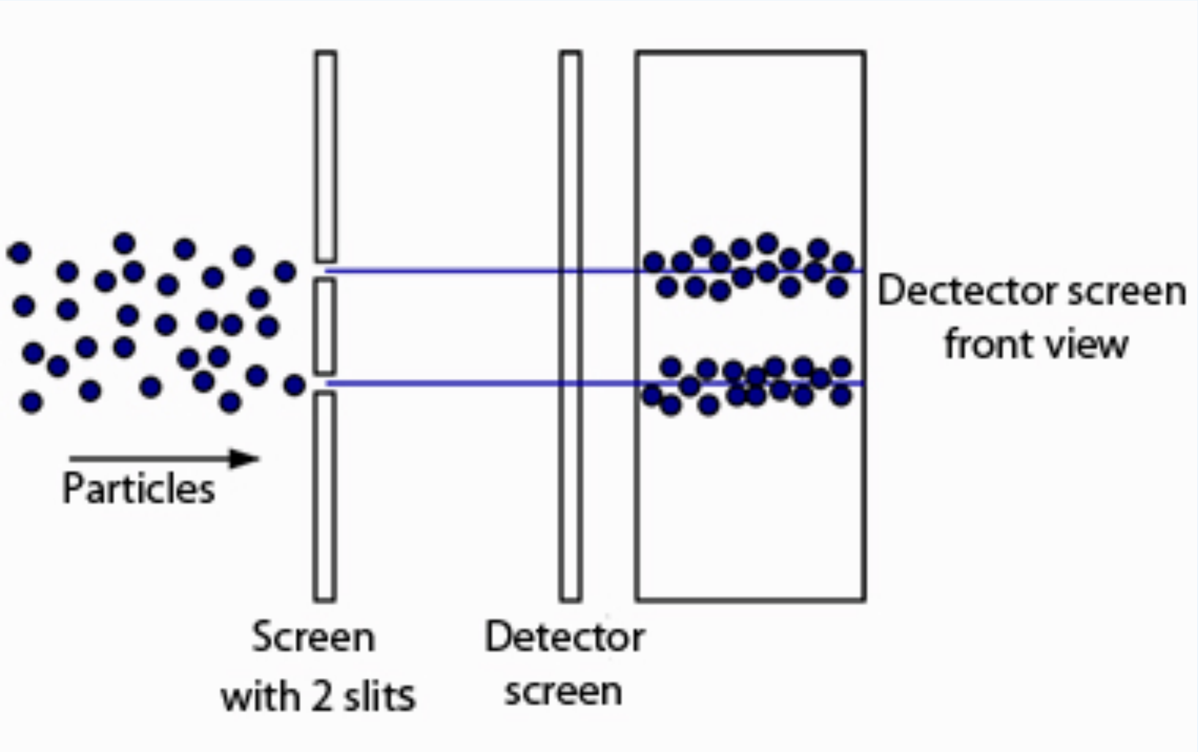
The **small De Broglie wavelength of electrons** indicates that they should exhibit **wave-like behaviour,** such as interference, in the appropriate conditions

Double-slit experiment in classical physics

Waves (light, water, …)



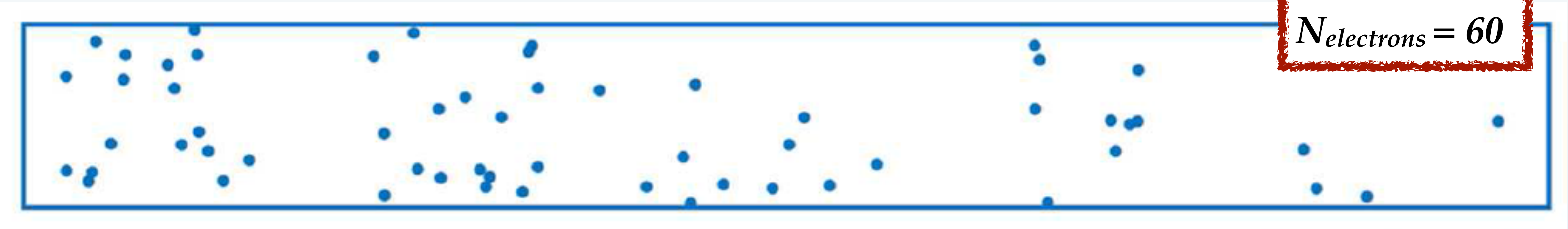
Matter particles



What happens if now we perform the experiment with electrons?

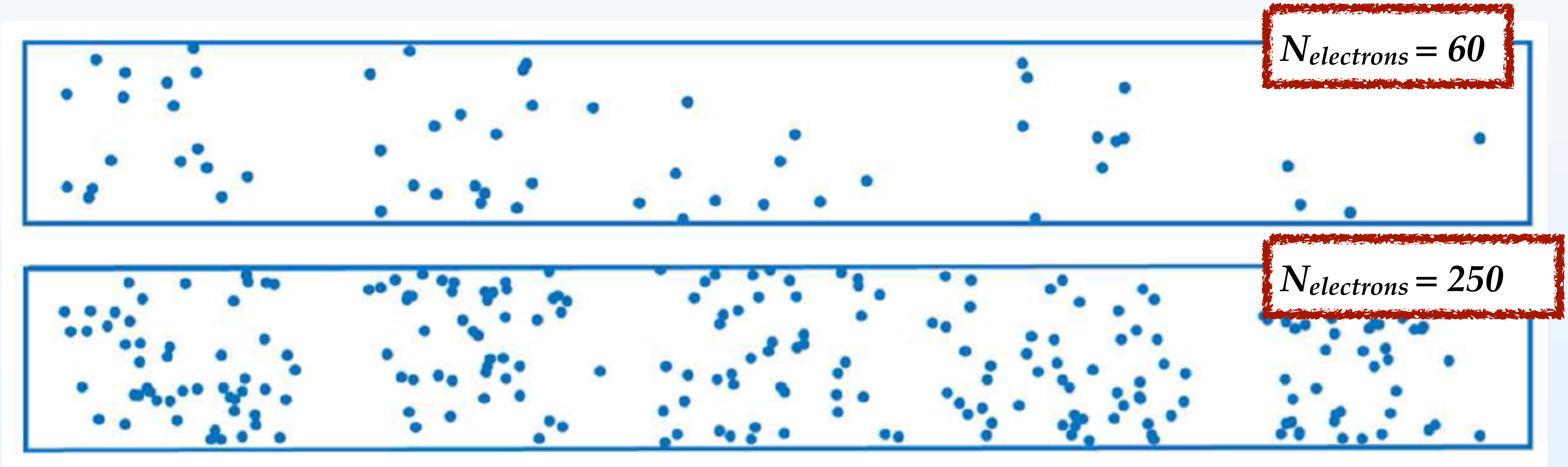
We fire electrons one-by-one to a double slit and detect them on a screen …

The double slit experiment

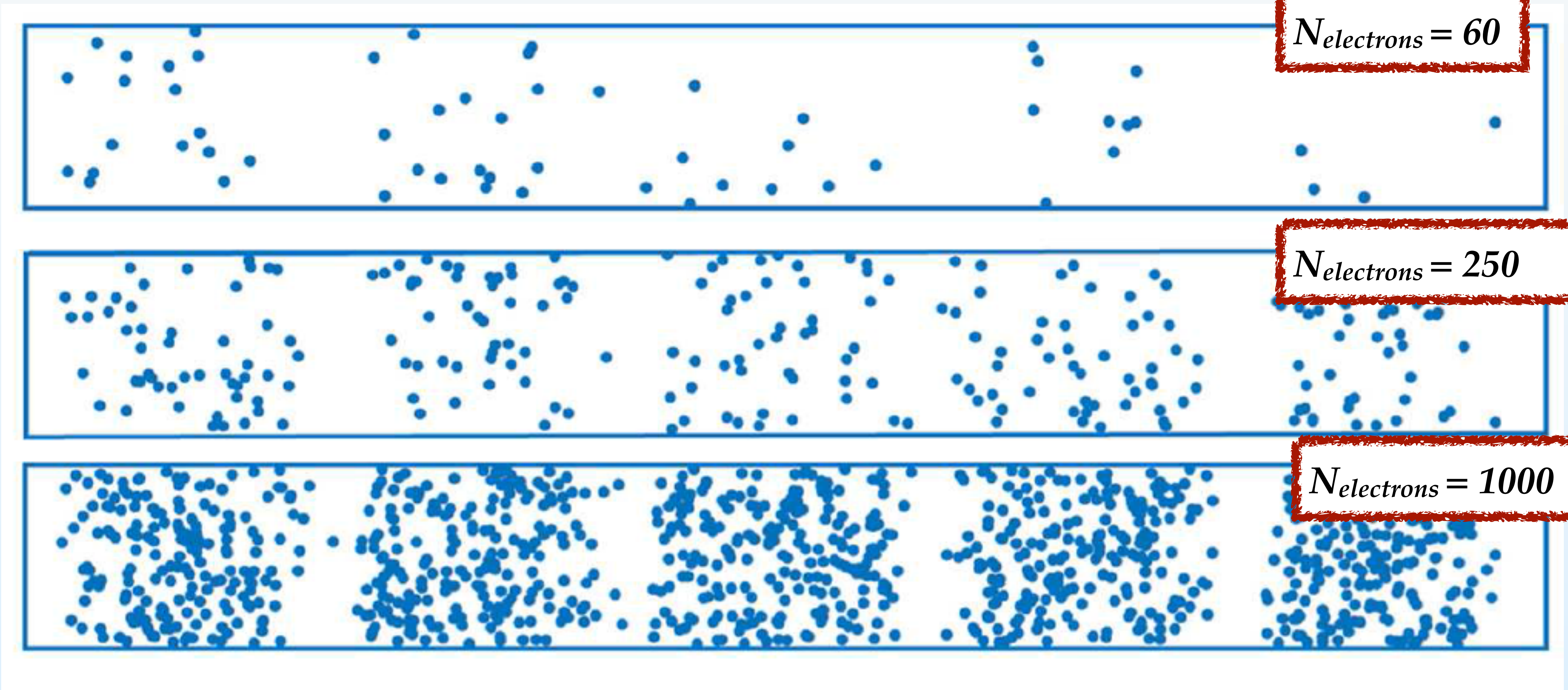


$N_{electrons} = 60$

The double slit experiment

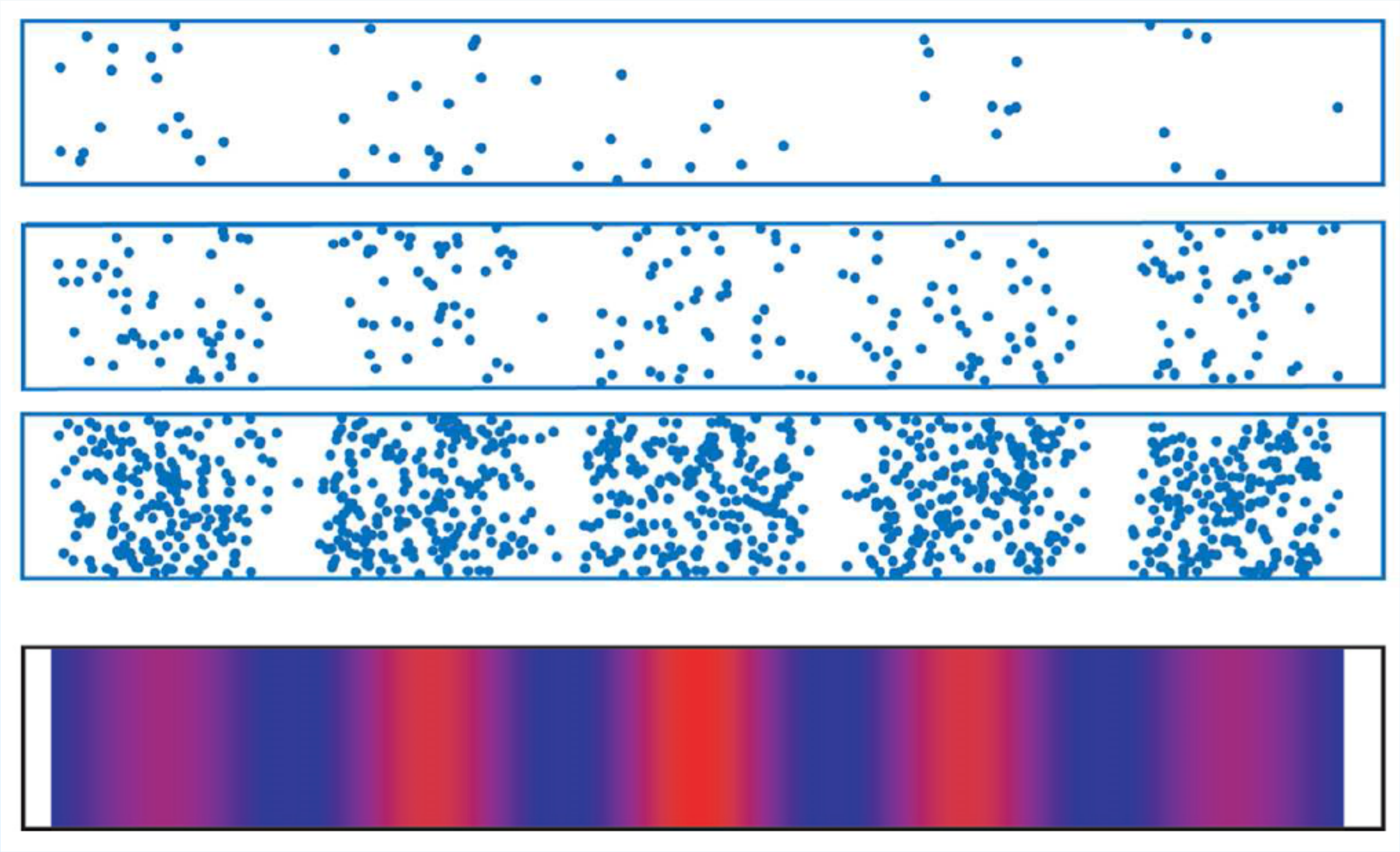


The double slit experiment



A wave-like interference patter arises!

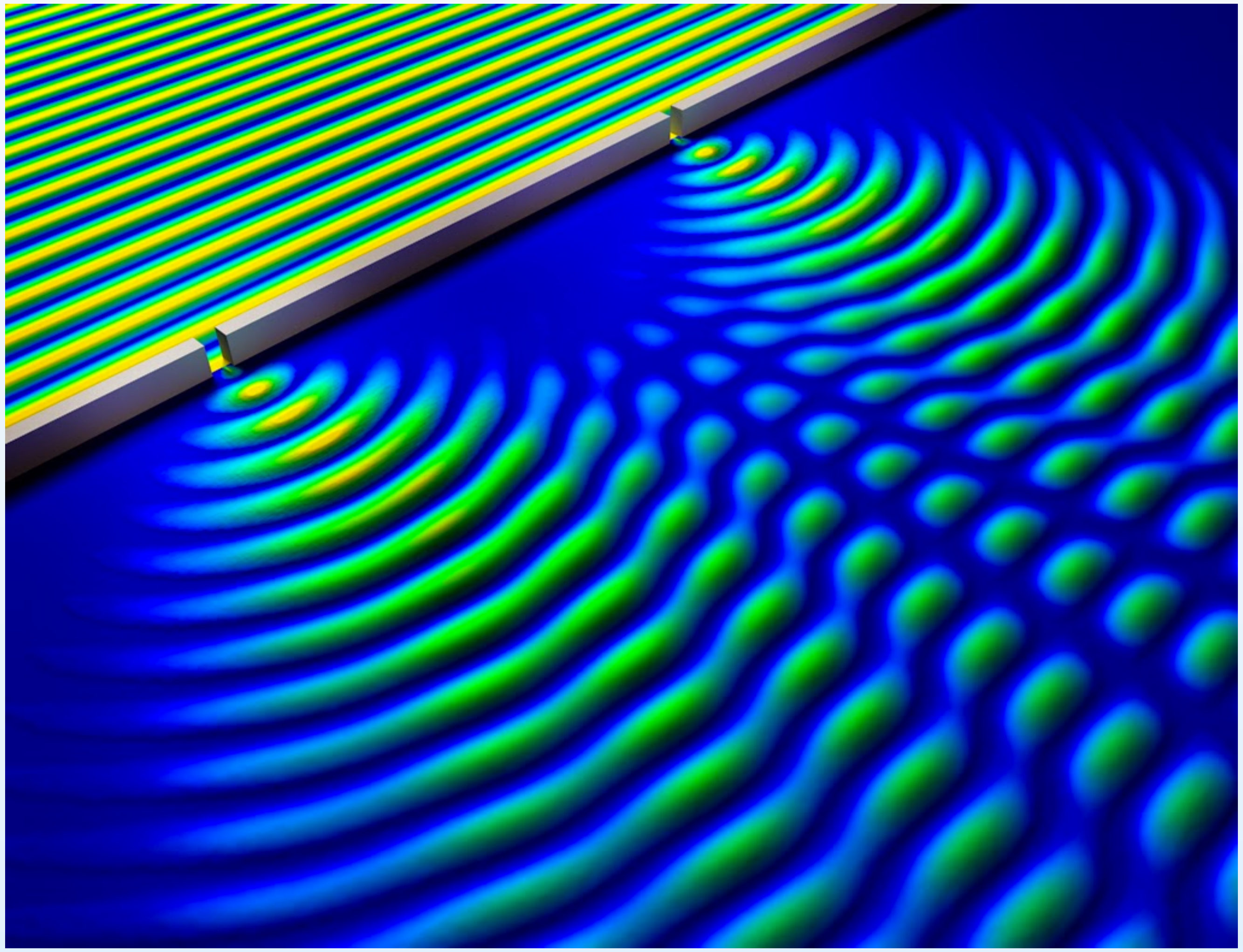
The double slit experiment



The double slit experiment

from http://www.toutestquantique.fr/

Particle-wave duality



The electrons behave as waves when travelling through the slits, and as particles when they impact on the detector screen: **particle-wave duality**

The **interference patter disappears** if we detect through which slit the electron traveled

The results of the double slit experiment have been reproduced by larger particles, such as **molecules composed by thousands of protons and electrons**

HC1: Key points

In the late XIXth and early XXth centuries, a series of landmark experiments demonstrated that **classical physics was not adequate** to describe some phenomena involving **small particles such as electrons and protons**, as well as some aspects of **electromagnetic radiation**:

- ☑ The analysis of the **black body radiation spectrum** showed that electromagnetic radiation was not emitted in a continuous range of energy, but rather it was **quantised**: energy can be only emitted in multiples of a basic amount

- ☑ Moreover, the **photoelectric effect** clearly demonstrated that this light quanta have a particle-like behaviour: **photons**

- ☑ Therefore, electromagnetic radiation (including light) exhibits **both wave and particle behaviours,** depending on the situation: **wave-particle duality**

- ☑ Conversely, the **double-slit experiment** shows that **matter particles exhibit also a wave-like behaviour** under some conditions: again, particle-wave duality

Quantum Mechanics is the mathematical language that describes all these remarkable (and peculiar) phenomena

QM interpretation

Quantum mechanics is h**ighly counterintuitive**, but admittedly we don't have much intuition of processes that take place at atomic scales or smaller

Quantum physics provides an **excellent quantitative description of a plethora of physical phenomena**, so let's learn how to use it to make predictions and leave delicate interpretation issues for a later stage

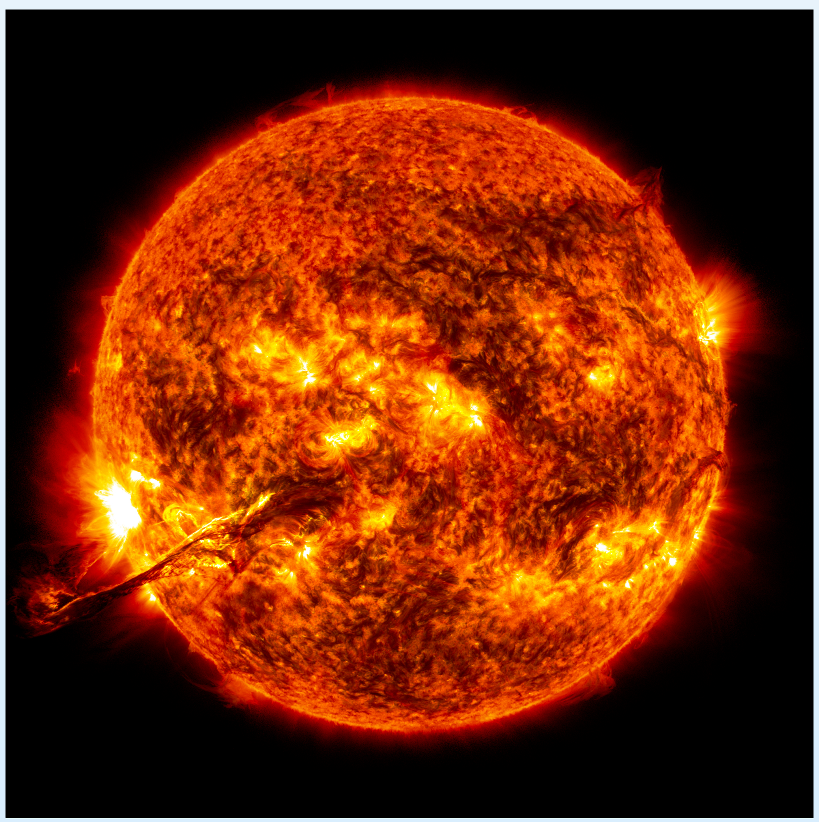
Feynman's interpretation of quantum mechanics:

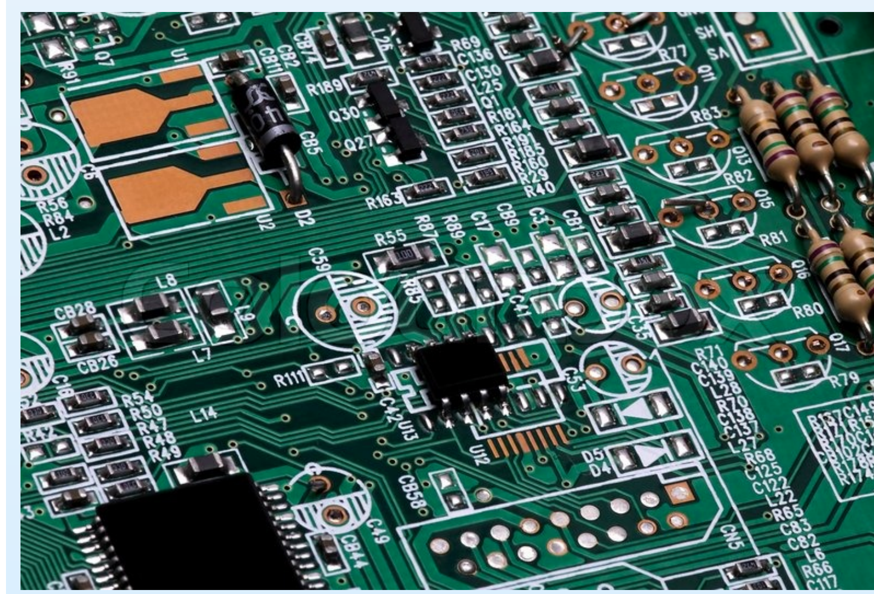
``Shut up and calculate!"

More than just small particles

Quantum theory is not only required to explain the properties of **small objects** like electrons, photons and atoms

Is crucial to understand a great number of **macroscopic phenomena**, from the **stability of solids** and **nuclear fusion in the stars** to **how your smartphone actually works!**





HC2

- **Monday 16.01, 13.30, collegezaal MF-A301**
- Preparation: study the **rest of Chapter 7 of A&DP**
- The goals of HC2 will be the following
  - Understand that **the state of a quantum system** is described by a mathematical entity known as the **wave function**, which is a solution of the **Schrödinger equation** (a quantum equation of motion)
  - Familiarise with the **physical interpretation of the quantum wave function**
  - Understand and apply the **mathematical description of quantum physics**, including hermitian operators, eigenvalue equations and orthogonality
  - Understand how e**xperimental observables can be extracted from the wave function**, and perform some calculations in simple cases
  - Understand and apply **Heisenberg's uncertainty principle**