Introduction to quantum theory of solids

Principles of quantum mechanics

Schrodinger's wave equation

Meaning, boundary conditions and application

Allowed and forbidden energy bands

Electrical conduction in solids

Fermi statistics in metals and semiconductors

Low-dimensional structures

Superconductivity

Material on above content is available in, Book on Semi-conductor Physics and Devices, Basic Principles by Donald A. Neamen, chapter 2 & 3. See the Book folder.

- Question: What do these have in common?
  - lasers
  - solar cells
  - transistors
  - computer chips
  - CCDs in digital cameras
  - superconductors
  - ....
- Answer:
  - They are all based on the quantum physics discovered in the 20th century.

Quantum Physics

- QP is "weird and counterintuitive"
  - "Those who are not shocked when they first come across quantum theory cannot possibly have understood it" (Niels Bohr)
  - "Nobody feels perfectly comfortable with it " (Murray Gell-Mann)
  - "I can safely say that nobody understands quantum mechanics" (Richard Feynman)
- But:
  - QM is the most successful theory ever developed by humanity
  - underlies our understanding of atoms, molecules, condensed matter, nuclei, elementary particles
  - Crucial ingredient in understanding of stars, …

Quantum mechanics

- **Quantum mechanics** (**QM**; also known as **quantum physics**, or **quantum theory**) is a branch of physics which deals with physical phenomena at nanoscopic scales where the action is on the order of the Planck constant.

- It departs from classical mechanics primarily at the *quantum realm* of atomic and subatomic length scales.

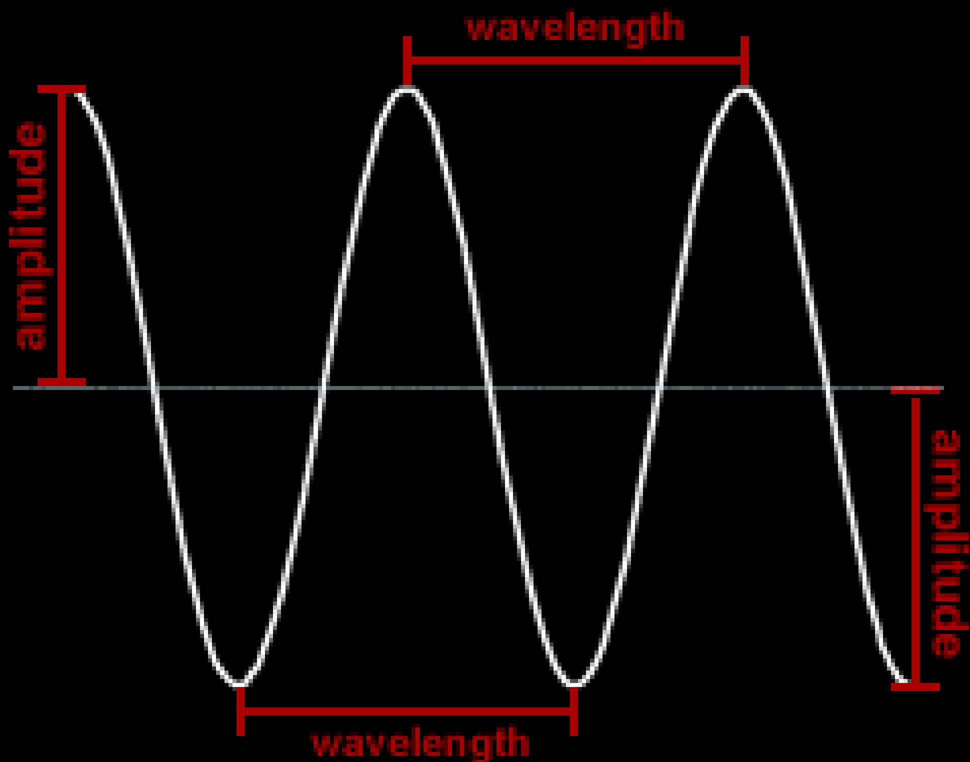
- Quantum mechanics provides a mathematical description of much of the dual *particle-like* and *wave-like* behavior and interactions of energy and matter.

Features of QP

- Quantum physics is basically the recognition that there is less difference between waves and particles than was thought before
- key insights:
  - light can behave like a particle
  - particles (e.g. electrons) are indistinguishable
  - particles can behave like waves (or wave packets)
  - waves gain or lose energy only in "quantized amounts“
  - detection (measurement) of a particle $\Rightarrow$ wave will change suddenly into a new wave
  - quantum mechanical interference – amplitudes add
  - QP is intrinsically probabilistic
  - what you can measure is what you can know

Light Waves

Until about 1900, the classical wave theory of light described most observed phenomenon.



Light waves:

<u>Characterized by:</u>

- Amplitude (A)
- Frequency (ν)
- Wavelength (λ)

Energy of wave α A^2

And then there was a problem…

In the early 20th century, several effects were observed which could not be understood using the wave theory of light.

Two of the more influential observations were:

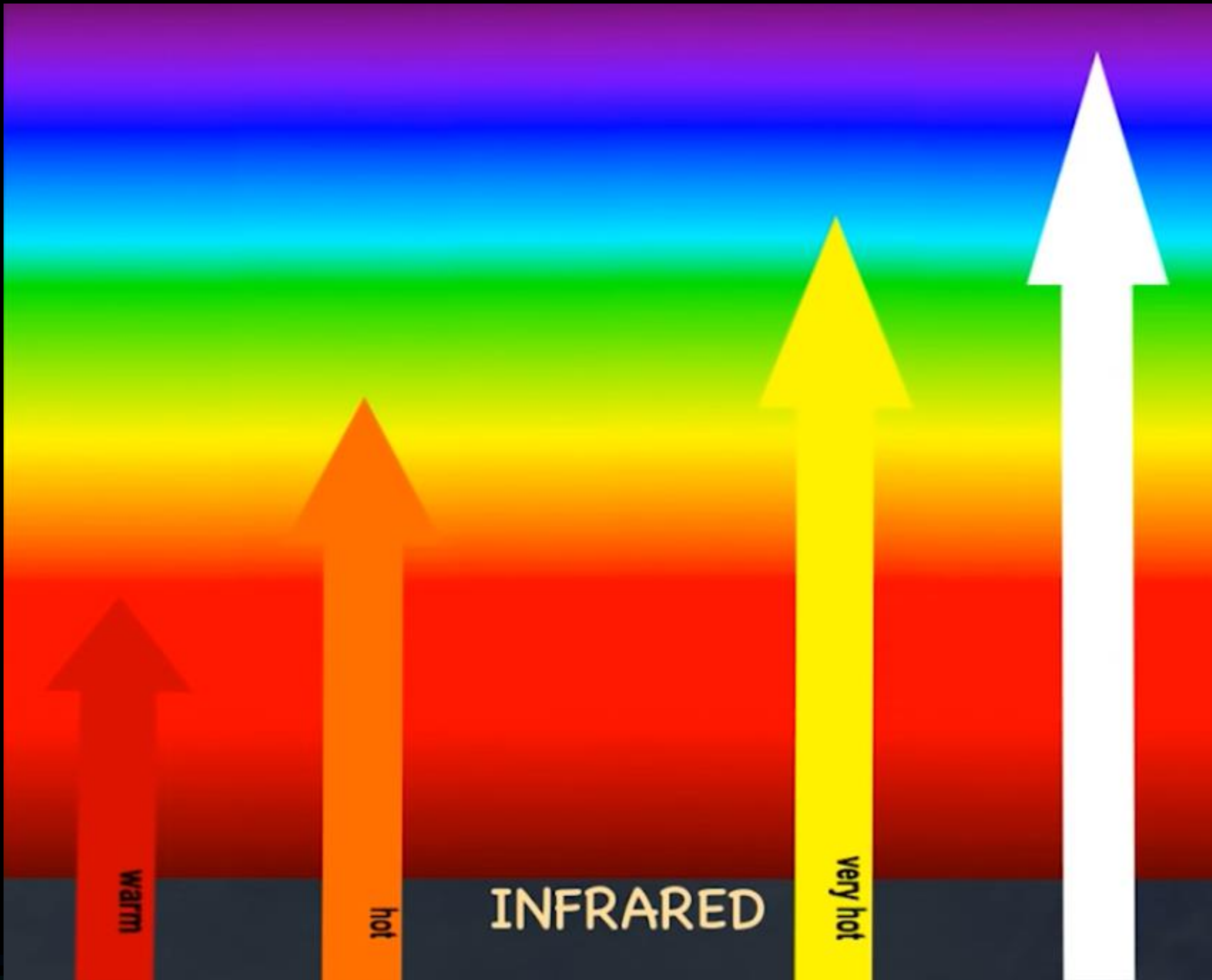
1) **The Photo-Electric Effect**

2) **The Compton Effect**

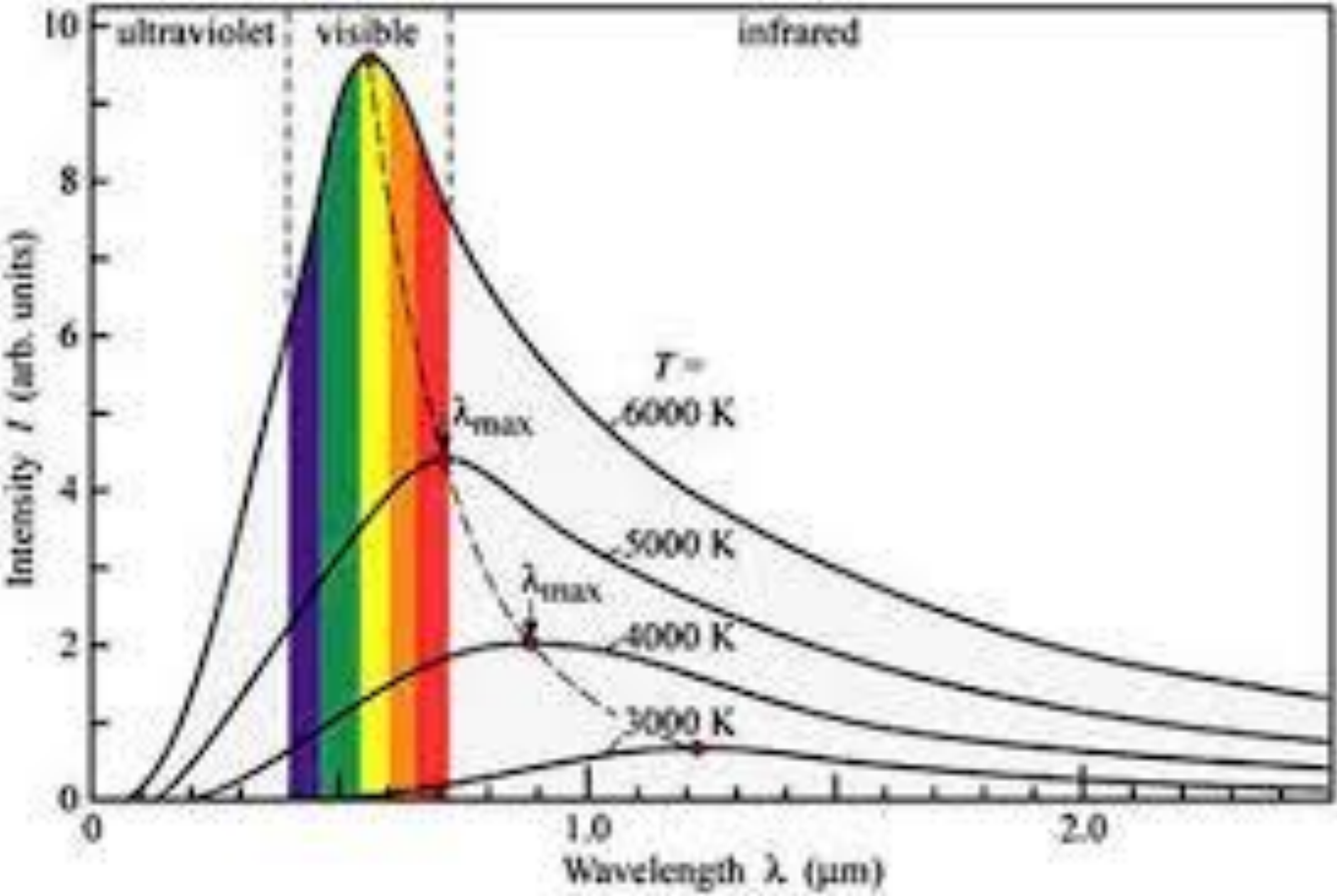
https://pediaa.com/difference-between-photoelectric-effect-and-compton-effect/

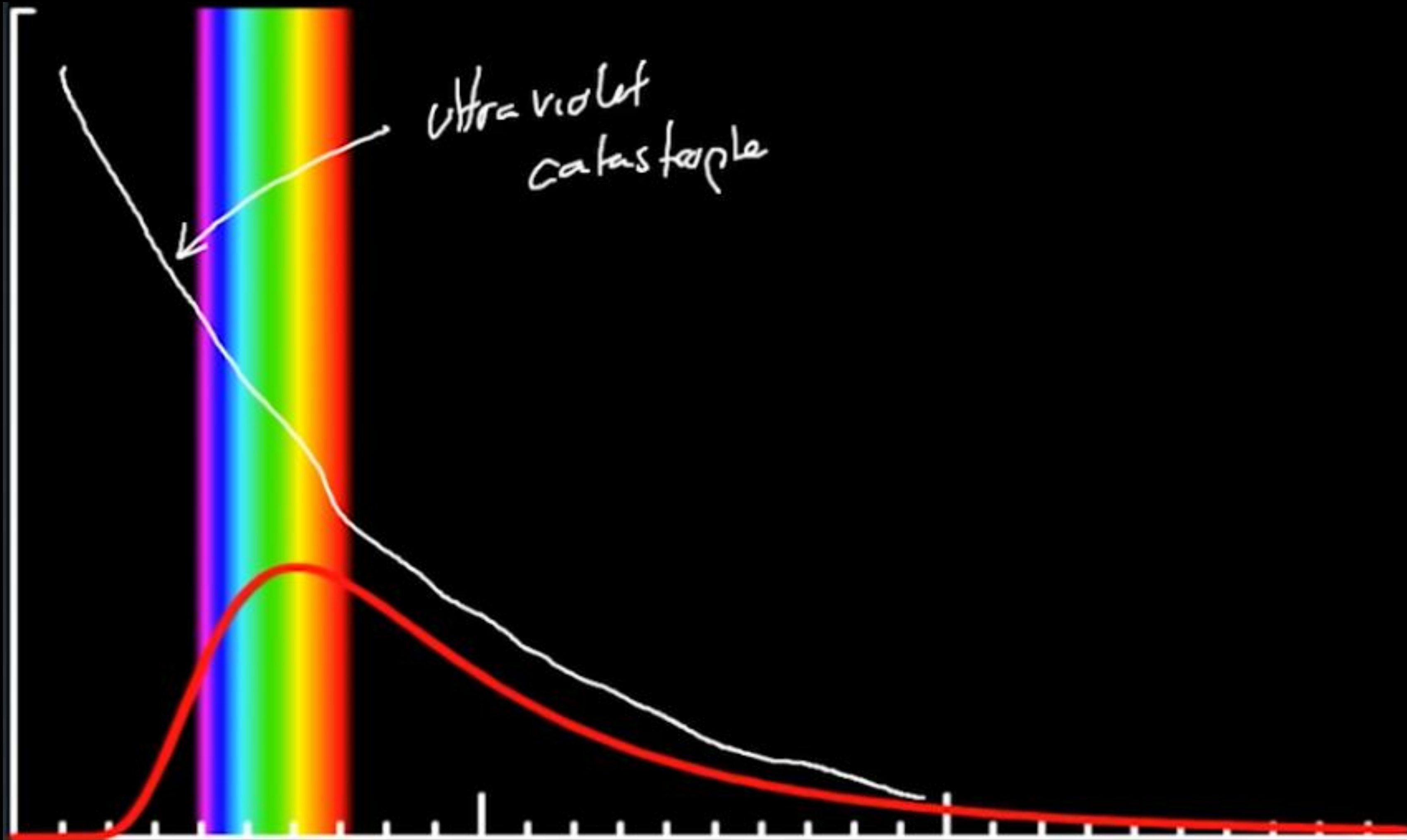
Max Planck and black-body radiation

Hot metalwork. The yellow-orange glow is the visible part of the thermal radiation emitted due to the high temperature. Everything else in the picture is glowing with thermal radiation as well, but less brightly and at longer wavelengths than the human eye can detect. A far-infrared camera can observe this radiation.


warm
hot
INFRARED
very hot

- As substances are heated they start to glow
- The hotter they are, the more glow
- The pattern is dependent on temperature NOT the substance used
- All objects emit radiation, and unless they receive energy, they will cool to their surroundings
- leads to Radiative cooling


ultraviolet
visible
infrared
T =
6000 K
5000 K
4000 K
3000 K
λmax
λmax
Intensity I (arb. units)
Wavelength λ (μm)
0
2
4
6
8
10
0
1.0
2.0



$$I = \frac{2\pi c k T}{\lambda^4}$$

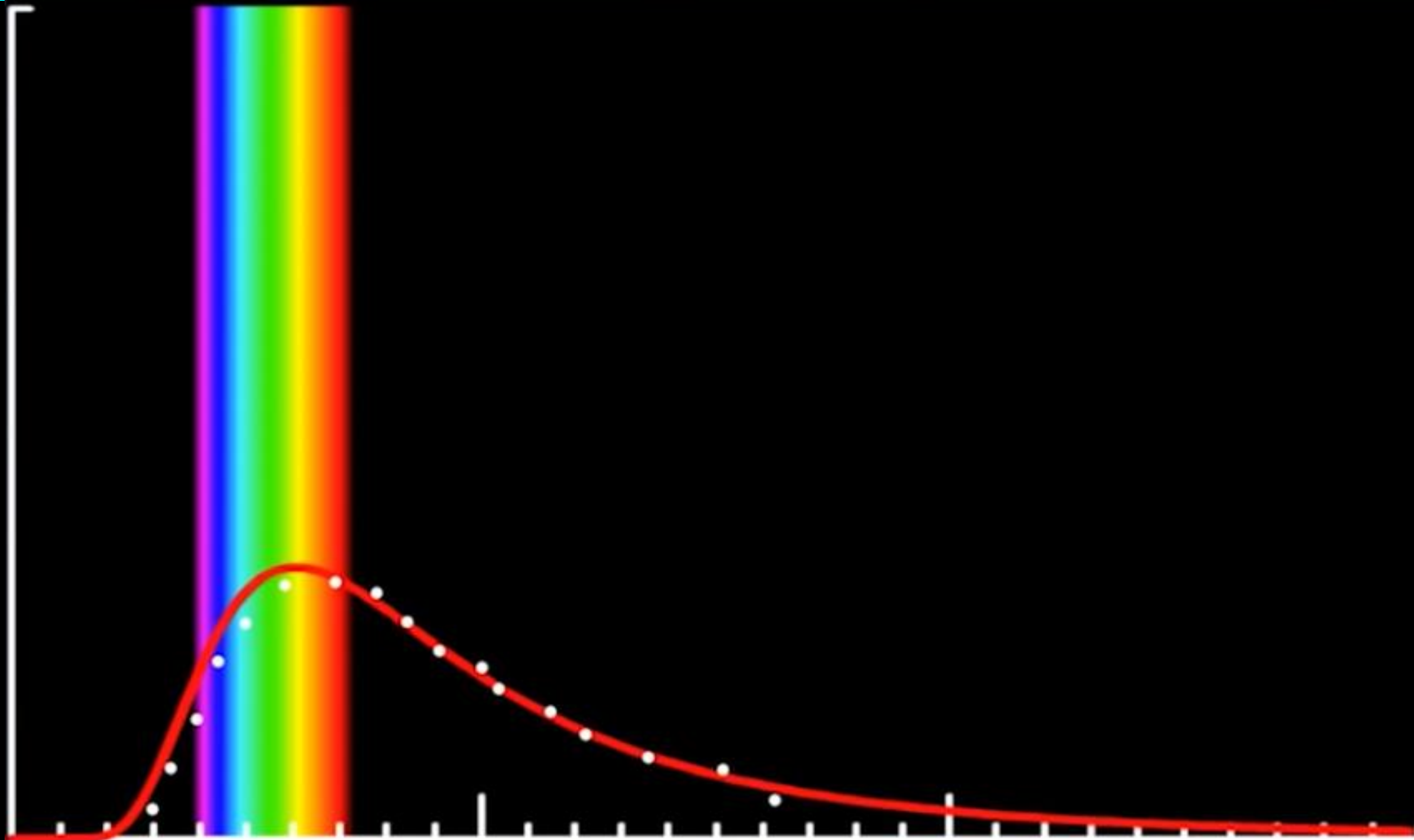
Max Planck and black-body radiation (contd..)

- The first model that was able to explain the full spectrum of thermal radiation was put forward by Max Planck in 1900.
- According to Planck, each energy element, E, is proportional to its frequency, *v*:

$E = h\,v$

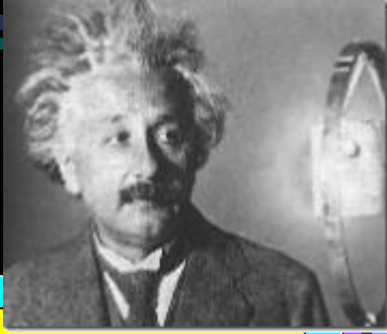
where *h* is Planck's constant = 6.63×10^{-34} J s,

Planck insisted that this was simply an aspect of the *processes* of absorption and emission of radiation and had nothing to do with the *physical reality* of the radiation itself. In fact, he considered his quantum hypothesis a mathematical trick to get the right answer rather than a sizable discovery.



$$P_\lambda = \frac{2\pi hc^2}{\lambda^5\left(e^{(hc/\lambda kt)}-1\right)}$$

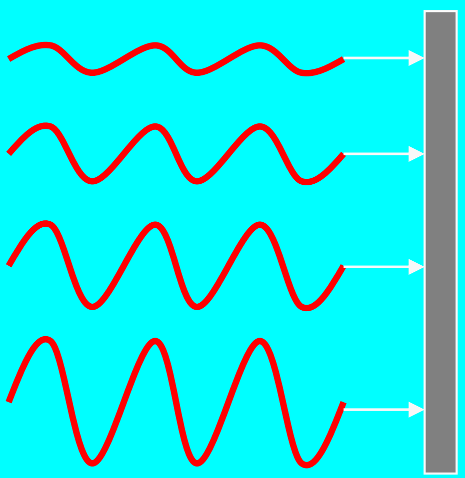
Photoelectric Effect (I)



"Classical" Method

Increase energy by increasing amplitude

electrons emitted ?



No

No

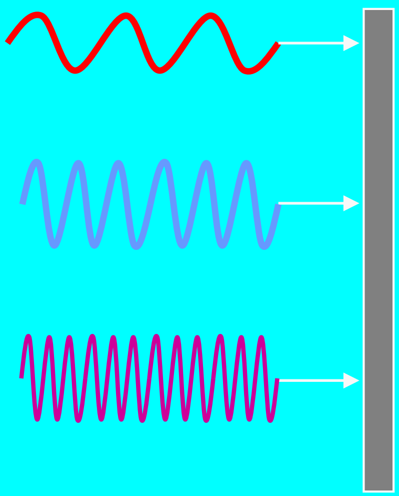
No

No

What if we try this ?

Vary wavelength, fixed amplitude

electrons emitted ?



No

Yes, with low KE

Yes, with high KE

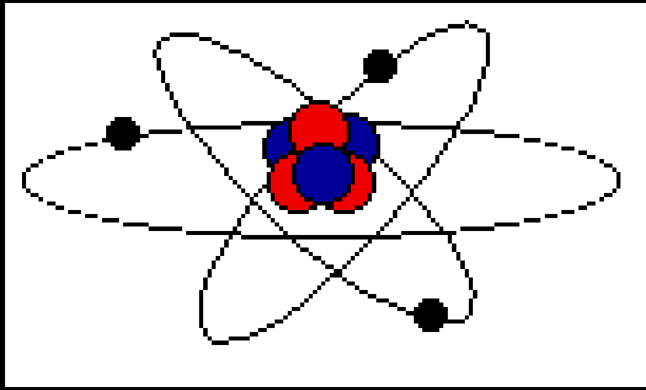
No electrons were emitted until the frequency of the light exceeded a critical frequency, at which point electrons were emitted from the surface! (Recall: small $\lambda \rightarrow$ large ν)

Photoelectric Effect (II)

- ❑ Electrons are attracted to the (positively charged) nucleus by the electrical force

- ❑ In metals, the outermost electrons are not tightly bound, and can be easily “liberated” from the shackles of its atom.

- ❑ It just takes sufficient energy…

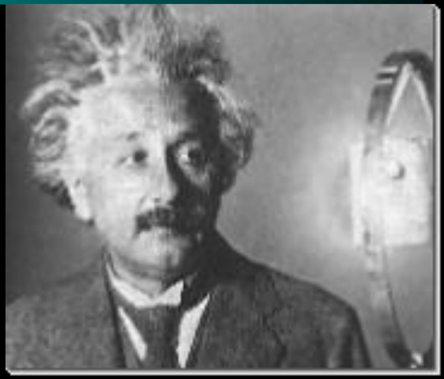


Classically, we increase the energy of an EM wave by increasing the intensity (e.g. brightness)

Energy α A^2

But this doesn’t work ??

PhotoElectric Effect (III)



- An alternate view is that **light** is acting like a **particle**

- The light particle must have sufficient energy to "*free*" the electron from the atom.

- **Increasing the Amplitude is simply increasing the <u>number of light particles</u>, but its <u>NOT increasing the energy of each one</u>!**

  ➔ Increasing the Amplitude does diddly-squat!

- However, if the energy of these "light particle" is related to their frequency, this would explain why higher frequency light can knock the electrons out of their atoms, but low frequency light cannot…

Photons

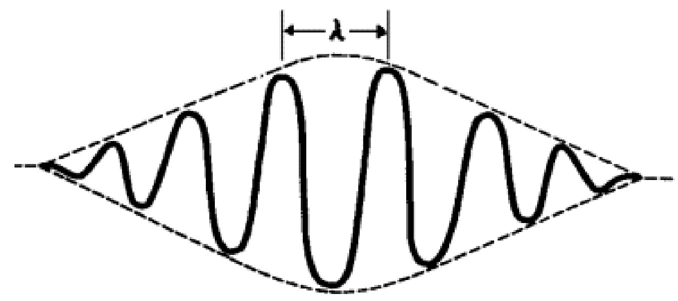


Figure 2

- <u>**Quantum theory**</u> describes light as a particle called a <u>**photon**</u>

- According to **quantum theory**, a **photon** has an **energy** given by

$$E = h\nu = hc/\lambda$$

where

h = Planck's constant = 6.6×10^{-34} [J s] and,

c = speed of light = 3×10^{8} [m/s]

λ = wavelength of the light (in [m])

- The energy of the light is <u>proportional to the frequency</u> (inversely proportional to the wavelength) ! The higher the frequency (lower wavelength) the higher the energy of the photon.

- 10 photons have an energy equal to ten times a single photon.

- <u>**Quantum theory describes experiments to astonishing precision**</u>, whereas the **classical wave description cannot**.

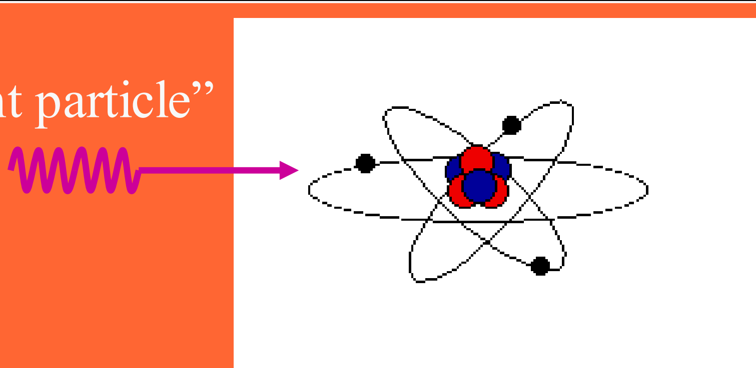
Photo-Electric Effect (IV)

- In this "quantum-mechanical" picture, the energy of the light particle (photon) must overcome the *binding energy* of the electron to the nucleus.

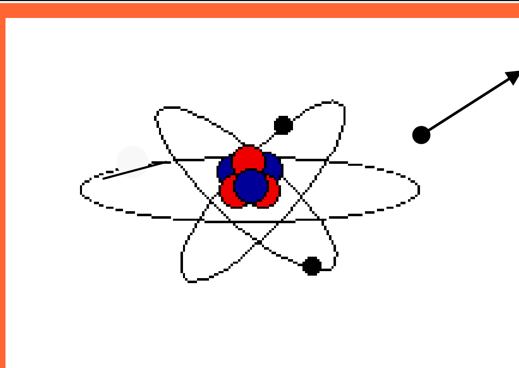
- If the energy of the photon exceeds the binding energy, the electron is emitted with a $KE = E_{photon} - E_{binding} = h(v - v_0)$

- The energy of the photon is given by $\mathbf{E=h}v$**,** where the constant $h = 6.6\times10^{-34}$ [J s] is Planck's constant and v_0, is the frequency of a photon whose energy is equal to the work function

"Light particle"

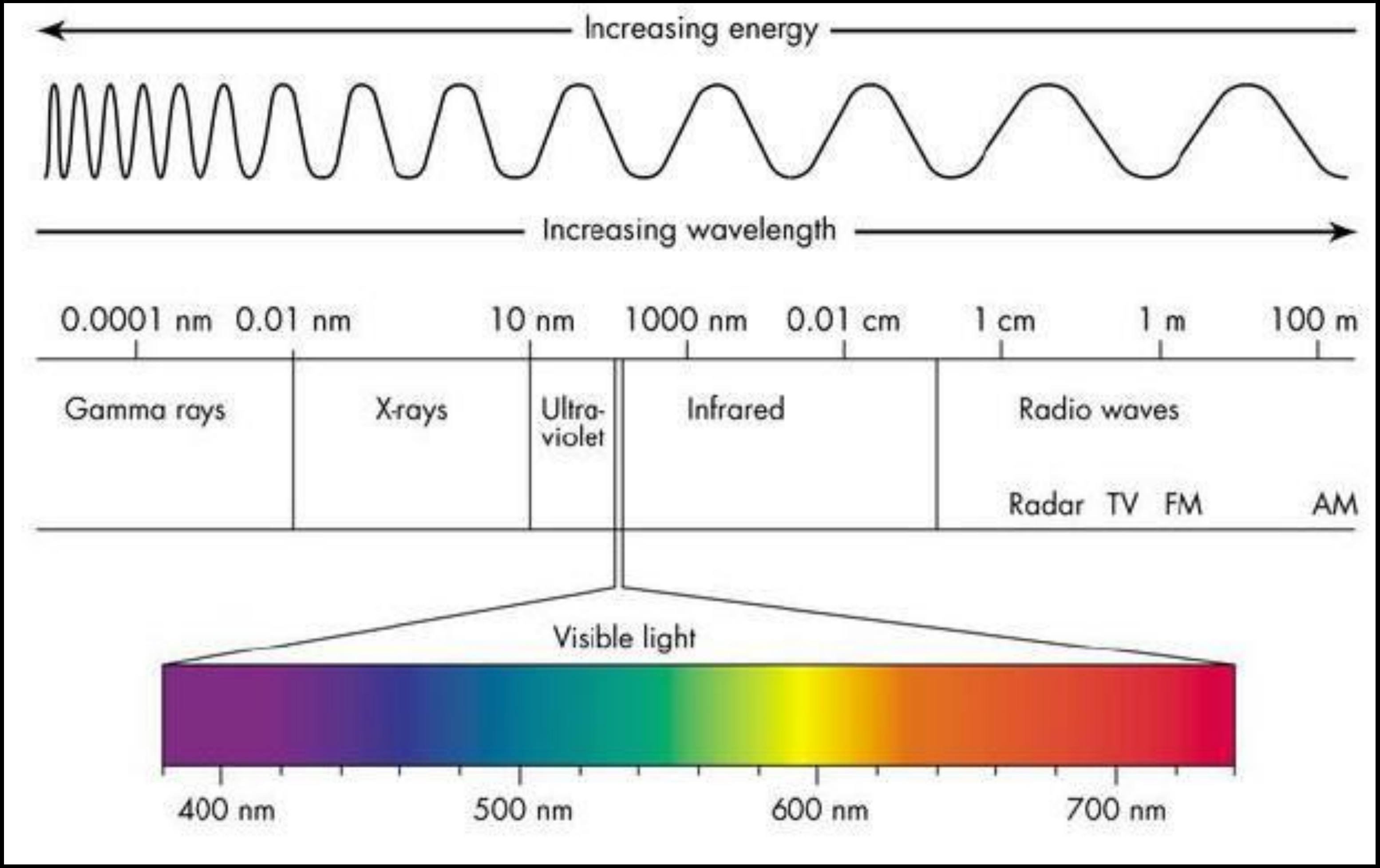


Before Collision



After Collision

The Electromagnetic Spectrum



$$E = h\nu = hc/\lambda$$

$h = 6.6 \times 10^{-34}$ [J*sec]
(Planck's constant)

Consequences of the light being quantized

- The relationship between the frequency of electromagnetic radiation and the energy of each individual photon is why ultraviolet light can cause sunburn, but visible or infrared light cannot.

- The total energy emitted per unit of time by a star (or by a piece of iron in a forge) depends on both the number of photons emitted per unit of time, as well as the amount of energy carried by each of the photons involved

Momentum

In physics, there's another quantity which we hold just as sacred as energy, and this is momentum.

For an <u>object with mass</u>, momentum is given by:

$$\boxed{\vec{p} = m\vec{v}}$$

The units are: [kg] [m/s] == [kg m/s]

Unlike energy, which is a scalar, momentum is a **vector.** That is it has both magnitude & direction. The direction is along the direction of the velocity vector.

The reason it is important in physics, is, because like Energy:
TOTAL MOMENTUM IS ALWAYS CONSERVED

Do photons carry momentum ?

DeBroglie's proposed that the a photon not only carries energy, but also carries momentum.

But, $p = mv$, and photon's have m=0, so how can it be that the momentum is not zero??

DeBroglie postulated that photons carry momentum, and their momentum is:

$$p = E / c$$

If we substitute: $E = hc/\lambda$ into this equation, we get:

$$p = h / \lambda$$

Momentum carried by a photon with wavelength λ

Wave–particle duality

- In 1923, Louis de Broglie reasoned that if light exhibits particle aspects, perhaps particles of matter show characteristics of waves.

- He postulated that a particle with mass m and a velocity v has an associated wavelength.

- The equation $\lambda = h/mv$ is called the de Broglie relation.

Video for double-slit experiment
http://upload.wikimedia.org/wikipedia/commons/e/e4/Wave-particle_duality.ogv

$$E = mc^2 \qquad E = \frac{hc}{\lambda}$$

$$m\cancel{c^2} = \frac{h\cancel{c}}{\lambda} \Rightarrow \boxed{\lambda = \frac{h}{mc}}$$

$$KE = \frac{p^2}{2m} \qquad \boxed{\lambda = \frac{h}{mv}}$$

$$\Downarrow$$

$$p = \sqrt{2m\,KE} \qquad \boxed{\lambda = \frac{h}{\sqrt{2m\,KE}}}$$

Wave–particle duality

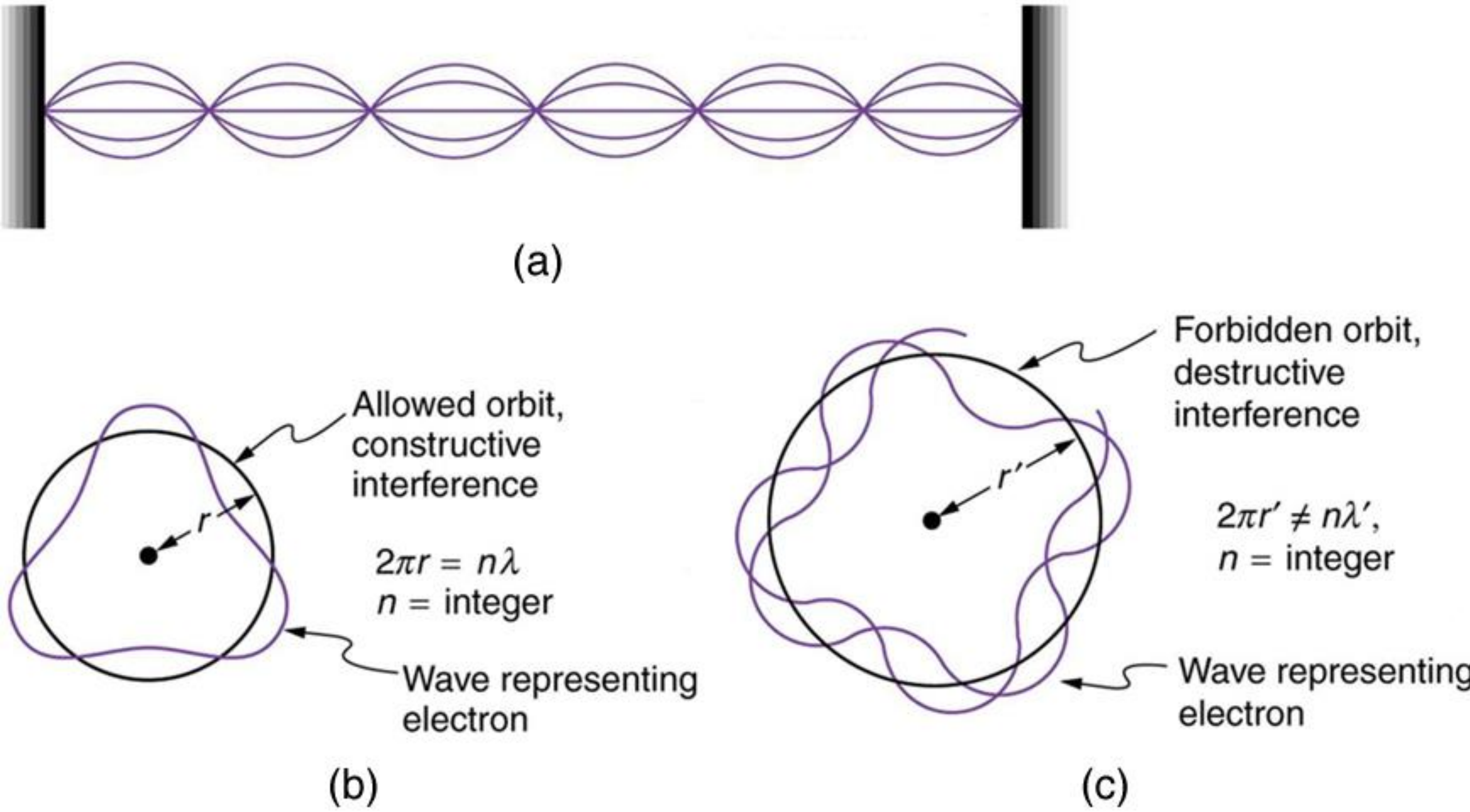
If matter has wave properties, why are they not commonly observed?

– The de Broglie relation shows that a baseball (0.145 kg) moving at about 60 mph (27 m/s) has a wavelength of about 1.7×10^{-34} m.

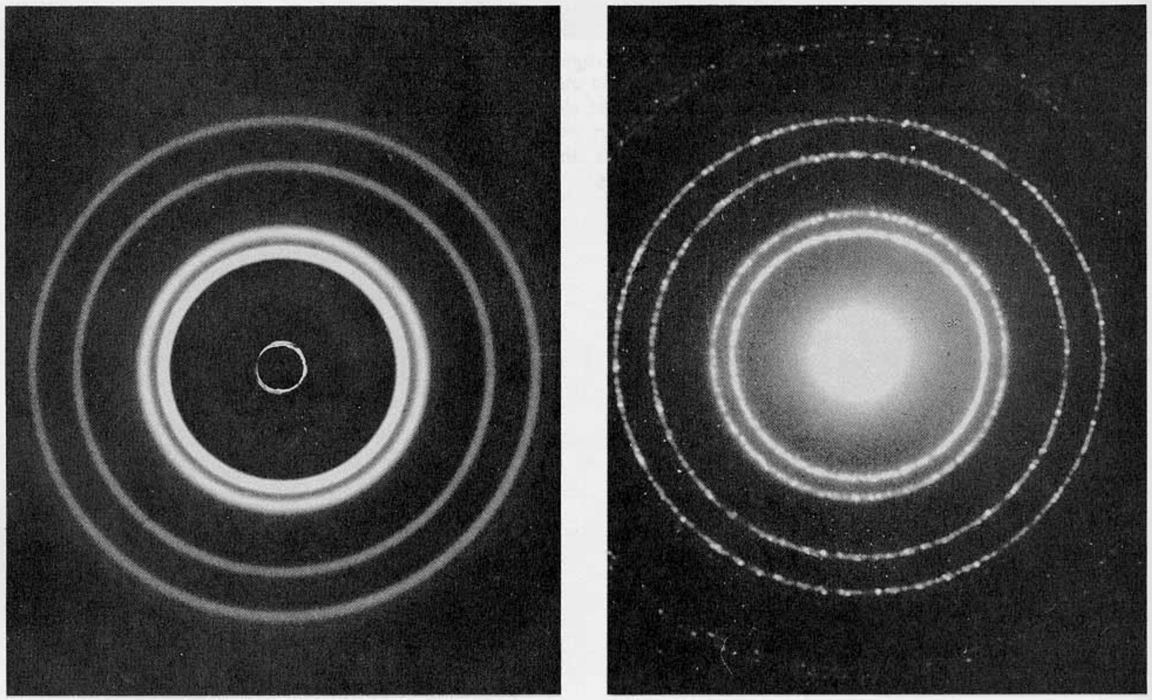
$$\lambda = \frac{6.63 \times 10^{-34}\ \frac{\text{kg}\cdot\text{m}^2}{s}}{(0.145\ kg)(27\ m/s)} = 1.7 \times 10^{-34}\ m$$

– This value is so incredibly small that such waves cannot be detected.

Fast electron	9×10^{-28}	5.9×10^{6}	1×10^{-10}
Alpha particle	6.6×10^{-24}	1.5×10^{7}	7×10^{-15}
1-gram mass	1.0	0.01	7×10^{-29}
Baseball	142	40.0	1×10^{-34}
Earth	6.0×10^{27}	3.0×10^{4}	4×10^{-63}


(a)
Allowed orbit,
constructive
interference
$2\pi r = n\lambda$
n = integer
Wave representing
electron
(b)
Forbidden orbit,
destructive
interference
$2\pi r' \neq n\lambda'$,
n = integer
Wave representing
electron
(c)

The diffraction pattern on the left was made by a beam of x rays passing through thin aluminum foil. The diffraction pattern on the right was made by a beam of electrons passing through the same foil.



Wave–particle duality

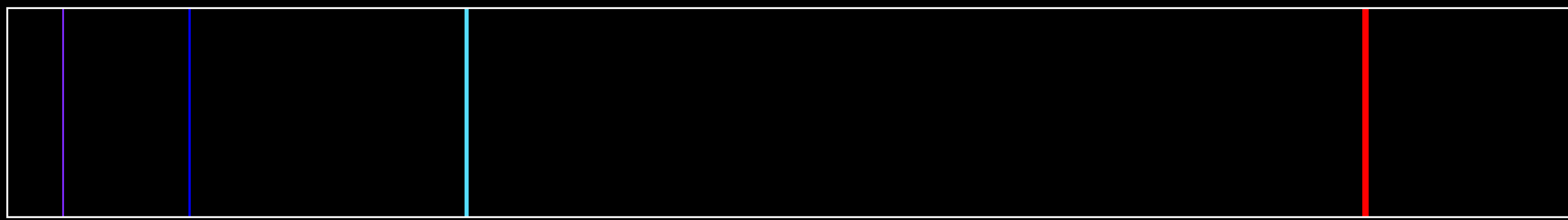
- If matter has wave properties, why are they not commonly observed?
  - Electrons have wavelengths on the order of a few picometers (1 pm = 10^{-12} m).
  - Under the proper circumstances, the wave character of electrons should be observable.
  - Molecules are of the dimension of a few pm, so the wave character of electrons is very important in molecules

Wave–particle duality (cont…)

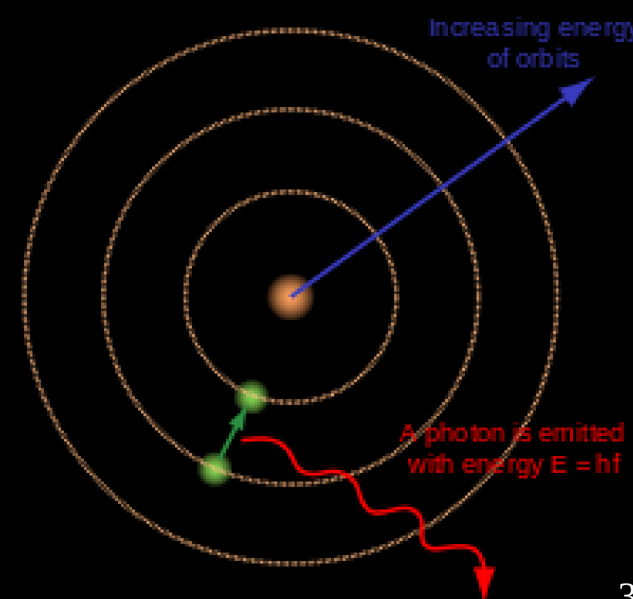
Although it is difficult to draw a line separating wave–particle duality from the rest of quantum mechanics, it is nevertheless possible to list some applications of this basic idea.

- Wave–particle duality is exploited in electron microscopy, where the small wavelengths associated with the electron can be used to view objects much smaller than what is visible using visible light.
- Similarly, neutron diffraction uses neutrons with a wavelength of about 0.1 nm, the typical spacing of atoms in a solid, to determine the structure of solids.
- *Explain or give reason for the above text in yellow*

The quantization of matter: the Bohr model of the atom

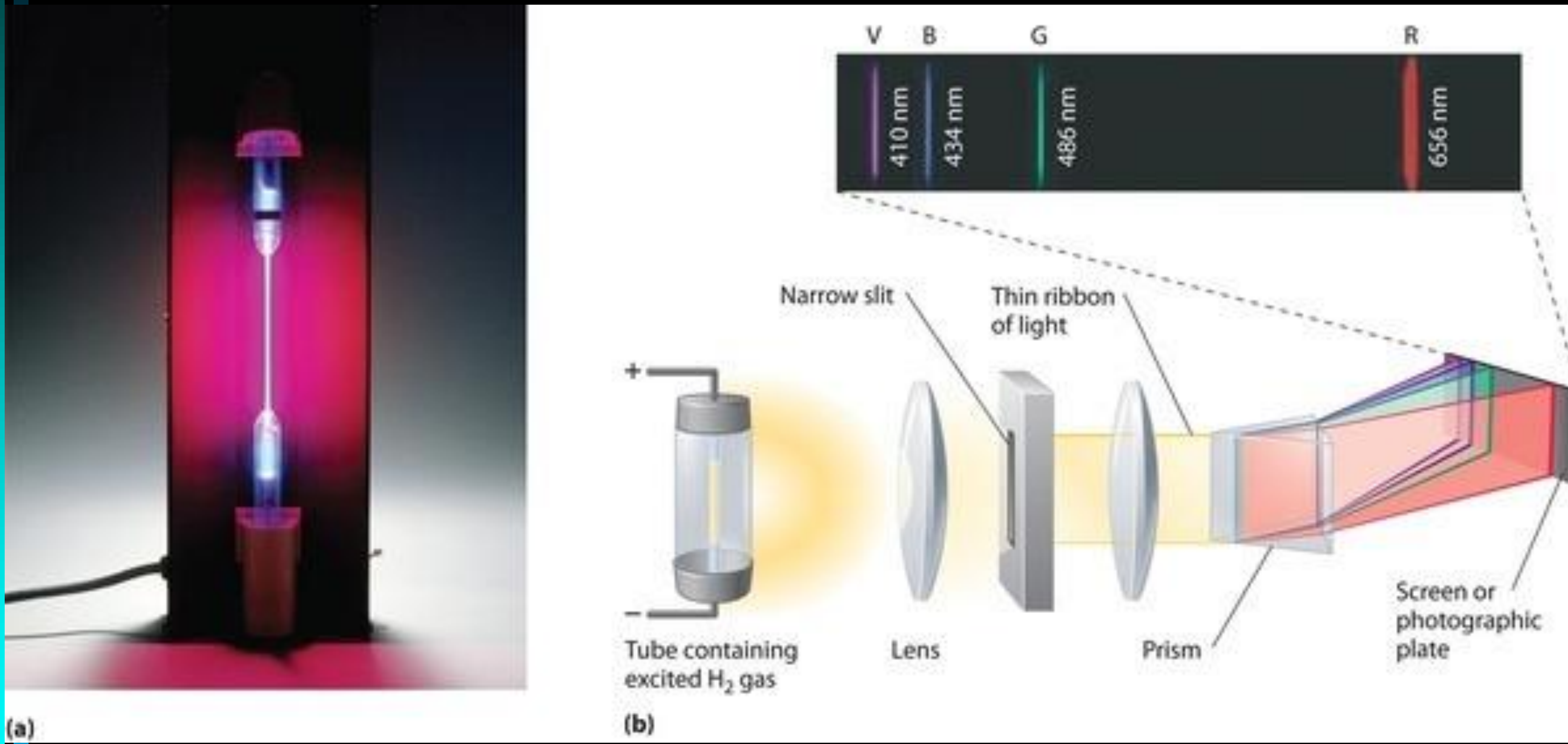


Emission spectrum of hydrogen. When excited, hydrogen gas gives off light in four distinct colors (spectral lines) in the visible spectrum, as well as a number of lines in the infrared and ultraviolet

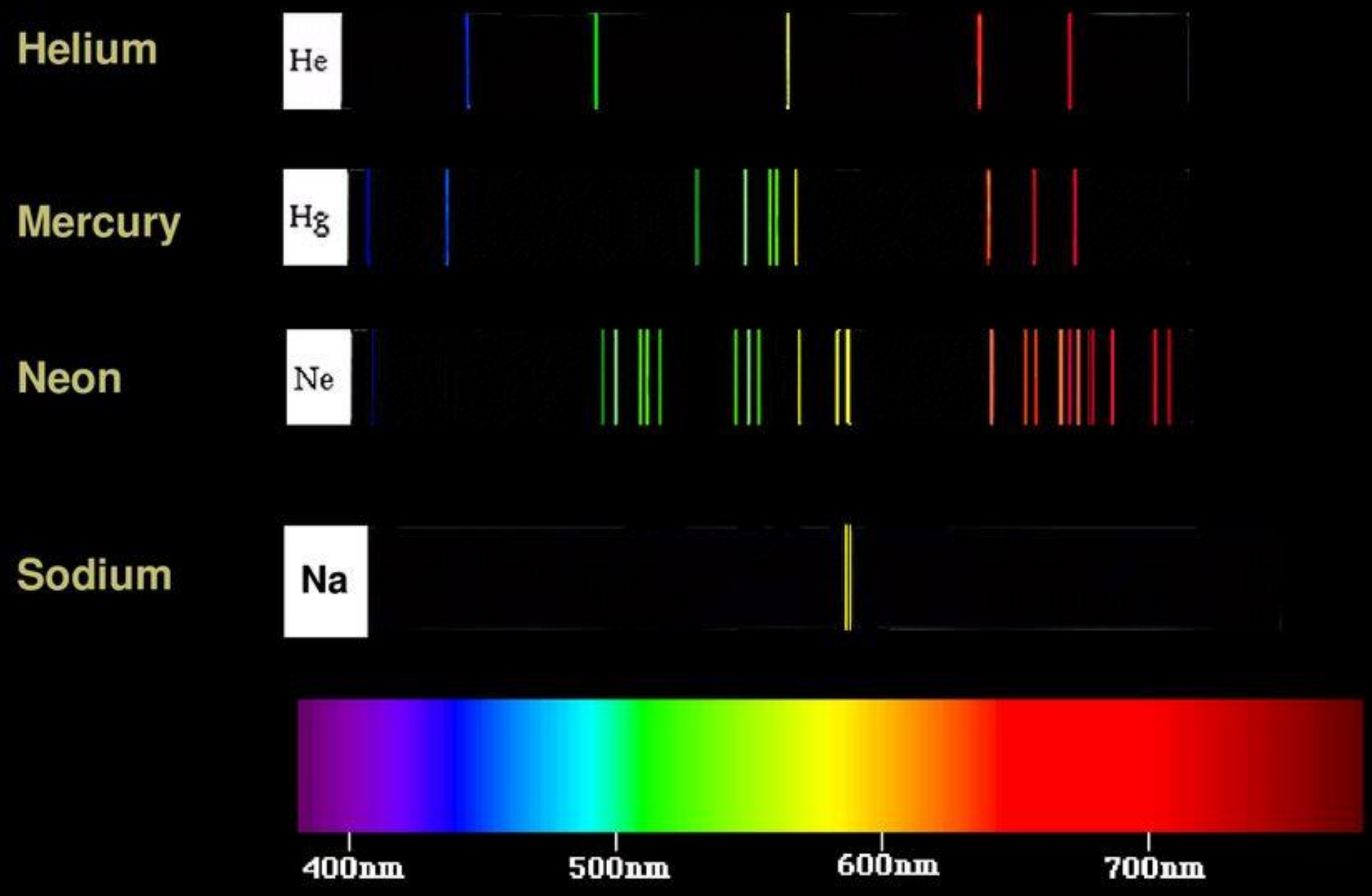


The discrete lines in emission spectra are due to some property of electrons in atoms being quantized.

The way that the electrons actually behave is strikingly different from Bohr's atom. This modern quantum mechanical model of the atom is discussed below.


V
B
G
R
410 nm
434 nm
486 nm
656 nm
Narrow slit
Thin ribbon of light
+
–
Tube containing excited H_2 gas
Lens
Prism
Screen or photographic plate
(a)
(b)

Bright Line (Emission) Spectra



Wave–particle duality (cont…)
Application to the Bohr mode

- De Broglie expanded the Bohr model of the atom by showing that an electron in orbit around a nucleus could be thought of as having wave-like properties.
- The electron's wavelength therefore determines that only Bohr orbits of certain distances from the nucleus are possible. In turn, at any distance from the nucleus smaller than a certain value it would be impossible to establish an orbit.
- De Broglie's treatment of quantum events served as a starting point for Schrödinger when he set out to construct a wave equation to describe quantum theoretical events.

Uncertainty principle

Quantum mechanics shows that certain pairs of physical properties, like position and speed, cannot both be known to arbitrary precision: the more precisely one property is known, the less precisely the other can be known. This statement is known as the uncertainty principle.

The uncertainty principle shows mathematically that the product of the uncertainty in the position and momentum of a particle (momentum is velocity multiplied by mass) could never be less than a certain value, and that this value is related to Planck's constant.

$$\Delta x \Delta p \geq h/2\pi$$

Uncertainty principle (cont..)

The second statement of the uncertainty principle is that it is impossible to simultaneously describe with absolute accuracy the energy of a particle and the instant of time the particle has this energy. Again. if the uncertainty in the energy is given by ΔE and the uncertainty in the time is given by Δt, then the uncertainty principle is stated as

$$\Delta E\, \Delta \mathrm{t} \geq h/2\pi$$

Although we cannot precisely define an electron's orbit, we can obtain the ***probability*** of finding an electron at a given point around the nucleus.

- Erwin Schrodinger defined this probability in a mathematical expression called a wave function, denoted ψ (psi).
- The probability of finding a particle in a region of space is defined by ψ^2.

Schrödinger equation

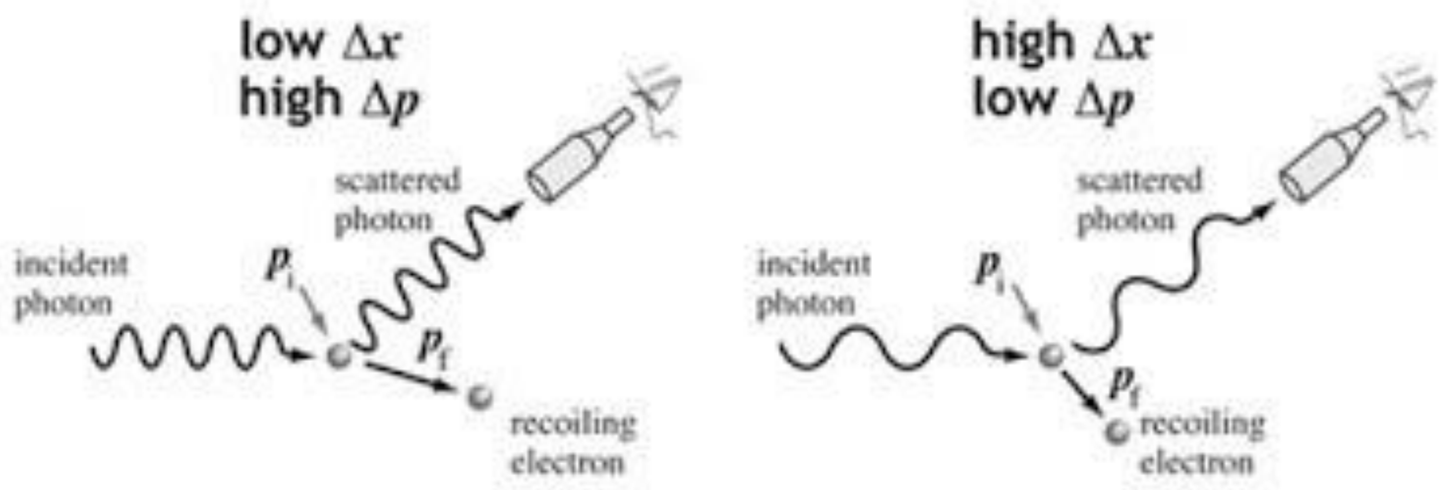
Schrödinger was able to calculate the energy levels of hydrogen by treating a hydrogen atom's electron as a classical wave, moving in a well of electrical potential created by the proton. This calculation accurately reproduced the energy levels of the Bohr model.

In quantum mechanics, the **Schrödinger equation** is a partial differential equation that describes how the quantum state of a physical system changes with time.

Heisenberg Uncertainty Principle

$$\Delta x\, \Delta p \geq \hbar$$

Δx = uncertainty in position
Δp = uncertainty in momentum
$\hbar$ = $h / 2\pi$



Schrödinger equation

Schrodinger, in 1926 provided a formulation called wave mechanics, which incorporated the principles of quanta introduced by Planck, and the wave-particle duality principle introduced by de Broglie.

Based on the wave-particle duality principle. we will describe the motion of electrons in a crystal by wave theory. This wave theory is described by Schrodinger's wave equation.

The one-dimensional, nonrelativistic Schrodinger's wave equation is given by

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

where Ψ (x,t) is the wave function, U (x) is the potential function assumed to he independent of time, m is the mass of the particle, and, i is the imaginary constant √-1