(Computational) Quantum Mechanics For Nanosciencies

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What is Quantum Mechanics (QM)?

- QM deals with small scales.
- QM can be abstract, counterintuitive and hard to grasp.
- QM is mathematically challenging.
- QM is not deterministic as it is associated with probabilities.
- Despite this, it is a linear theory, so there is harmony in the equations and there is no chaos as in Classical Mechanics (CM).

What is Quantum Mechanics (QM)?

- **Richard Feynman:** "I think I can safely say that nobody understands QM.”

- “There is no general consensus as to what its fundamental principles are, how it should be taught, or what it really means.”

- “QM was not created by one individual”, like other theories (e.g., GR, EM).

- **<u>The purpose of this class is to teach you how to DO and USE quantum mechanics.</u>**

Reference: Griffiths 1995

What is Quantum Mechanics (QM)?

- **D. Griffiths:** “I do not believe one can intelligently discuss what quantum mechanics means until one has a firm sense of what quantum mechanics does."

- “Not only is quantum theory conceptually rich, it is also technically difficult.”

  e.g. Linear algebra, complex numbers, partial derivatives, Fourier analysis, classical mechanics, electrodynamics.

- “Using the right tool makes the job *easier,* not more difficult”

  e.g. Legendre, Hermite, and Laguerre polynomials, spherical harmonics, Bessel, Neumann, and Hankel functions, Airy functions, Hilbert spaces, Hermitian operators, Clebsch- Gordan coefficients, and Lagrange multipliers.

Reference: Griffiths 1995

What is Quantum Mechanics (QM)?

- “Don't let the mathematics (which, for us, is only a tool) interfere with the physics.”

- “QM represents an abrupt and revolutionary departure from classical ideas, calling forth a wholly new and radically counterintuitive way of thinking about the world.”

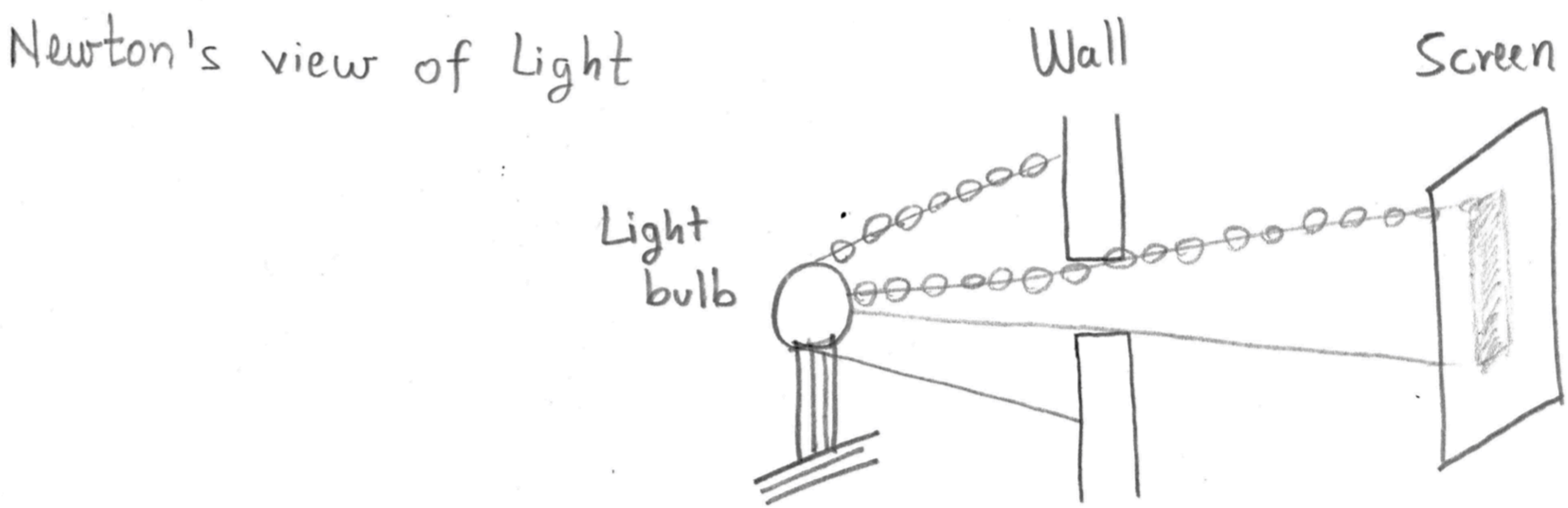
- **<u>QM is a (mathematical) framework to do physics (at small scales).</u>**

Reference: Griffiths 1995

Brief history of QM

<u>Experiments and basic ideas</u> that led to the formulation of QM:

- The earliest ideas that would eventually lead to the formulation of QM emerged from trying to understand the nature of light.
- In the 1600's, I. Newton proposes light is made of a beam of particles, based on this experiment:

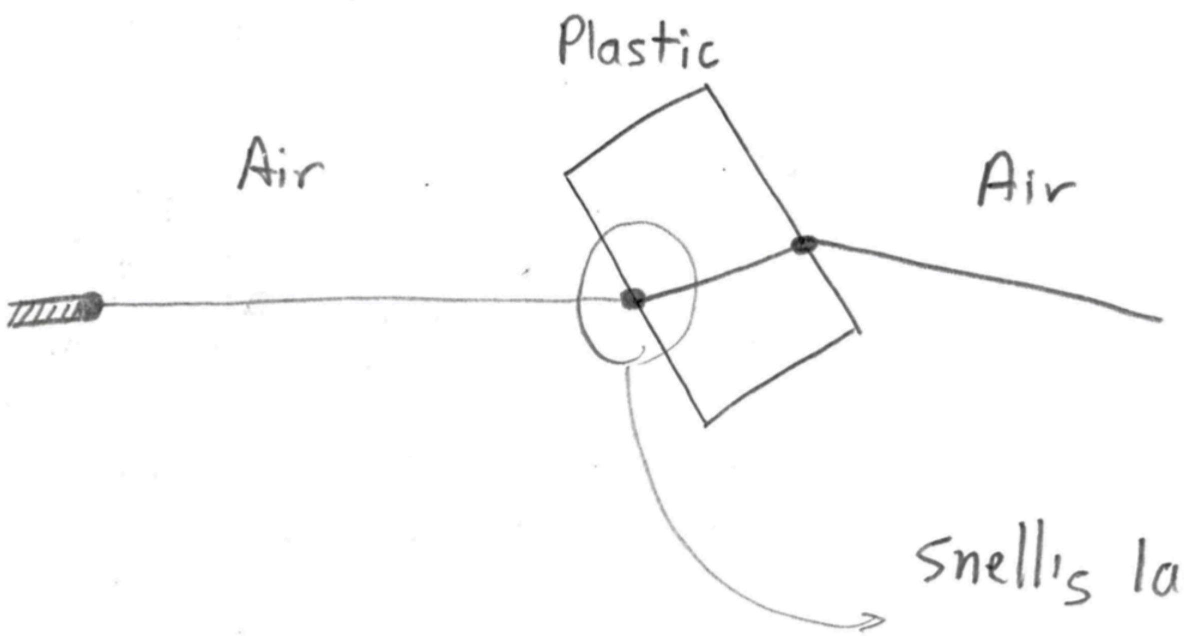


Applet: https://phydemo.app/ray-optics/simulator/

Brief history of QM

- Also in the **1600's,** R. Hooke proposes light is made of waves based on refraction experiments. Refraction can be explained by considering light as composed of waves.

Refraction:



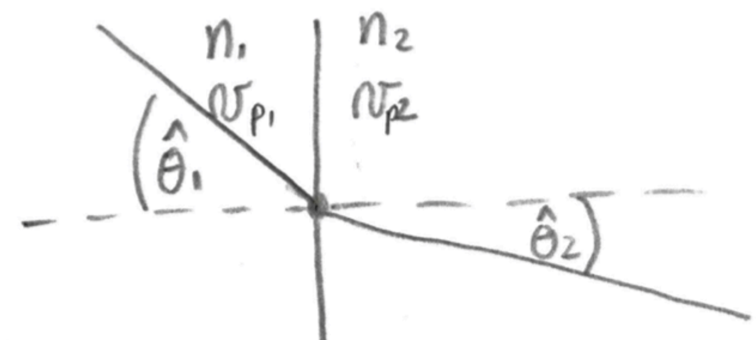
$n \equiv$ refractive indices $\equiv \frac{c}{v_p} = \frac{ck}{\omega}$

$v_p \equiv$ phase velocities $= \frac{\omega}{k} = \frac{\lambda}{T}$

$\hat{\theta}_1 \equiv$ incidence angle

$\hat{\theta}_2 \equiv$ refraction angle

Snell's law



$$\boxed{\frac{\sin\hat{\theta}_1}{\sin\hat{\theta}_2} = \frac{v_{p1}}{v_{p2}} = \frac{n_2}{n_1}}$$

$$\omega = \frac{ck}{n} \Rightarrow \frac{d\omega}{dk} = \overbrace{\frac{c}{n}}^{v_p} - \frac{c}{n^2}\frac{dn}{dk} \equiv \text{group velocity}$$

Applet: https://phet.colorado.edu/sims/html/bending-light/latest/bending-light_en.html

Brief history of QM

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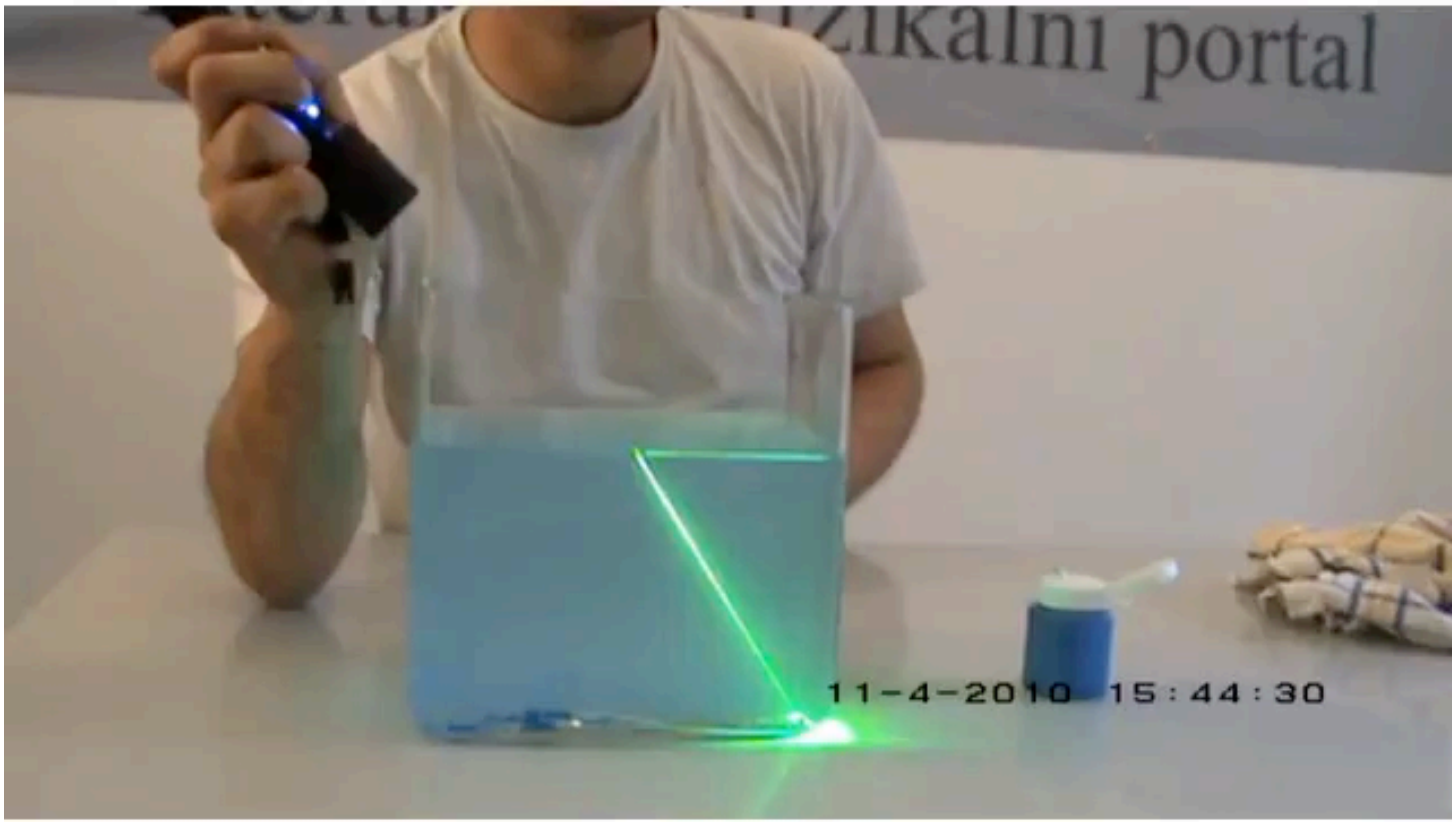


Video: https://www.youtube.com/watch?v=m9cUy6B--xc

Brief history of QM

- **1800's** - Experiments on interference and diffraction probe Hooke's ideas correct.
- **1800's** - K. Maxwell compiles the EM equations. Light is EM radiation.

Gauss' law: $$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

Gauss' law for magnetism: $$\nabla \cdot \mathbf{B} = 0$$

Maxwell–Faraday equation (Faraday's law of induction): $$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

Maxwell–Ampère equation (circuital law): $$\nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}$$

Reference: https://www.cantorsparadise.com/maxwells-equations-7484212839b1

Particle nature of EM radiation

- **End of 1800's** - Black-body radiation could not be explained by EM theory framework.

An object can absorb/emit radiation: $\left\{ \begin{array}{l} \text{Absorption} \uparrow T \\ \text{Emission} \downarrow T \end{array} \right.$

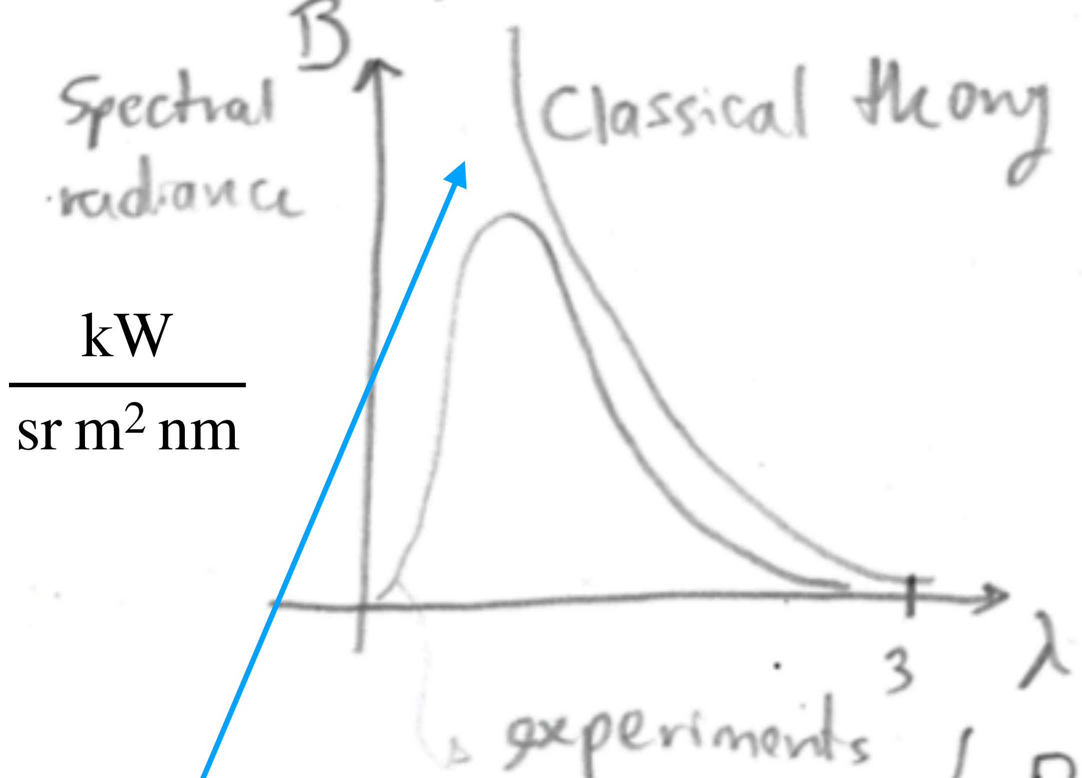
Kirchoff's law: Abs = Emission $\Rightarrow$ $T = ct.$ $\Leftrightarrow$ thermal eq.

Black body: Does not reflect radiation

Particle nature of EM radiation

- **End of 1800's** - Black-body radiation could not be explained by EM theory framework.

Black body radiation:



UV catastrophe

$$\begin{cases} B_\lambda(T) = \dfrac{2ck_BT}{\lambda^4} \\ B_\nu(T) = \dfrac{2\nu^2 k_BT}{c^2} \end{cases}$$

Rayleigh-Jeans law

$$k_B = 1.38\times10^{-23}\ \text{m}^2\,\text{kg}\,\text{s}^{-2}\,\text{K}^{-1}$$

$$\begin{cases} B_\lambda(T) = \dfrac{2hc^2}{\lambda^5}\dfrac{1}{e^{\frac{hc}{\lambda k_BT}}-1} \\ B_\nu(T) = \dfrac{2h\nu^3}{c^2}\dfrac{1}{e^{\frac{h\nu}{k_BT}}-1} \end{cases}$$

Planck's law

Particle nature of EM radiation

- **1900 -** M. Planck proposes quantisation of EM radiation

Planck: EM can only be em./abs in discrete packets:

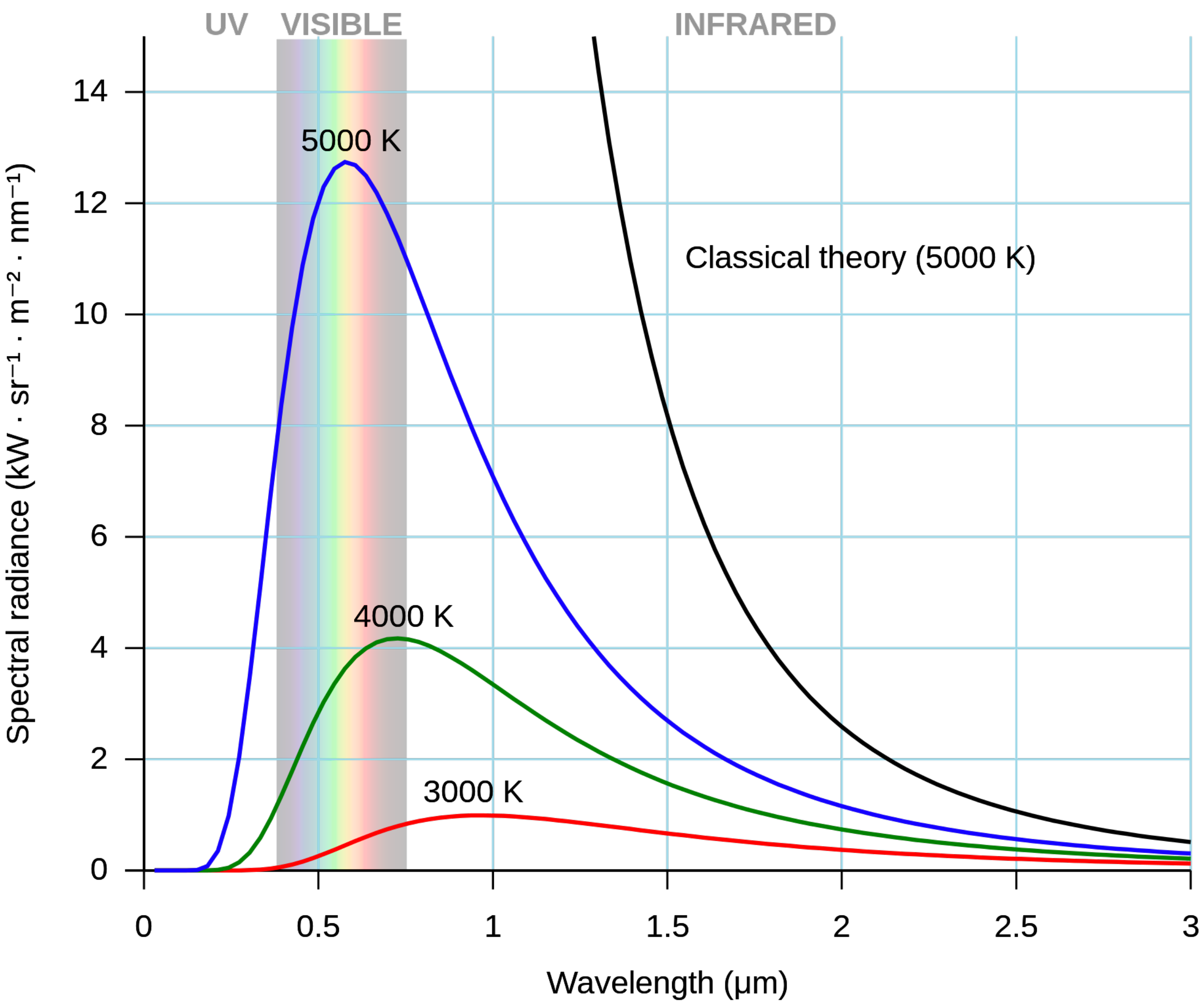
$$\boxed{E_{quanta} = h\nu = h\frac{c}{\lambda}}$$

- $E = h\nu = \hbar\omega$
- $\vec{p} = \hbar\vec{k}$

$\hbar = \frac{h}{2\pi}$

De Broglie relation:

$$\boxed{\lambda = \frac{2\pi}{k} = \frac{h}{p}} \Rightarrow E = pc$$



UV catastrophe

Reference: https://en.wikipedia.org/wiki/Ultraviolet_catastrophe

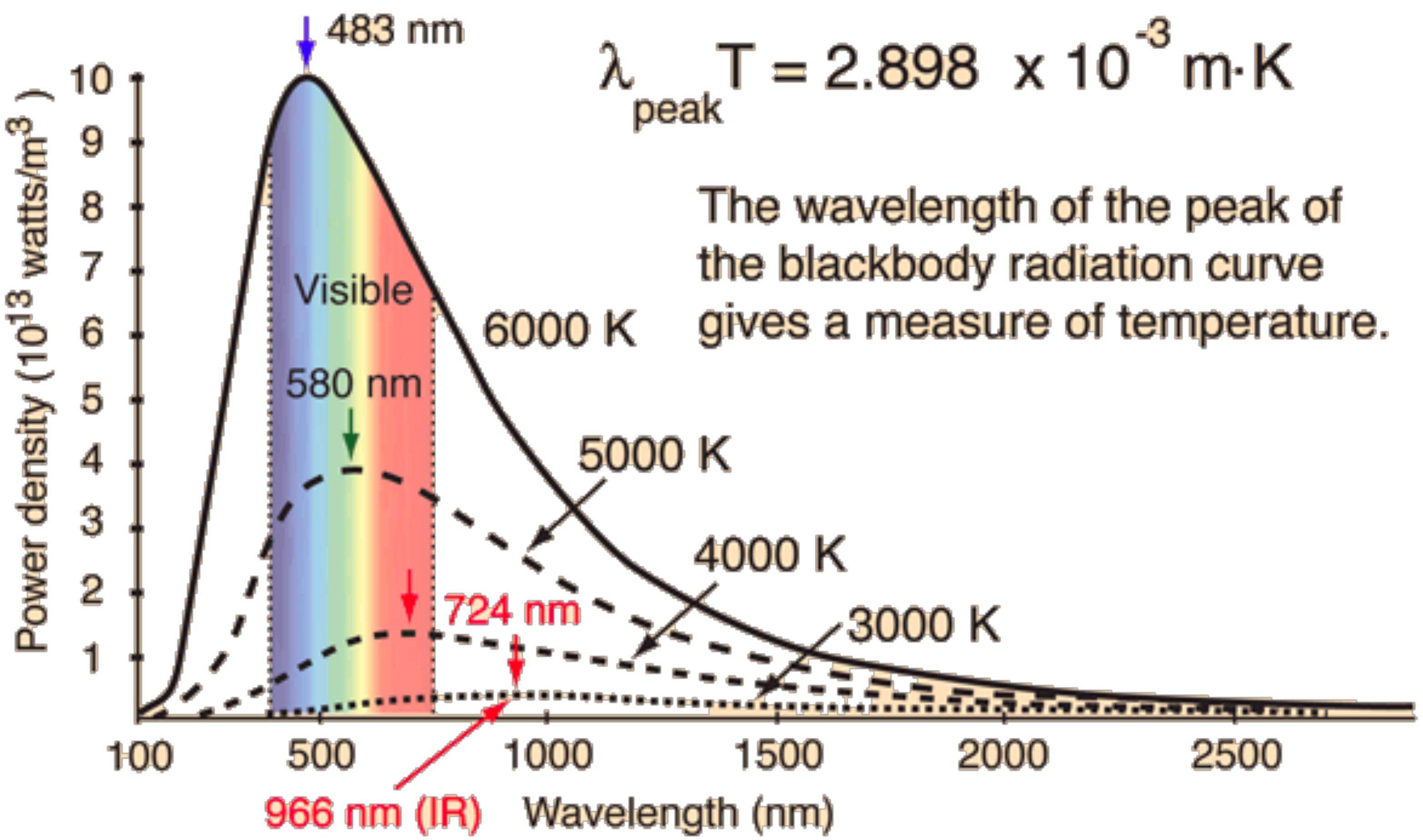
Particle nature of EM radiation

- **Wien's displacement law:**

λ at which an object emits more radiation.

$$\lambda_{max\,(peak)} = \frac{b}{T} \quad ; \quad b = 2.898 \times 10^{-3}\, mK$$

$$\nu_{peak} = \frac{\alpha}{h} kT \approx 5.879 \times 10^{10} \frac{Hz}{K} \cdot T$$



Reference: http://hyperphysics.phy-astr.gsu.edu/hbase/wien.html

Particle nature of EM radiation

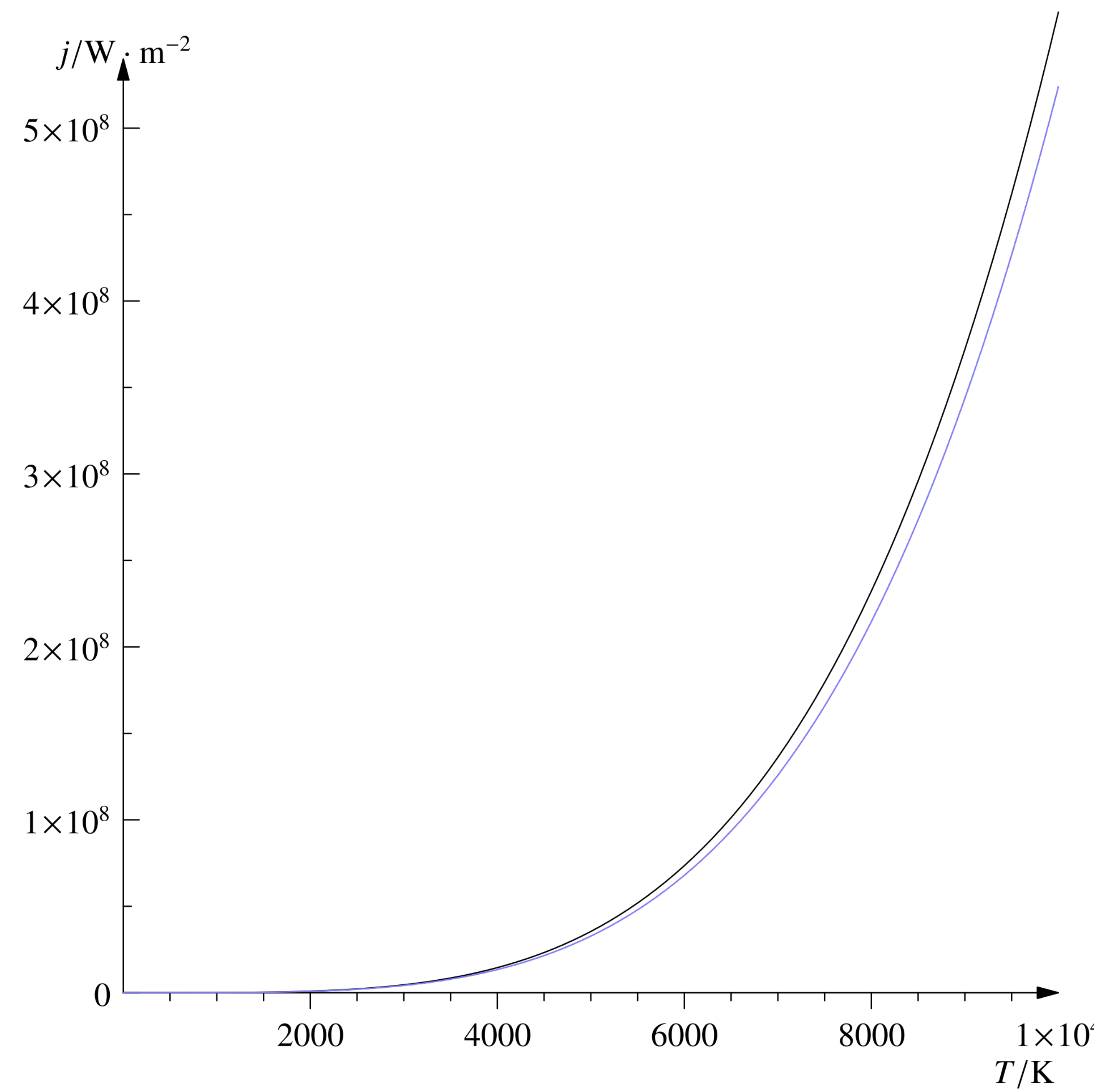
- **Stefan-Boltzmann law:**

Total radiation emitted at all λ:

$$j = \sigma T^4 \quad \left[\frac{W}{m^2}\right]$$

$$\sigma = \frac{2\pi^5 k^4}{15 c^2 h^3} = 5.67 \times 10^{-8} \frac{W}{m^2 K^4}$$

↳ SB constant



Reference: https://en.wikipedia.org/wiki/Stefan%E2%80%93Boltzmann_law