ATOMIC PHYSICS

<u>End of 19th Century</u>:

• Almost all of physics seemed to be explained by mechanics, thermodynamics & electromagnetism

• Only a few "minor" problems remained to be resolved. Otherwise physics was thought to be almost complete, it was just a question of time…

• Nature of problems: There were quite solid "buildings" of Mechanics, Electricity and Magnetism without communications between them.

• There were also mysterious effects that lacked explanation, but they did not affect machinery, weaponry, or agriculture. Only a few people were bothered by these unsolved problems.

The dilemma of Mechanics and E&M

The problem can be stated in the following form there are three statements

- Galilean transformations of coordinates and absolute time.

- The speed of light is constant in all frames of reference.

- All laws of Nature are the same in all inertial frames of reference.

- These three statements contradict each other. One has to be dropped to resolve the problem.

The special theory of relativity

- Einstein's solution – special theory of relativity: two postulates, 1905:

- All inertial frames of reference are equally suitable for the description of physical phenomena.

- The speed of light in vacuum is the same for all observers and is independent of the motion of the source.

- The toll for this is the Lorentz transformations of space-time with a set of consequences – the effects not intuitively simple for most people

Nature and nature's laws lay hid in night,
God said, "Let Newton be," and all was light.
It did not last; the devil howling "Ho!
Let Einstein be!" restored the status quo.

Alexander Pope – Sir John Collins

Three big problems with light (EM radiation) that were unresolved:

- Blackbody radiation

- Photoelectric effect

- Atomic spectra

Today we will start discussion of how "fixing" these three problems has changed the world.
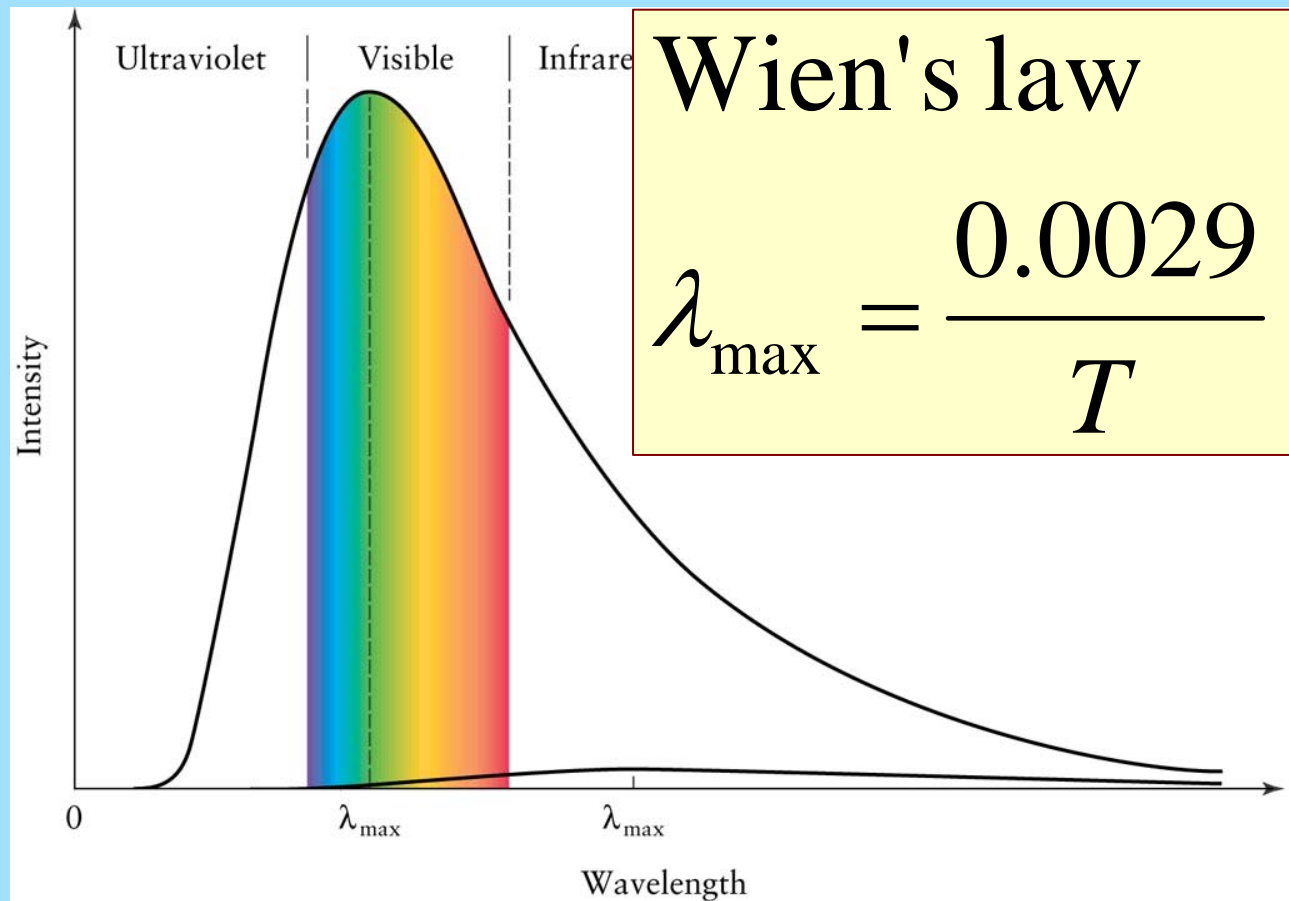
BLACKBODY RADITATION

Bodies emit heat radiation that depends on their temperature.

Stefan's law

$$P \sim T^4$$

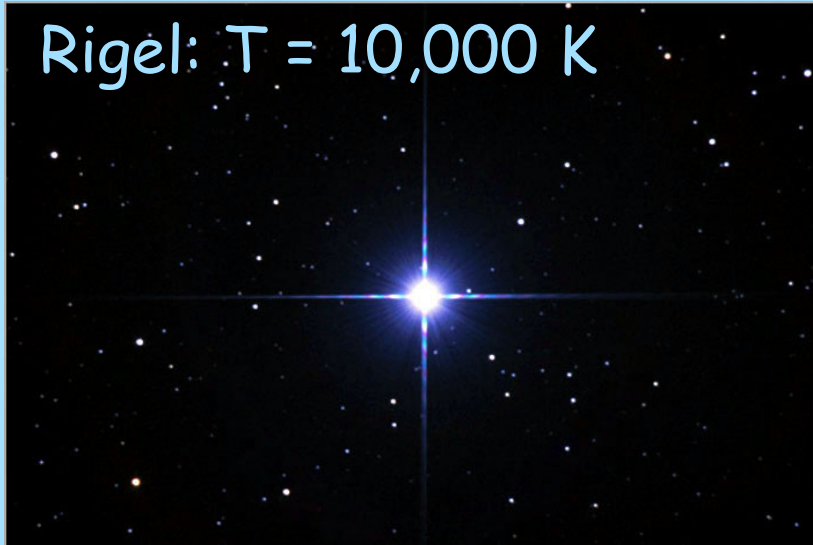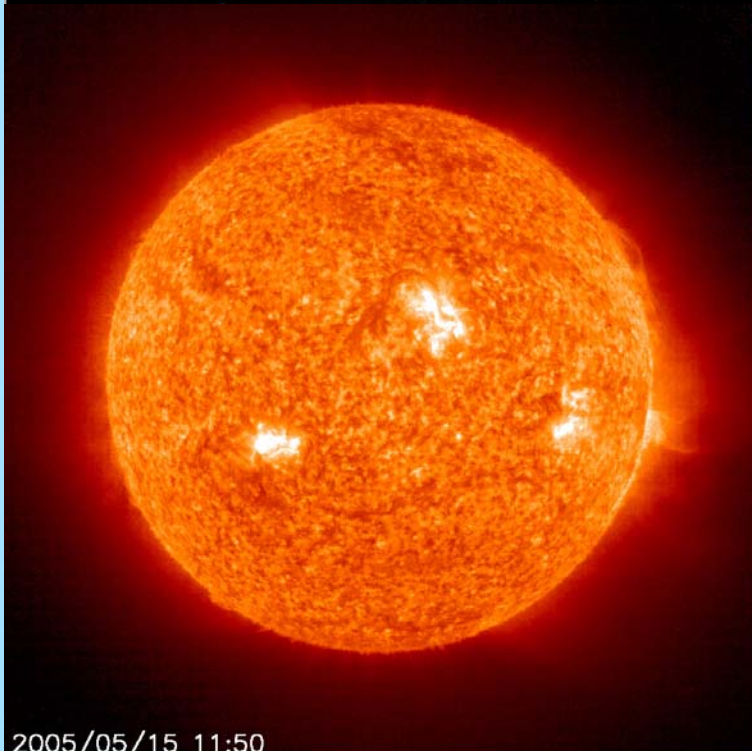The power of EM radiation emitted by an object is proportional to the fourth power of its temperature (K)

Ultraviolet | Visible | Infrared

Intensity

λ_{max} λ_{max}

Wavelength

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Wien's law

$$\lambda_{max} = \frac{0.0029}{T}$$

Color of stars is due to their temperature

Rigel: T = 10,000 K

Betelgeuse: T = 3,200 K

Size of Star

Size of Earth's Orbit

Size of Jupiter's Orbit

Sun: T = 5,800 K

2005/05/15 11:50
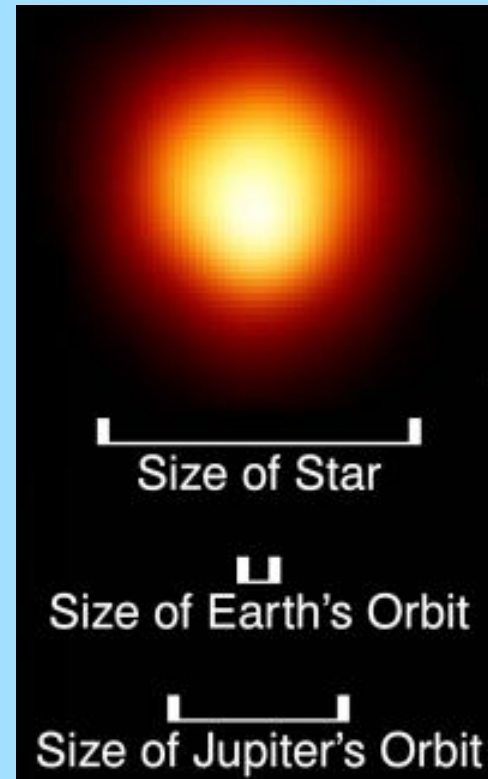
Blackbody Radiation

BBR is due to EM waves emitted by vibrating atoms.
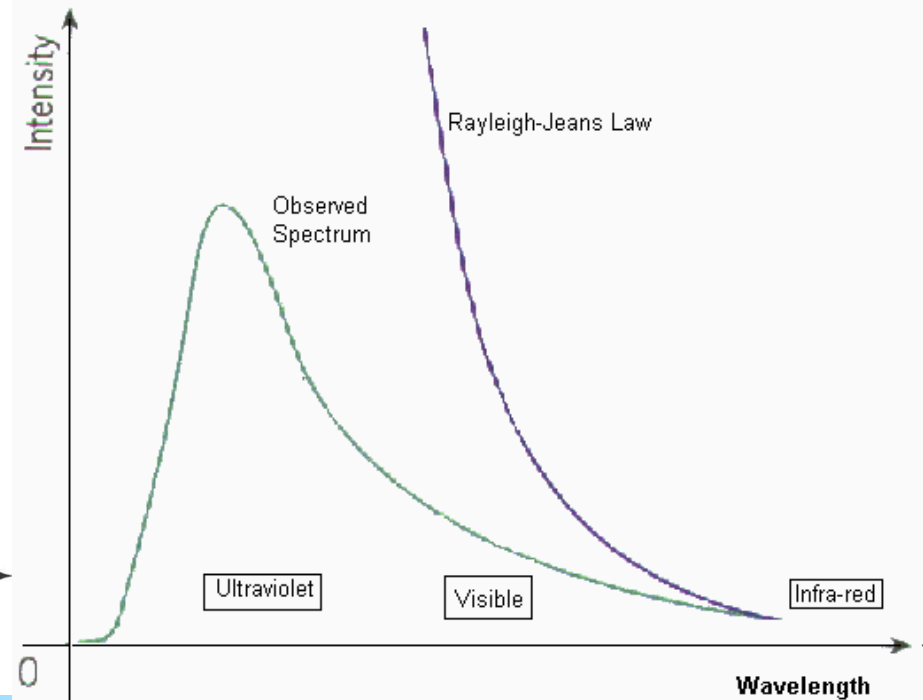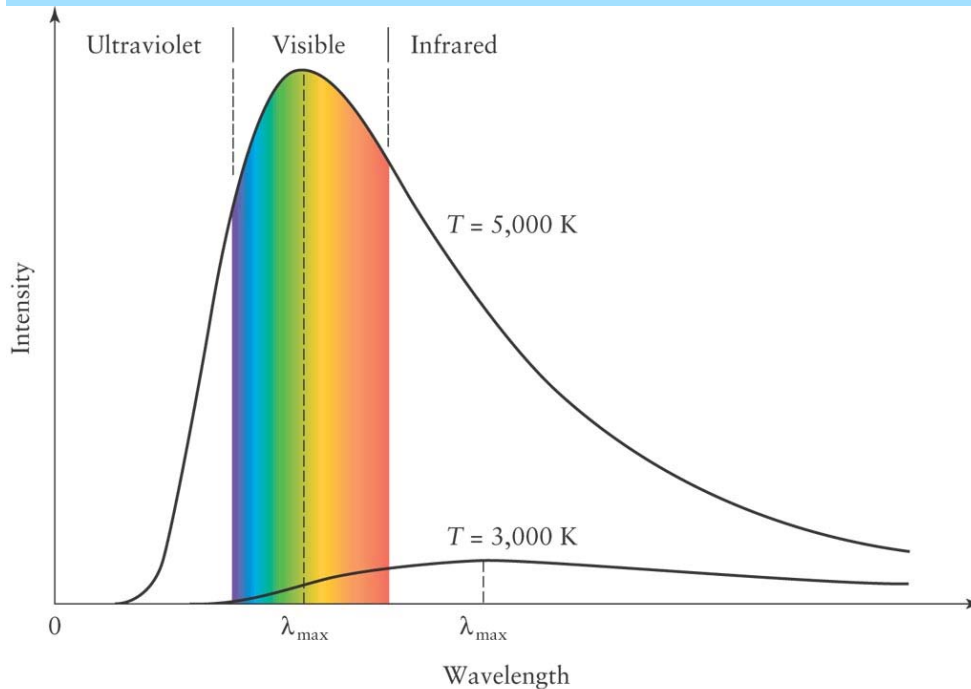
Experiment:

1. Wien's law – maximum emission at λ_{max}

2. Radiation is in equilibrium with matter

Theory:

1. No "maximum emission wavelength"

2. Ultraviolet catastrophe

Photo-electric effect

When light is shone on metal , the surface may become positively charged. This is because electrons gain energy from the light waves, and are able to leave the metal's surface.

Experiment:

- The frequency of the light must be above a certain threshold value for that metal for electrons to be emitted. For example blue light causes sodium to emit electrons but red light does not.
- Incredibly weak beams of light can cause electrons to be emitted.
- The kinetic energy of the electrons depends only on the frequency of the light. A very weak ultraviolet beam will give electrons a higher kinetic energy than a very bright blue beam of light.
- The electrons are emitted very quickly after the radiation is turned on

Theory:

- The electrons should eventually absorb enough energy to be emitted, regardless of frequency.
- Light waves are expected to spread out and no electrons are expected to obtain the energy to escape.
- The kinetic energy of the electrons depends on the intensity of the light
- Electron emission should increase with time…

Spectra

What is different between the spectrum emitted by a regular light bulb and the spectra emitted by the discharge tubes ?

• The spectrum of the light bulb is a continuous band of colors: <u>Continuous spectrum</u>.

• It is light emitted due to the temperature of the filament (Blackbody radiation)

• The spectra emitted by the discharge tubes show distinctive lines of color: <u>Emission-line spectra</u>.
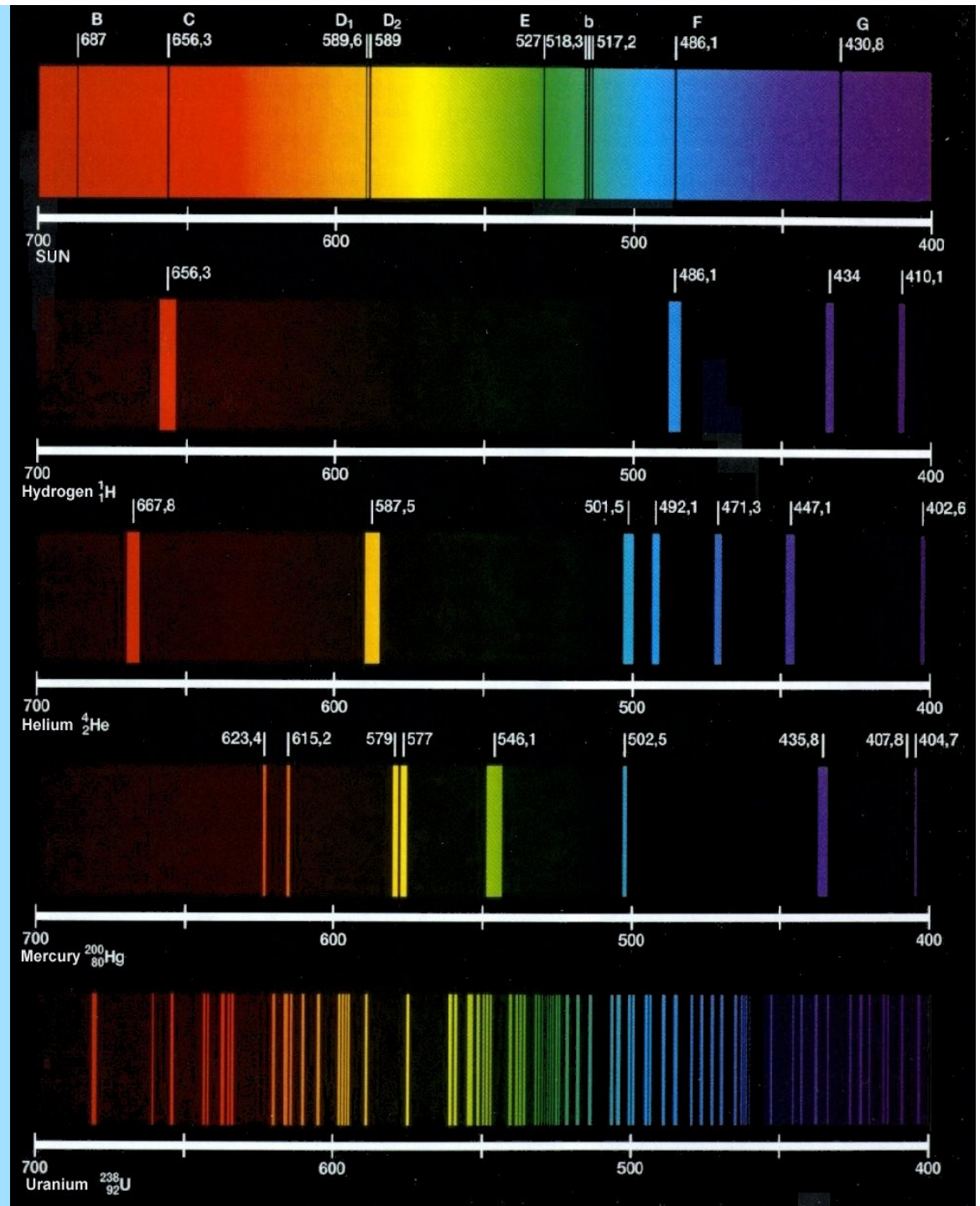
Absorption spectra
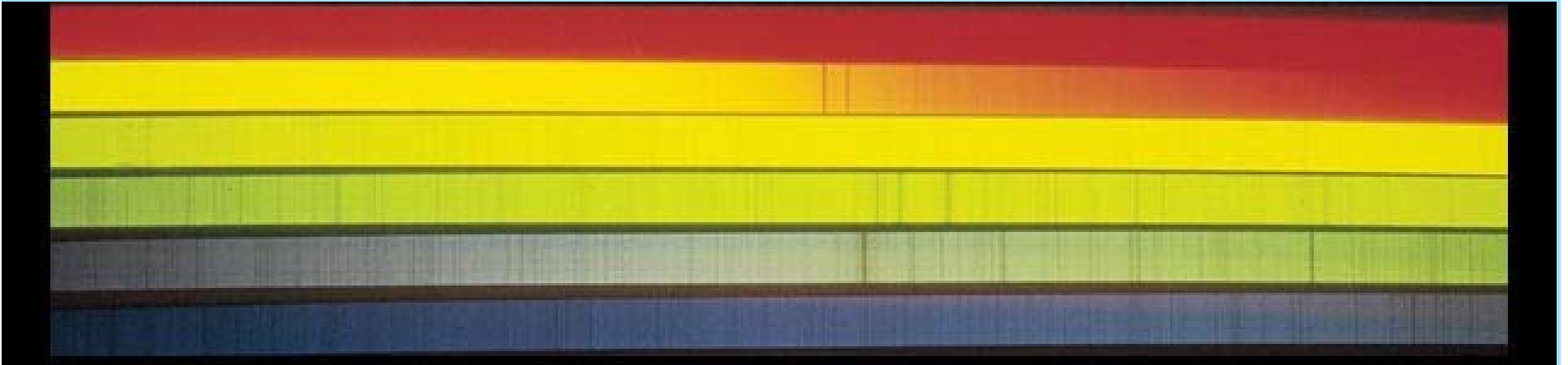
The spectrum from the Sun discovered by Fraunhofer, 1824
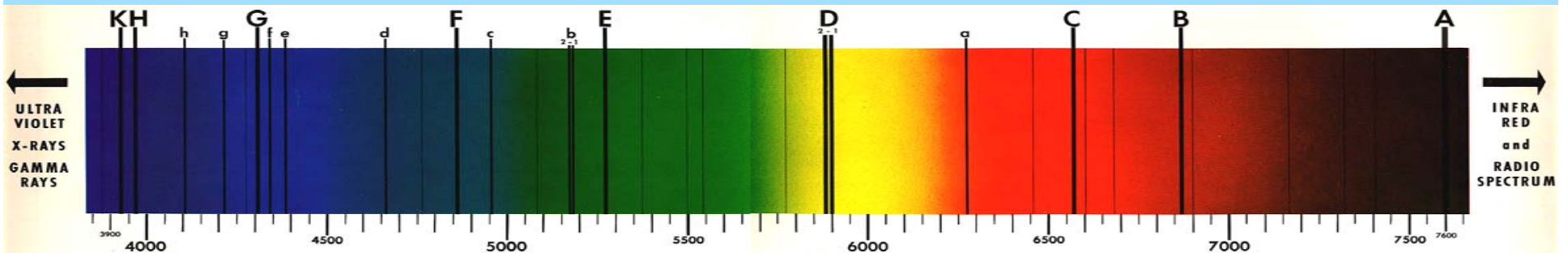
Ok, blackbody radiation, but what are these lines?

Emission spectra

1. When "heated" gases emit only on certain wavelengths rather than continuous BBR spectrum.

2. The spectrum is uniquely defined by the gas.

Black body radiation

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First explained by Max Planck

Assumption: The light is emitted in "portions", called quanta. The energy of each quantum is proportional to its frequency

$E = h\,f$, where $h = 6.626 \times 10^{-34}$ J s

f - frequency of oscillating atoms – the energy is quantized – comes in portions for a given frequency: e.g. if light is emitted at frequency f, the emitted energy will be 0, hf, 2hf, 3hf,… nhf, (n+1)hf,…

This assumption led to the Plank's formula for BBR that becomes Rayleigh-Jeans formula in the limit of long waves

Photons

- Einstein took the next step by working out that all radiation is quantized. He argued that an oscillating charge can accept or lose energy in small values of $\Delta E = h\Delta f$. This energy is lost as electromagnetic radiation.

- This radiation must be emitted in small packets, each containing ΔE. He then suggested that each energy of radiation will have its own frequency.

- The radiation from an object is not continuous – it consists of a series of "packets" of energy. Radiation is a "packet of energy" but is also a wave because it has a frequency. These became known as photons.

Photons – particles and waves

Photons reveal properties of both particles and waves:

- Wave properties: frequency, wavelength, interference, diffraction, polarization, reflection, refraction, etc.
- Particle properties: carries a quantum of energy = hf, carries linear momentum = h/λ.

These particle properties are essential for the explanation of BBR: the quantization of energy in such a way gives Planck's formula, the property of momentum explains the equilibrium of radiation and matter.

Particle – wave duality is one of the most striking and essential features of the modern physics

Photoelectric effect

$$hf = W + KE$$

- Einstein: the light arrived in photons. One photon gave all its energy to one electron.

- The electron must gain a certain amount of energy to overcome the forces that hold it inside the metal.

- One electron can only accept one photon of energy, so this must have the required frequency to have the necessary escape energy, so the intensity will not make any difference to this. Brighter light means there are more photons, so more electrons can be emitted, but it is the frequency of the light that decides the energy of the photon and so the electron's kinetic energy.

- Electrons can also be emitted very quickly because it only requires one photon for emission to occur, not the gradual build up of wave energy.

- The kinetic energy of escaped electrons is a linear function of frequency

How much energy does a photon of light have ?

Example: Red light, $f = 4.7 \times 10^{14}$ Hz

$E_{red} = h\,f = (6.63 \times 10^{-34}\ J\,s)\,(4.7 \times 10^{14}\ s^{-1})$

$$= 3.12 \times 10^{-19}\ J$$

Convenient unit of energy: 1 electron gains in a 1 Volt battery:

$E = q\,V = (1.6 \times 10^{-19}\ C)\ (1\ V) = 1.6 \times 10^{-19}\ J$

$$= 1\ \text{Electron} \times \text{volt} = 1\ eV$$

So, $E_{red} = 3.12 \times 10^{-19}\ J / 1.6 \times 10^{-19}\ J/eV$

$$= 1.95\ eV$$

Ranges in energies E = hf/e in eV

Red light: E = 1.65 eV - 1.99 eV

Yellow light: E = 2.11 eV - 2.23 eV

Blue light: E = 2.52 eV - 2.77 eV

UV: E = 3.10 eV - 4 keV

X-rays: E = 40 eV - 400 keV

Example: to escape a certain metal surface, electrons should overcome 5 eV threshold. What radiation is needed to cause photoelectric effect? What would be the average kinetic energy of escaping electrons if it is irradiated with UV radiation at 6 eV?

UV is needed, KE = hf – W = 6 – 5 = 1 eV

The threshold for PE (W – work function) depends on the material

How do we determine the frequency?

$$E = hf \qquad \Rightarrow \qquad f = \frac{E}{h}$$

$$h = 6.626 \cdot 10^{-34} \text{ J} \cdot \text{s}$$

$$\frac{1\text{eV}}{h} = \frac{1.602 \cdot 10^{-19} \text{ J}}{6.626 \cdot 10^{-34} \text{ J} \cdot \text{s}} = \frac{1}{4.136 \cdot 10^{-15} \text{s}}$$

$$h = 4.136 \cdot 10^{-15} \text{ eV/Hz}$$

Our example - threshold energy $E = 5 \text{ eV}$

$$f = \frac{5 \text{ eV}}{4.136 \cdot 10^{-15} \text{ eV/Hz}} = 1.2 \cdot 10^{15} \text{ Hz}$$

Atomic model

  - The size of the nucleus is very small compared to the orbit radius

  - Electrons orbit nuclei as planets orbit around the Sun – the Coulomb force

  - Problem: rotating electrons (due to centripetal acceleration) emit EM waves – bound to loose energy and fall on the nucleus – no stable atoms...

- Atoms are made of a positively charged nucleus (protons + neutrons) and a "cloud" of negatively charged electrons that surround the nucleus.

- The electrons do not emit radiation while on the orbit

E. Rutherford (1871-1937)

N. Bohr (1885-1962)

The Bohr model of the atom

• Both energy and angular momentum are quantized

• Electrons move in specific "orbits". Only certain orbits are allowed. Orbits are characterized by their energy and angular momentum

• The orbits do not have to be spherical

• Electrons can jump from one orbit to another by absorbing or emitting energy.

Hydrogen atom
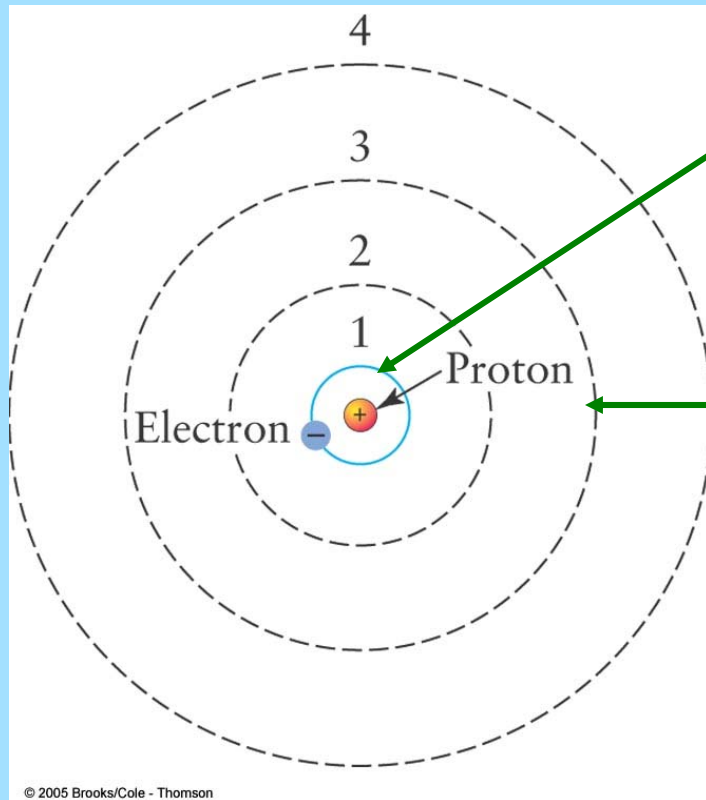
Innermost orbit (number 1) has lowest energy = "ground state"

Higher orbits have larger energy = "excited states".

- To get from a lower energy orbit to a higher energy orbit the electron needs to absorb energy.

- To "fall" back to a lower energy orbit the electron needs to emit (get rid of) some energy.

Typically, the energy is emitted as photons (electromagnetic radiation).

Photon

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Absorption of light:

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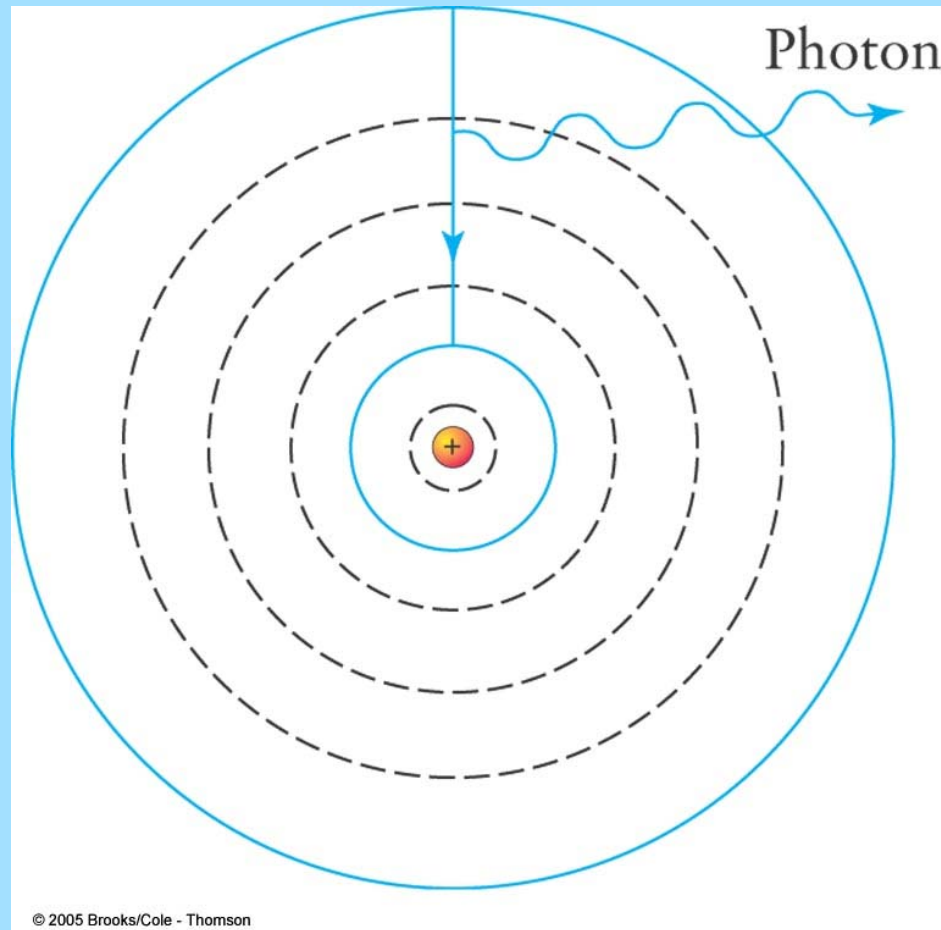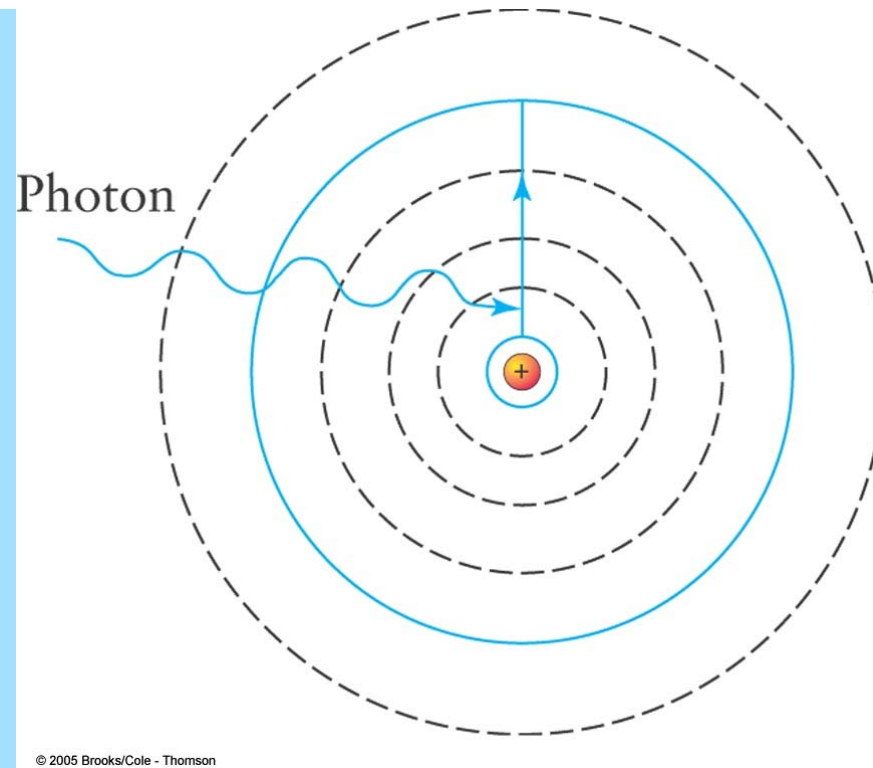
Absorption-
line spectrum:

Continuous source

Gas cloud

Prism

Red

Violet

Spectrum

Dark lines

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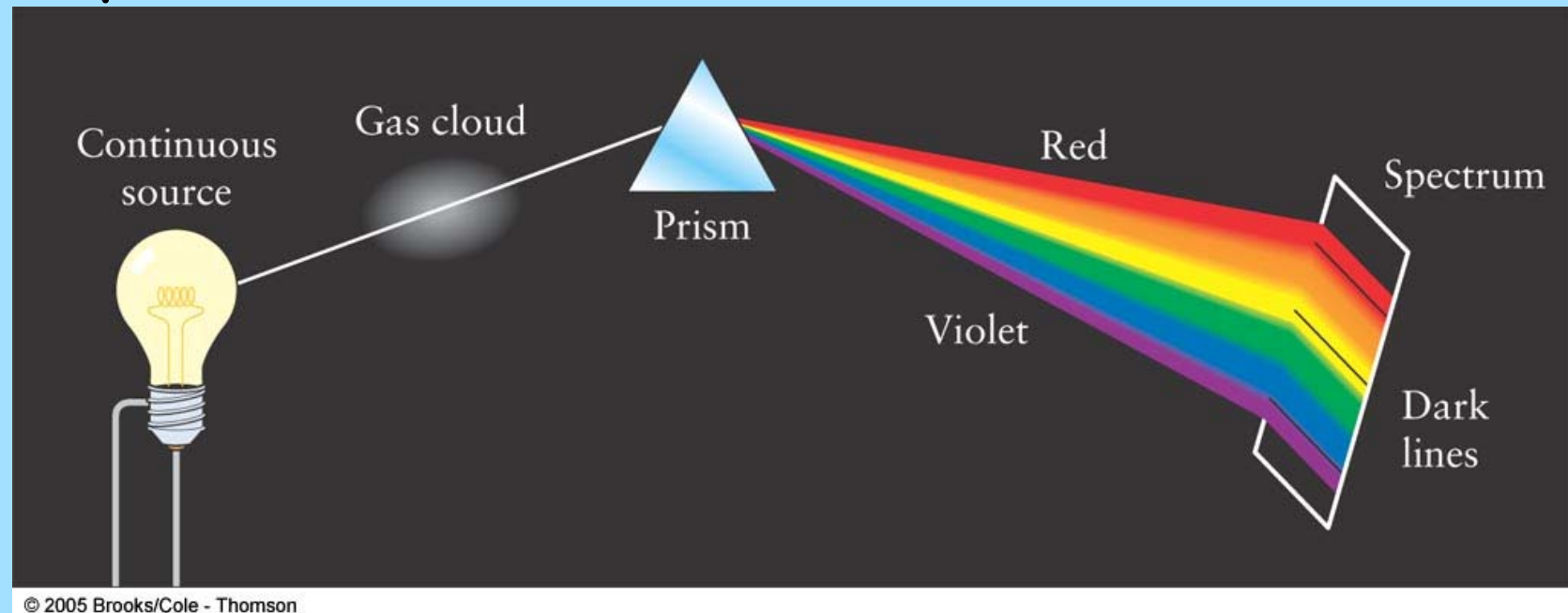
Energy levels (Energies of orbits) in hydrogen:

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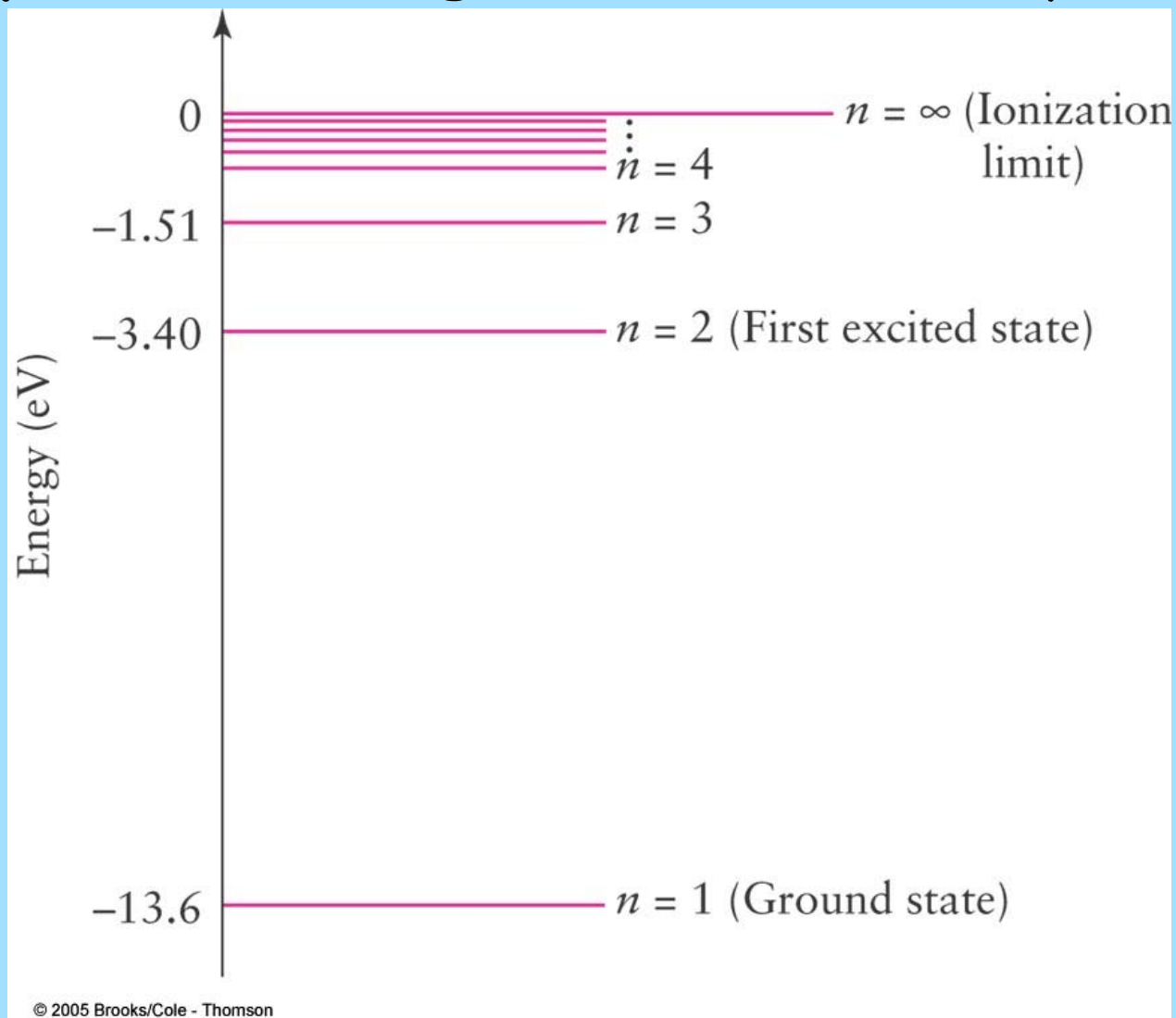
Why are these energies negative ?

Because the electrons are bound to the atom and energy is required to remove them.

An electron that is all by itself at rest, far away from any other charge, would have zero potential energy and zero kinetic energy, i.e. its total energy would be zero.

Electron bound to a positively charged nucleus, has negative potential energy and positive kinetic energy, but the total energy is negative.

It would take energy to remove the electron, i.e. to make its energy equal to zero again. This energy is called the IONIZATION ENERGY.

Question:

An electron in an excited state (n = 3) falls back to the ground state (n=1). How much energy is released (emitted) ?

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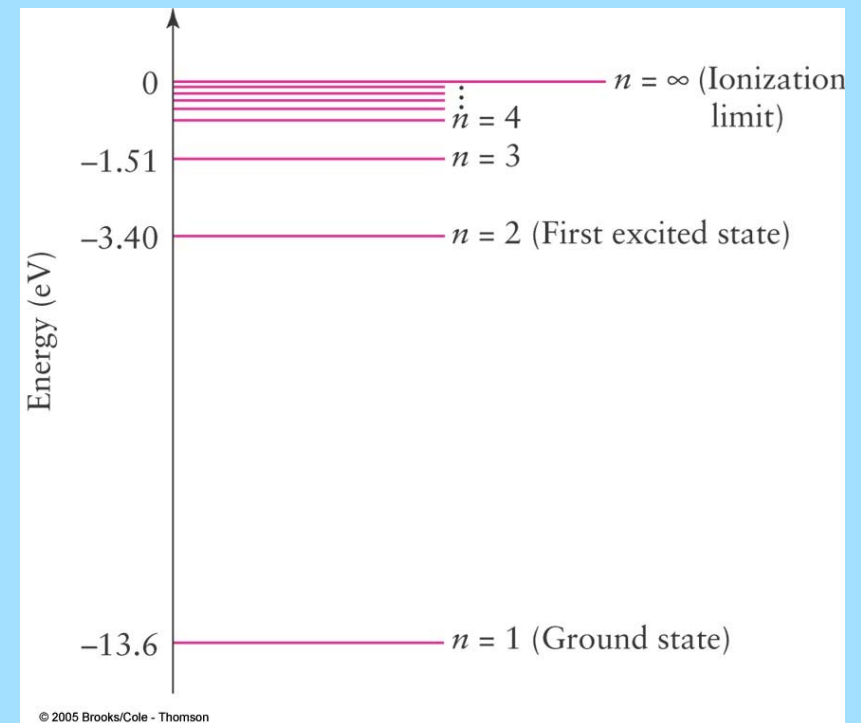
The energy of the electron changes from –1.51 eV to –13.60 eV. Therefore
(-1.51 eV)-(-13.60 eV) = 12.09 eV is released.

Energy absorbed or emitted by an electron moving from an orbit m to an orbit n:

$$\Delta E = E_n - E_m$$

If an electron jumps from orbit 2 to orbit 4, does it absorb or emit energy ?

1. Absorb

2. Emit

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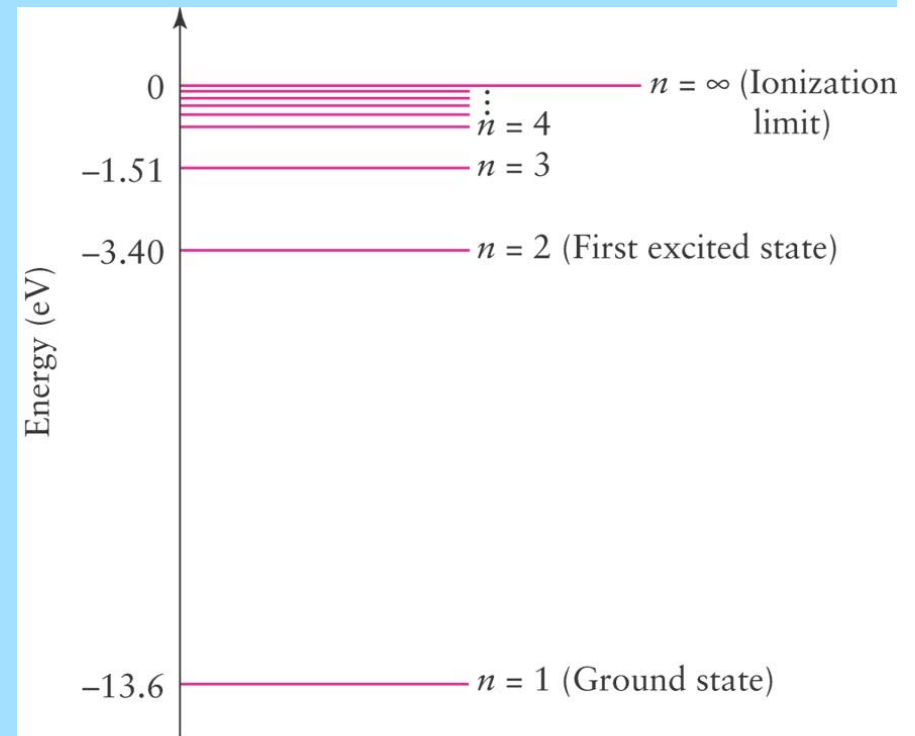
An electron jumps from the n=3 orbit to the n=2 orbit. What is the frequency of the light that is emitted?

$\Delta E = E_3 - E_2 = -1.51$ eV $- (-3.4)$ eV
$\qquad\qquad = 1.89$ eV

ΔE is the energy of the photon emitted:

$\Delta E = h\,f$

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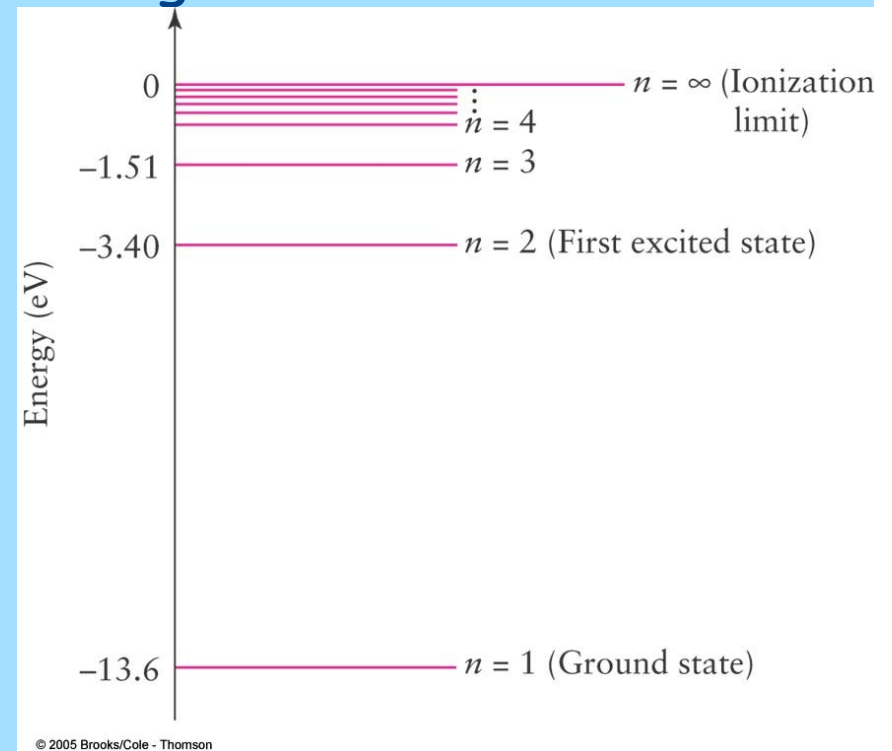
$f = \Delta E/h = (1.89 \text{ eV})/(4.136 \times 10^{-15} \text{ eV/Hz})$

$\qquad = 4.57 \times 10^{14}$ Hz (Red, visible light)

Hydrogen spectrum

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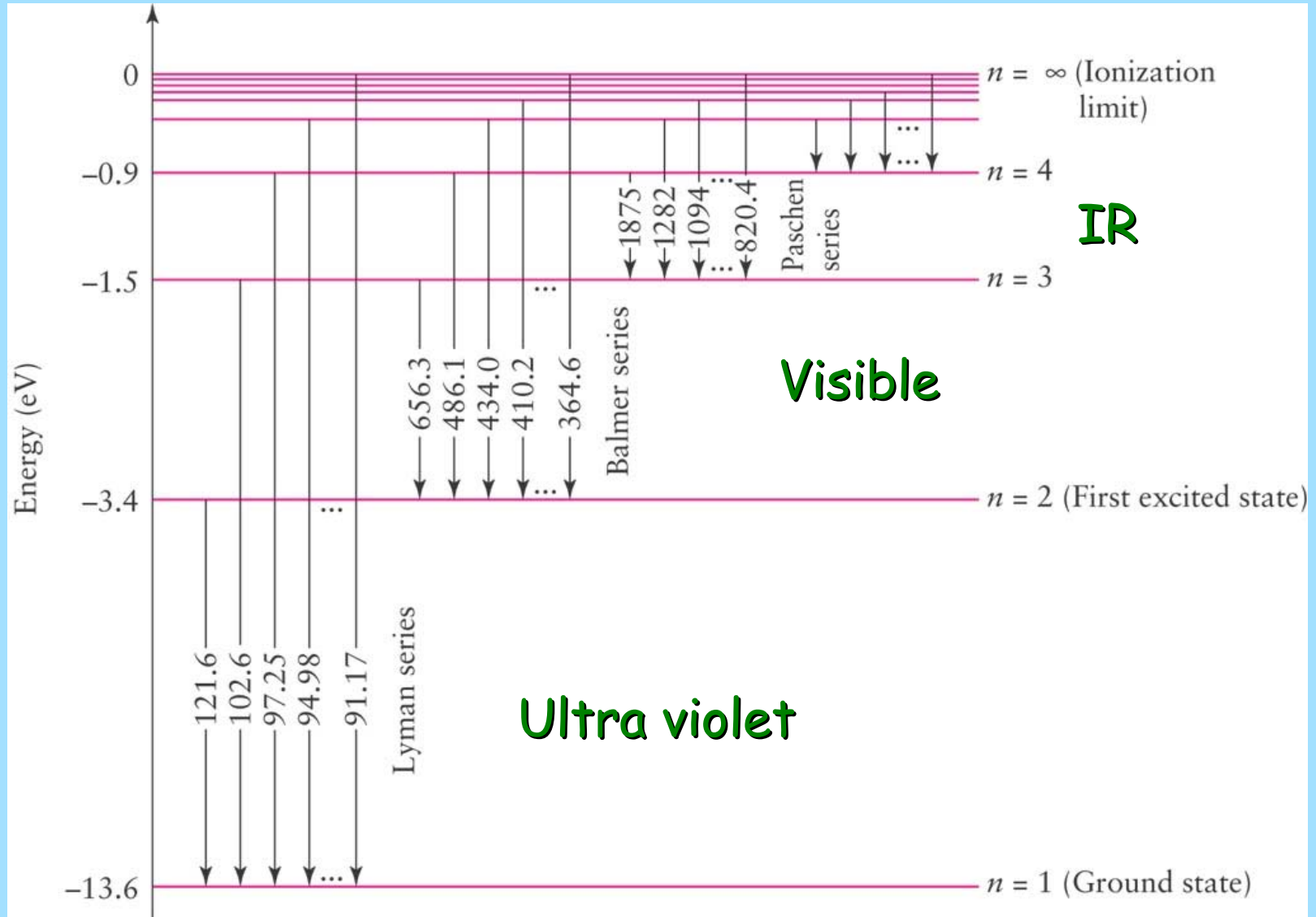
Atomic physics – quantum mechanics

- Blackbody radiation: Energy of vibrating atoms comes in portions – quanta with E = hf.

- In general, light comes in chunks, called photons with energy E = h f and momentum $p = h/\lambda$

- Electrons in atoms have specific orbits: the orbits are quantized and not continuous.
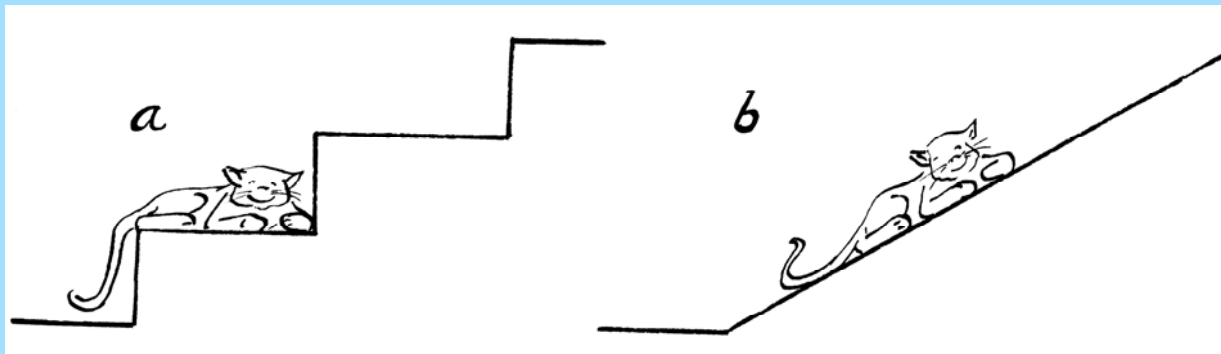
Energy absorbed or emitted by an electron moving from an orbit m to an orbit n:

$$\Delta E = E_n - E_m \quad \text{- final minus initial}$$

- If positive, electron energy increases – a photon is absorbed,

- Negative – emitted

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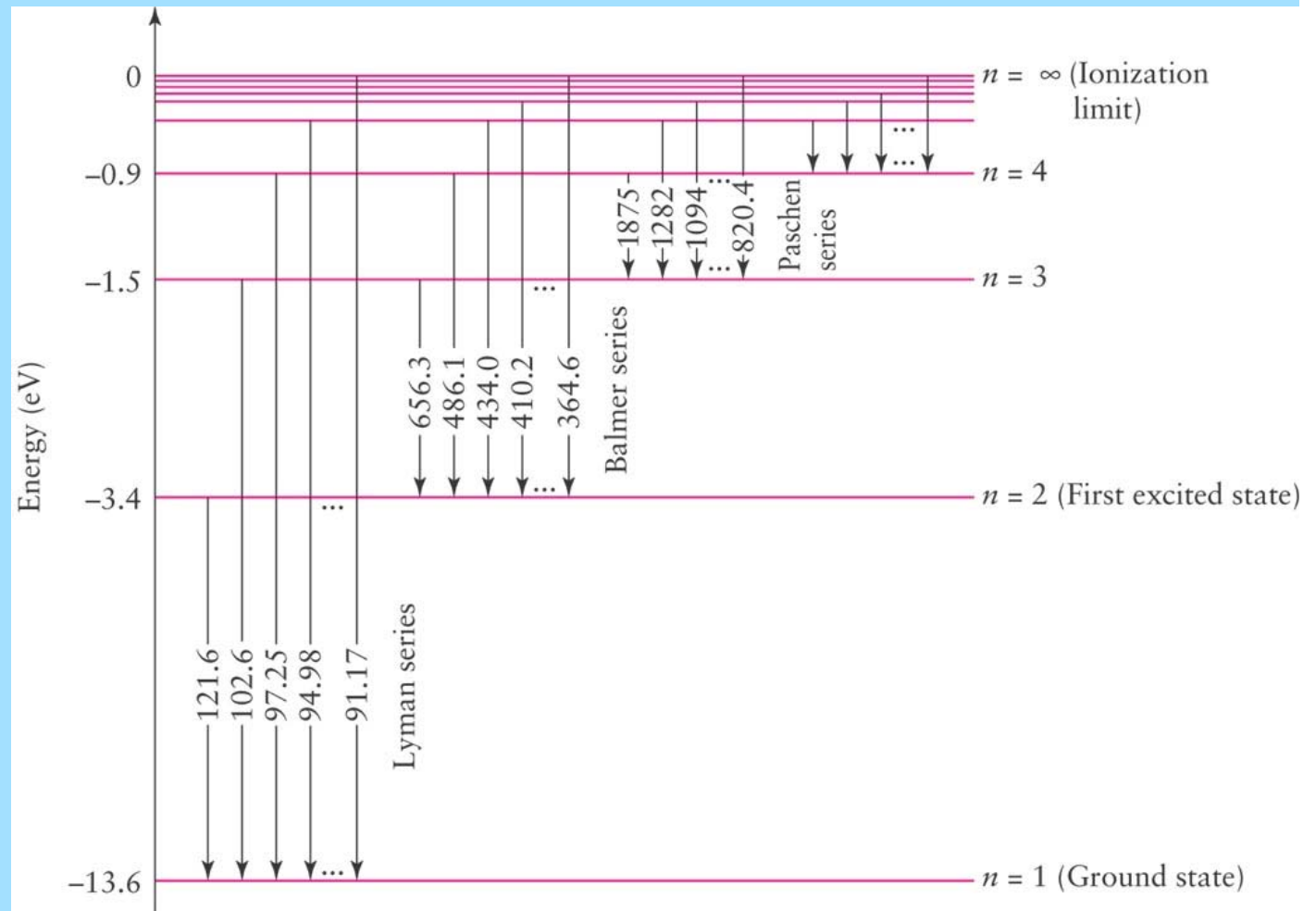
Atomic model

- Atoms are made of a positively charged nucleus (protons + neutrons) and a "cloud" of negatively charged electrons that surround the nucleus.

- The electrons do not emit radiation while on the orbit

- Both energy and angular momentum are quantized

- Electrons move in specific orbits. Only certain orbits are allowed. Orbits are characterized by their energy and angular momentum

- The orbits do not have to be spherical

- Electrons can jump from one orbit to another by absorbing or emitting energy.

Phenomenology calls for a fundamental theory

- The Bohr's model is based on two assumptions – postulates that require quantization. The model works, but it cannot explain why.

- Blackbody radiation and photoelectric effect – same thing: photons have to be put on a solid ground…

General features of the new phenomena:

- In the microscopic world (atoms, electrons, photons), (some) properties change in discontinuous ways, they are quantized.
- EM radiation reveals dualistic properties being both waves and particles

Can electrons (and other particles) act as waves?

1923: Any particle with momentum mv "has" a wavelength h/mv – de Broglie wavelength

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

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

More general statement: photon has zero mass, but this formula gives a momentum to a photon:

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

Prince Louis-Victor de Broglie
   (1892-1987)

Application to Bohr model

If electrons are waves, they have to "fit" their orbit, if not they will interfere destructively.

(a)   (b)
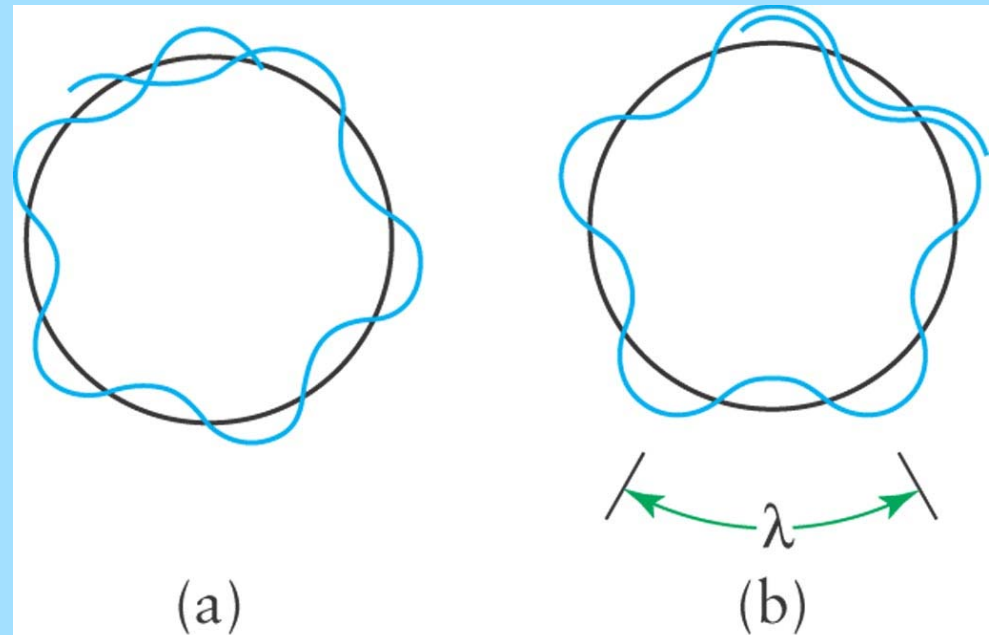
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Therefore: $2 \pi r = n \lambda = n h/(m v)$, with n = 1,2,3,...

From this: $L = m r v = n h/(2 \pi)$

The angular momentum of the electron is quantized exactly as required by Bohr model

Experimental proof

Davisson & Germer, 1925

Send electrons through a thin metal foil

Observed: Diffraction & Interference!!!

X-rays
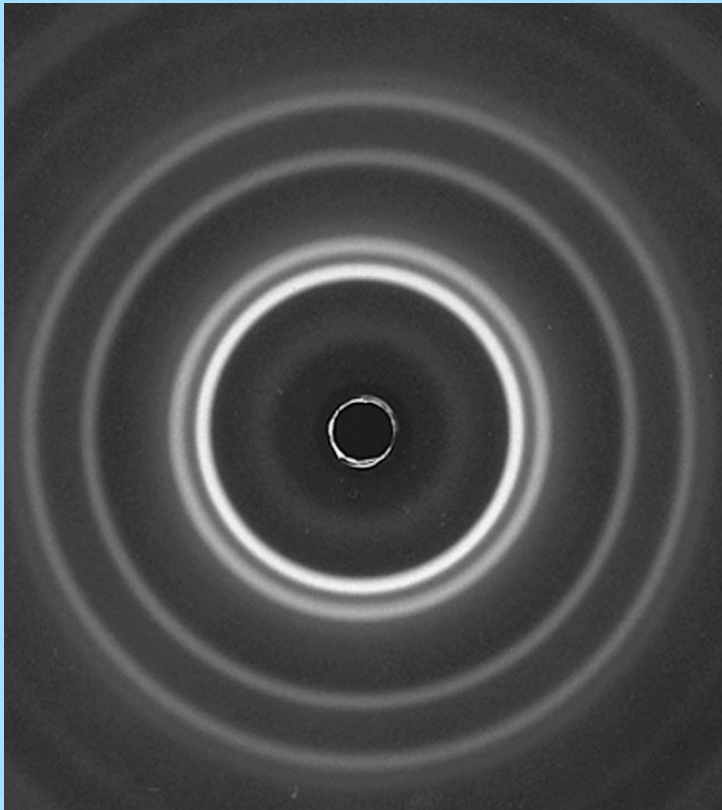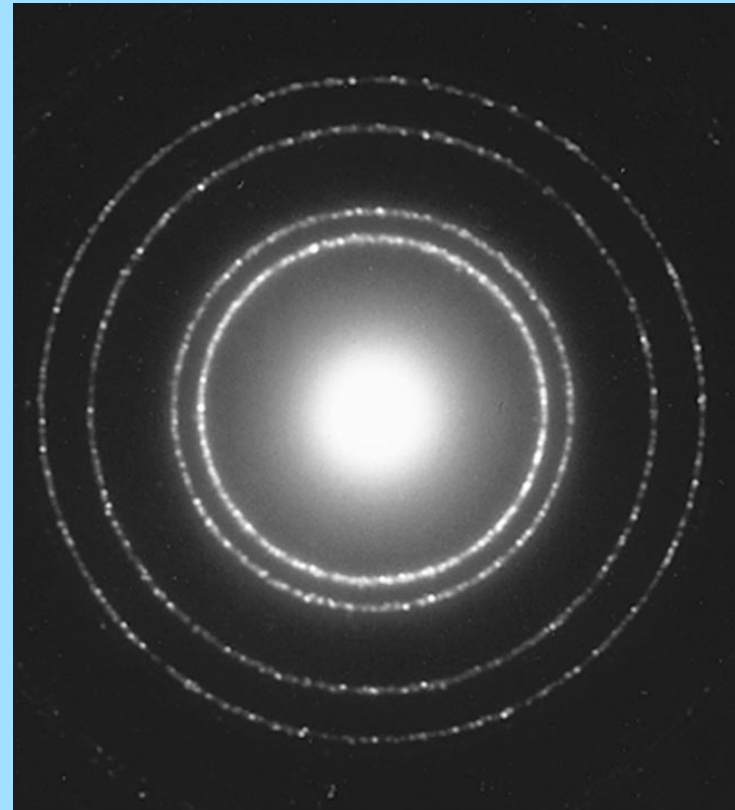
Electrons

# Bragg scattering of electrons on the crystal surface
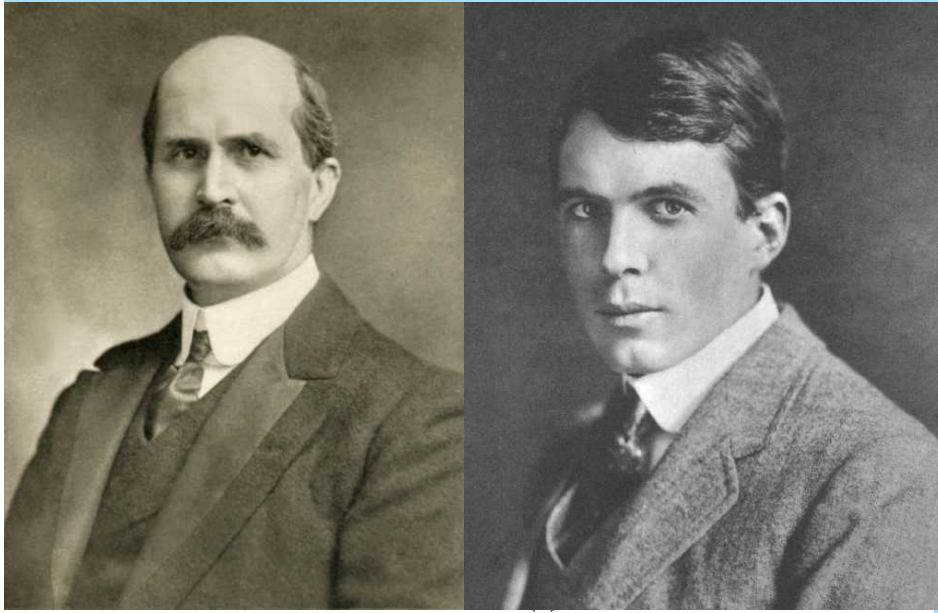
Sir W.H. Bragg and his son Sir W.L. Bragg in 1913 discovered X-ray diffraction and interference but it turned out that the same result could be obtained using electron or other particles' scattering
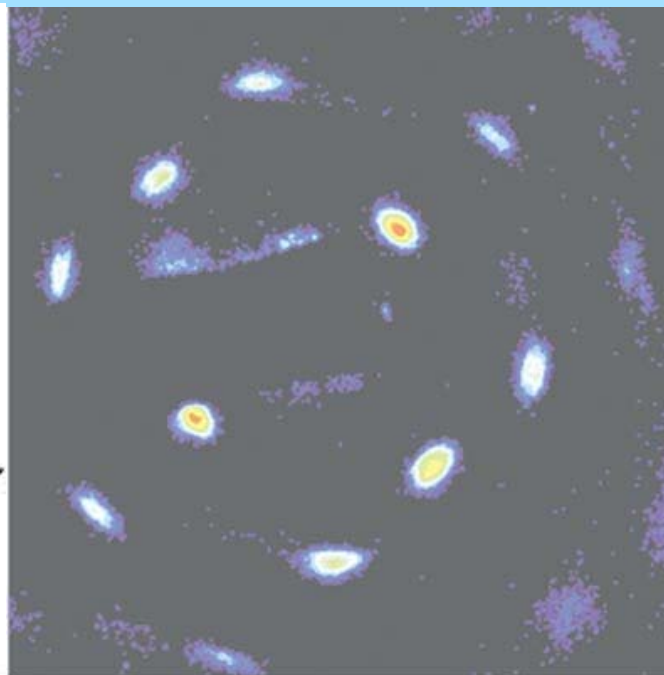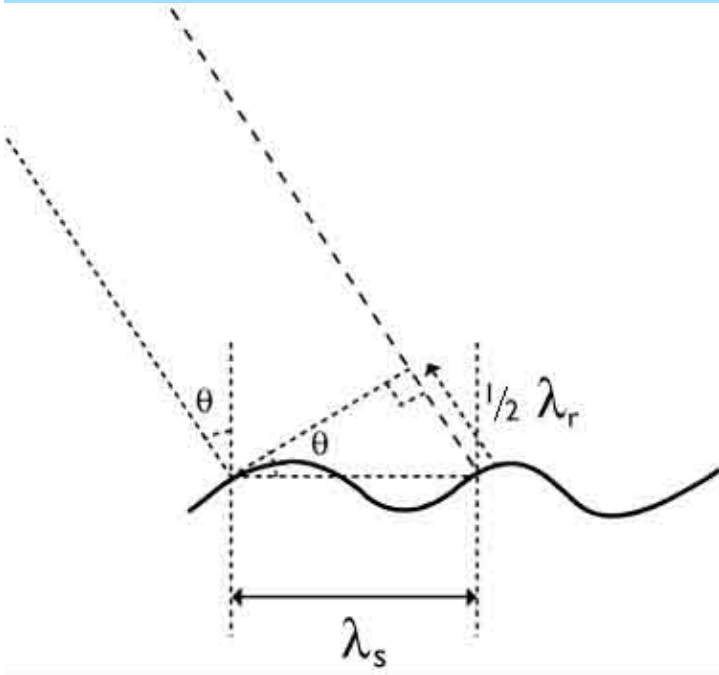
Electron microscopy

TEM – transmission electron microscope – electrons instead of light – Max Knoll and Ernst Ruska, Germany, 1931
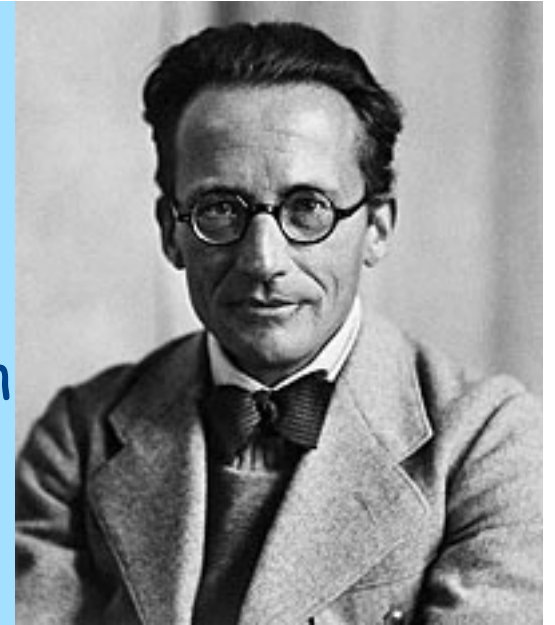
SEM – scanning electron microscope 1942-1965
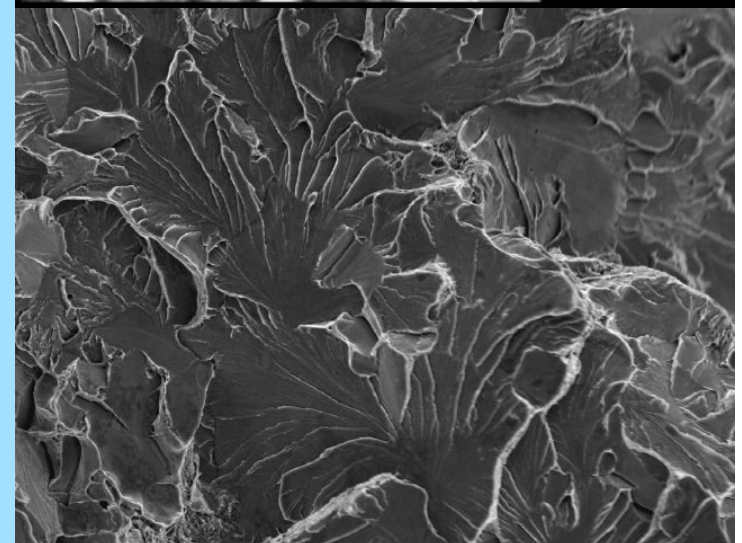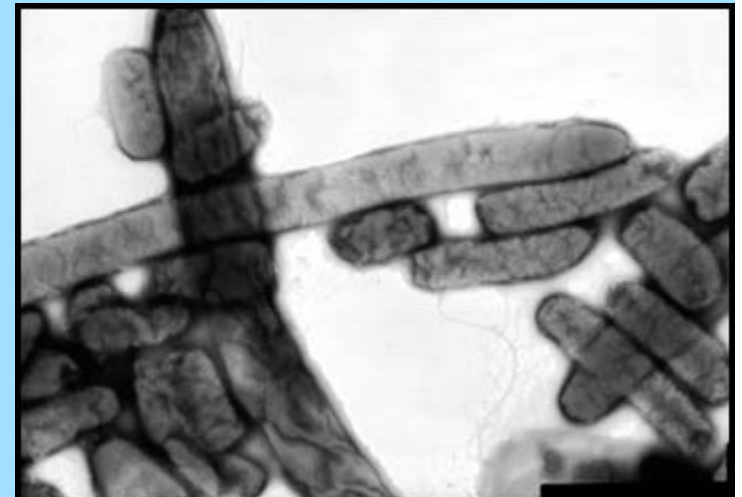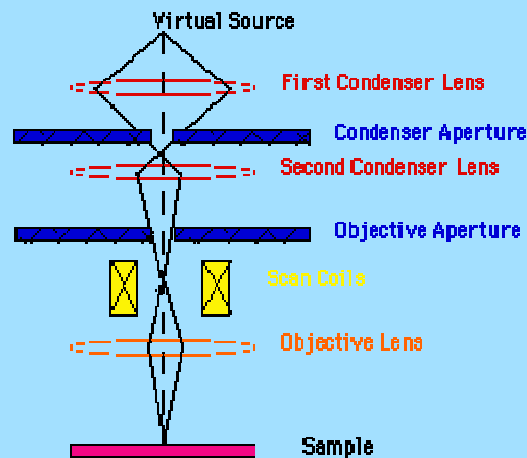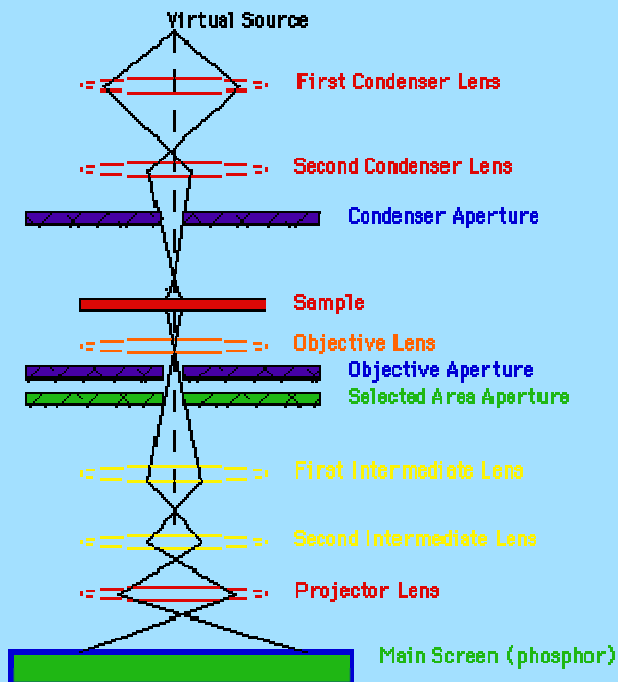
The theory...

1926 – six papers – wave mechanics

- Introduce a wave to describe an electron (or other particle) – try to mimic an EM wave

Erwin Schrödinger (1887-1961)

- Introduce a wave function that would obey a wave equation

- Find solutions of this equation for hydrogen atom and other systems

- Hydrogen atom – Bohr model!

What does the wave function have to do with an electron?

Heisenberg's Formulation of quantum mechanics, 1925

• Particles have wave-like properties.

• Therefore they cannot be thought of as well-defined points in space with well-defined momentum.

• Their position and momentum are not 100% determinable.

"The more precisely
the POSITION is determined,
the less precisely
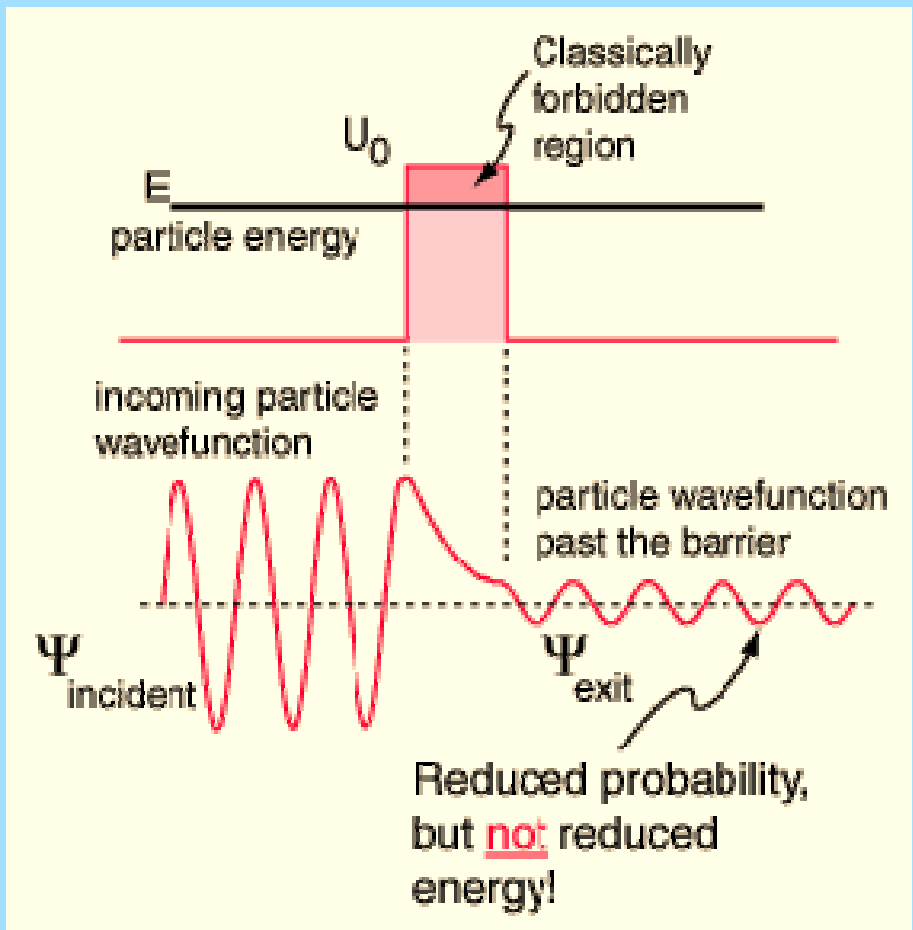the MOMENTUM is known"

$$\Delta x \; \Delta(mv) \geq h$$
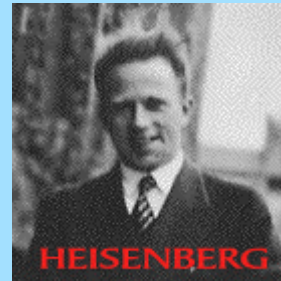
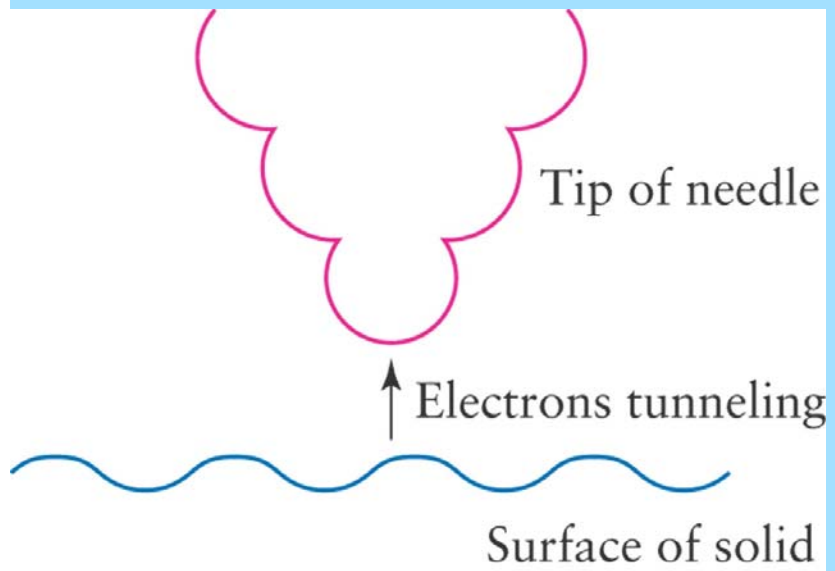HEISENBERG

Werner Heisenberg
(1901-1976)

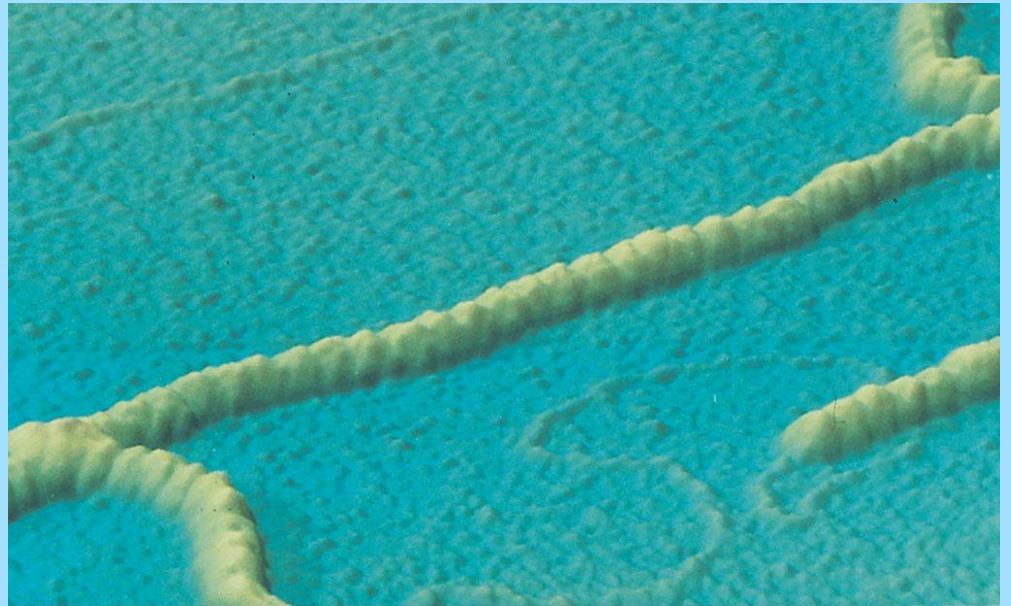# Tunneling:

Another "strange" result of the wave nature of electrons.

Electrons can move "ghostlike" through a barrier.

Used in read-heads for hard drives, transistors, Scanning Tunneling Microscopy

Tip of needle

Electrons tunneling

Surface of solid

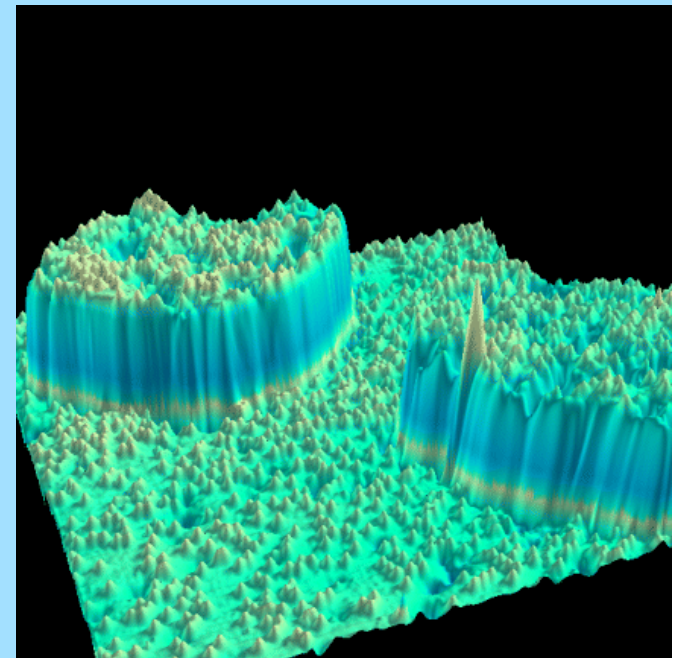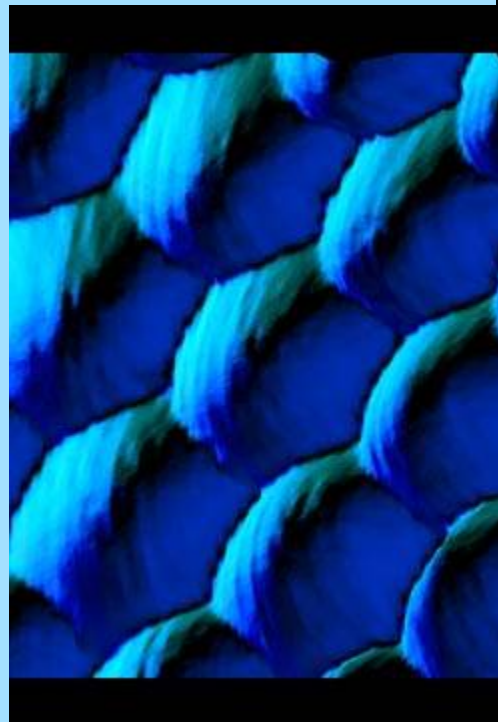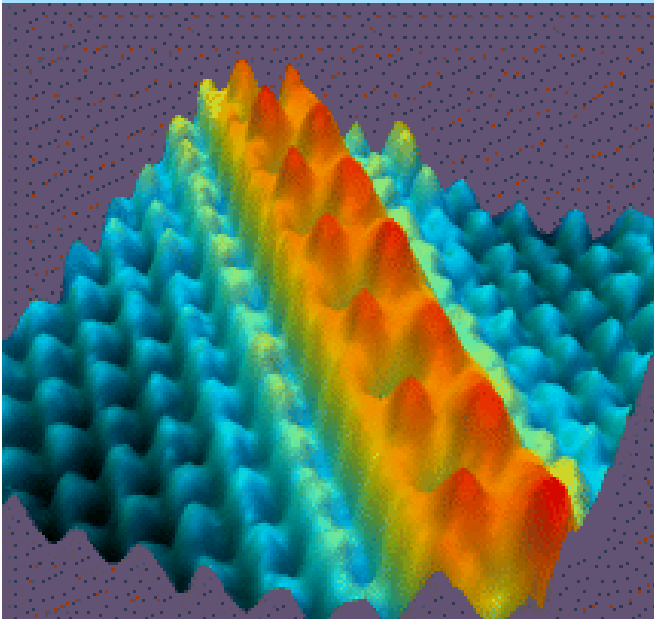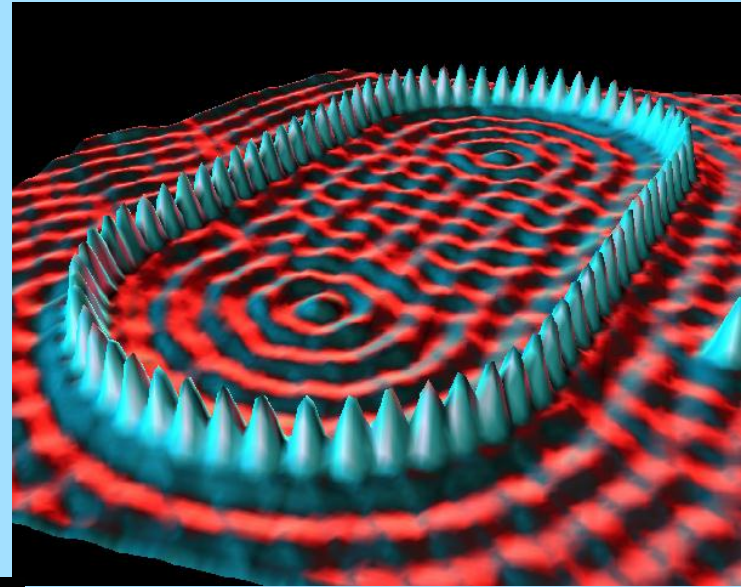© 2005 Brooks/Cole - Thomson

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Contemporary application: scanning microscopy

Gerd Binnig and Heinrich Rohrer, 1983 – STM

Consequences of quantum mechanics
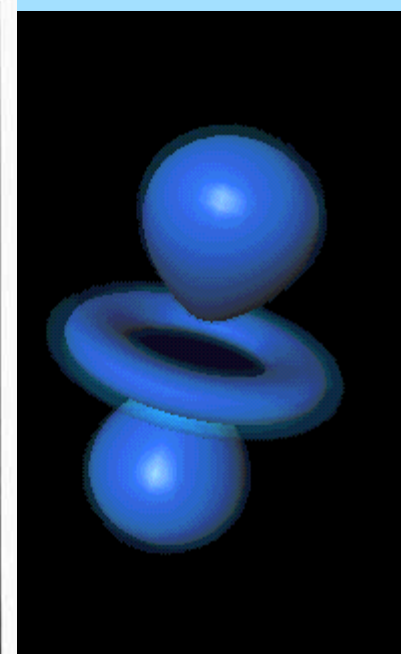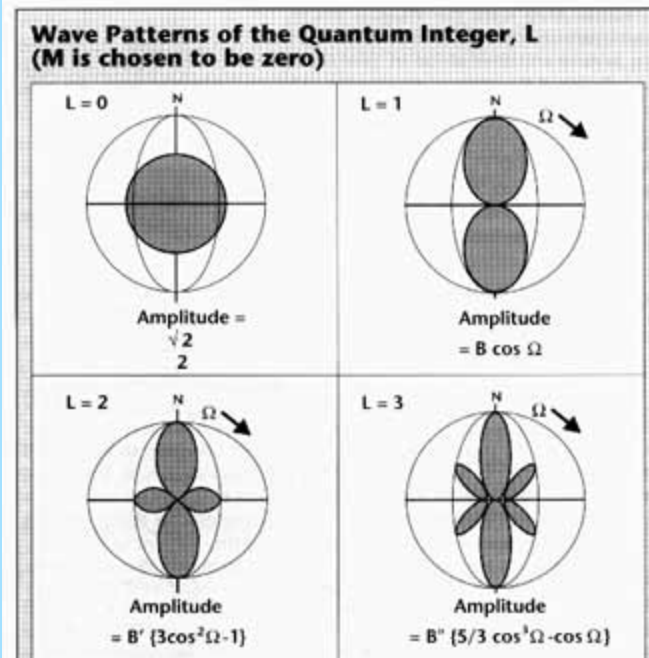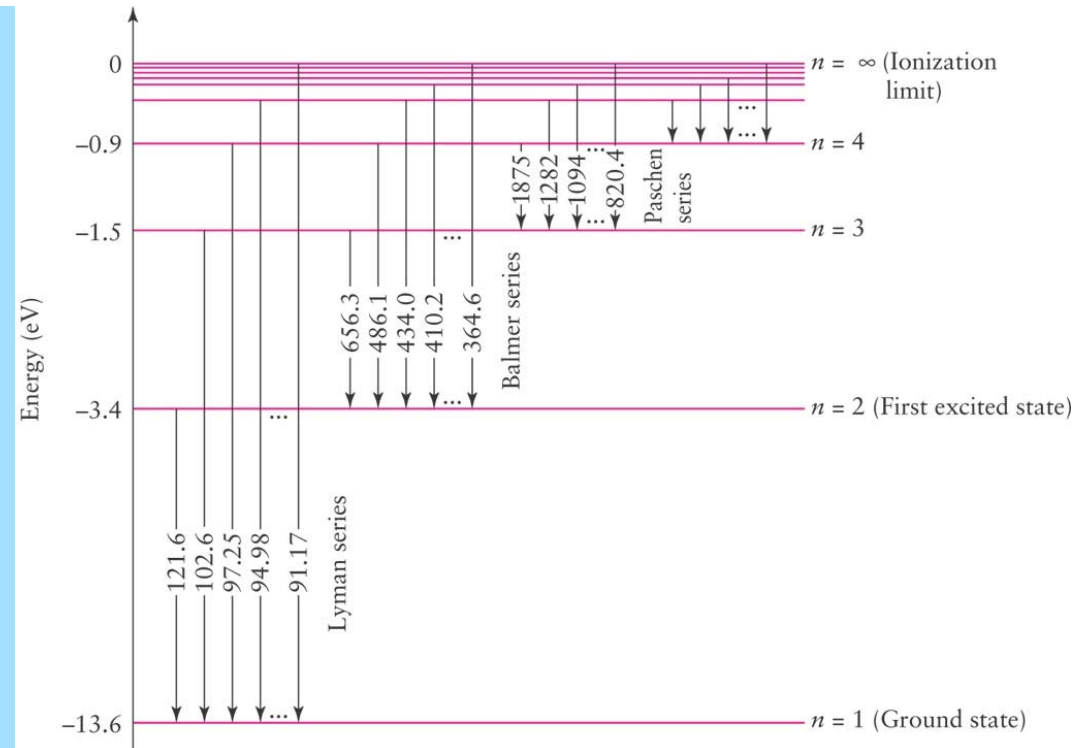
- For small particles, trajectories are ill-defined

- On the atomic scale and smaller, the particles cannot be localized

- The wave function gives a probabilistic description to a particle

- The physical quantities can be determined in a probabilistic way using the wave function

- It is not possible to predict a result of measurement with certainty – only a probability of result can be calculated.

- Not all quantities can be measured at the same time due to uncertainty principle

- Well – it's a new look at measurement…

Back to atomic model

- Electrons occupy orbitals according to their energy and angular momentum

- It is not possible to tell where on the orbital the electron resides

- We can only determine the probability to find it at a certain location...

- ... probability of it having a certain velocity, etc.

- Clouds of probability

Energy (eV)

0 — $n = \infty$ (Ionization limit)

−0.9 — $n = 4$

−1.5 — $n = 3$

1875
1282
1094
820.4
Paschen series

656.3
486.1
434.0
410.2
364.6
Balmer series

−3.4 — $n = 2$ (First excited state)

121.6
102.6
97.25
94.98
91.17
Lyman series

−13.6 — $n = 1$ (Ground state)

Wave Patterns of the Quantum Integer, L
(M is chosen to be zero)

L = 0
N
Amplitude = $\dfrac{\sqrt{2}}{2}$

L = 1
N
Ω
Amplitude = B cos Ω

L = 2
N
Ω
Amplitude = B' {3cos²Ω−1}

L = 3
N
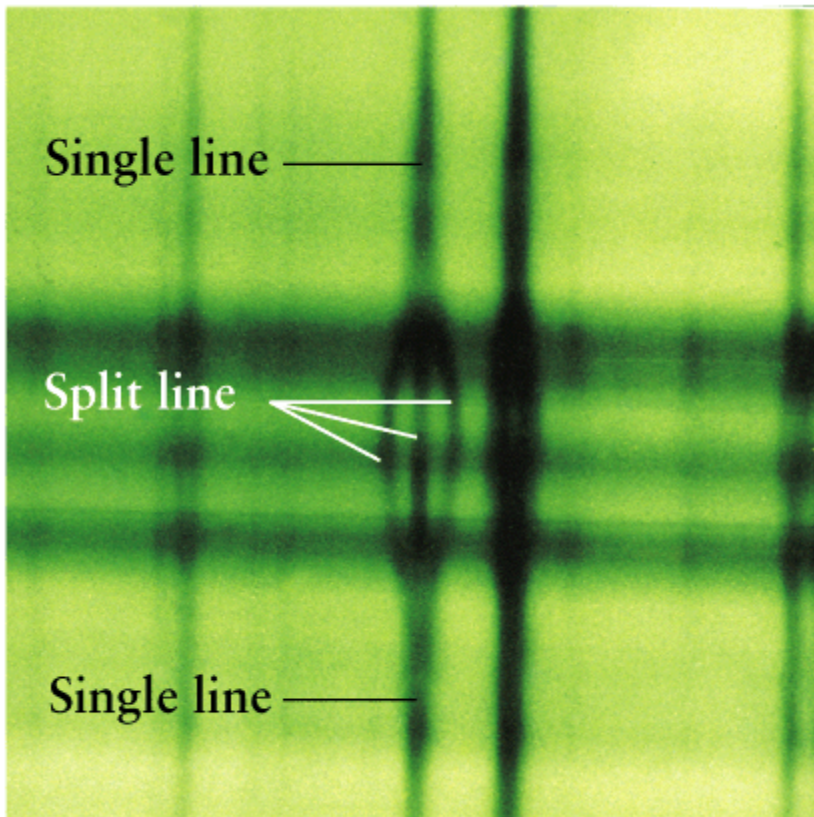Ω
Amplitude = B'' {5/3 cos³Ω −cos Ω}
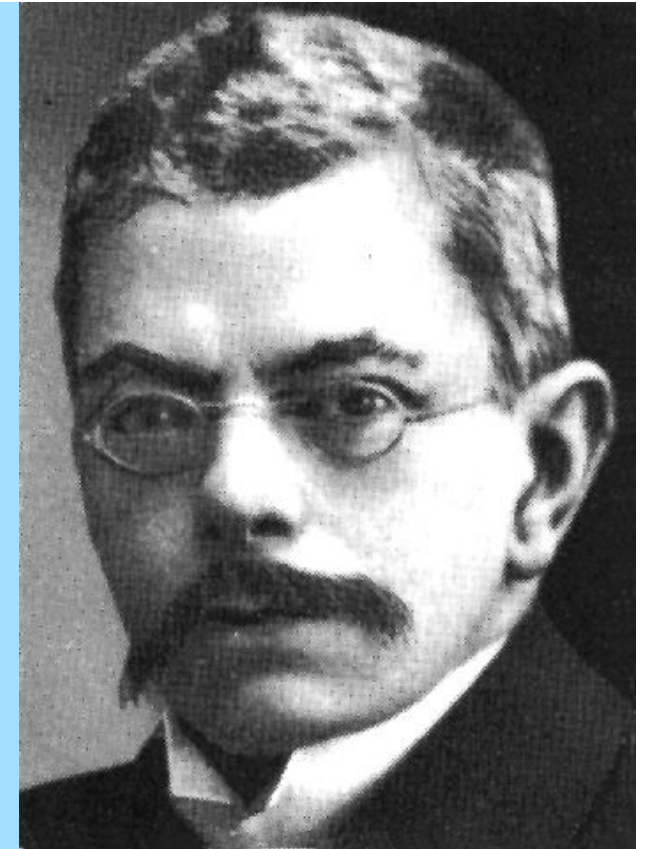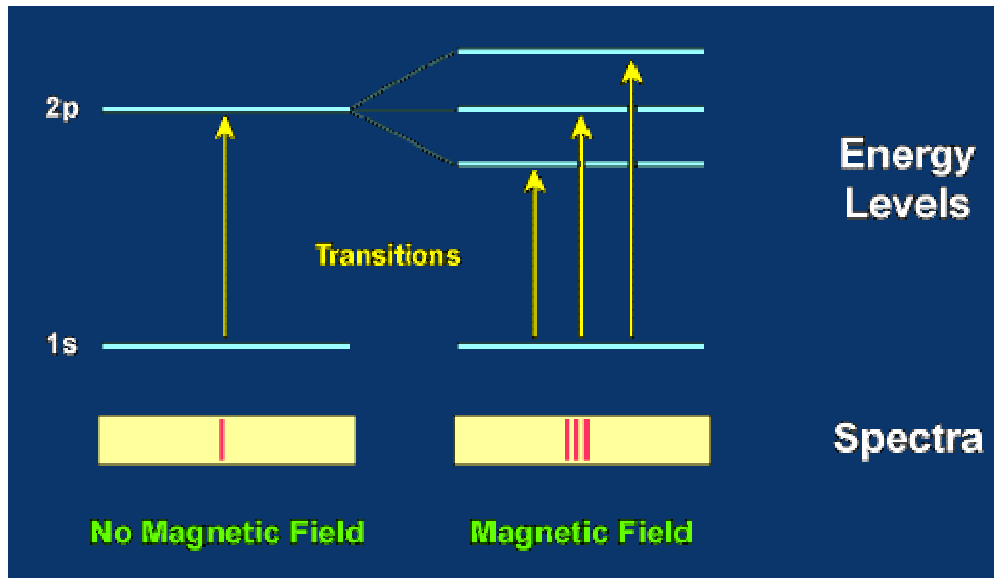
Pieter Zeeman
(1865-1943)

The energy levels split in magnetic field

Fine structure of levels has been found in 1920s...

- To explain the fine structure of atomic levels introduced spin – intrinsic moment of electron (and other particles), 1928

- In some sense, similar to spinning in one or other direction with respect to a certain axis, but it is wrong to think about an electron as a spinning ball since it has to spin at a speed exceeding the speed of light

- According to Heisenberg uncertainty principle, only one projection of the spin can be determined (spin up or down)

- Electrons and some other particles such as protons and neutrons have a spin of $h/4\pi$.

Wolfgang Pauli
(1901-1958)

■The Bohr model explained the hydrogen atom quite well, but not other atoms.

■In a more complicated atom, why don't all the electrons occupy the ground state? Why do they fill the orbitals?

Pauli: the wave functions of particles that have a spin of h/4π are such, that no two particles can be in the same state! – Exclusion principle

*No two electrons in the same atom can occupy the exact same state.*

Each energy (n=1,2,...) level has a certain number of quantum states. Once all of these are filled up, the next higher energy level becomes occupied.

(a)   Orbit 1

(b)   Orbit 2

(c)   Orbit 2

(d)   Orbit 2
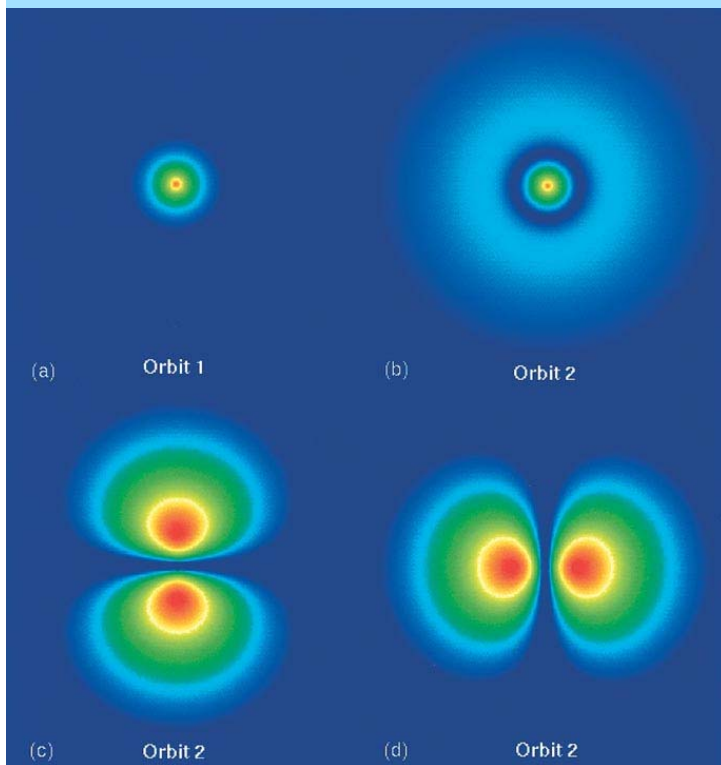
Table 10.1 Ground-State Configurations of Several Atoms

Element	Atomic Number	Number of Electrons in Level $n = 1$	$n = 2$	$n = 3$
Hydrogen	1	1	0	0
Helium	2	2	0	0
Lithium	3	2	1	0
Carbon	6	2	4	0
Oxygen	8	2	6	0
Neon	10	2	8	0
Sodium	11	2	8	1
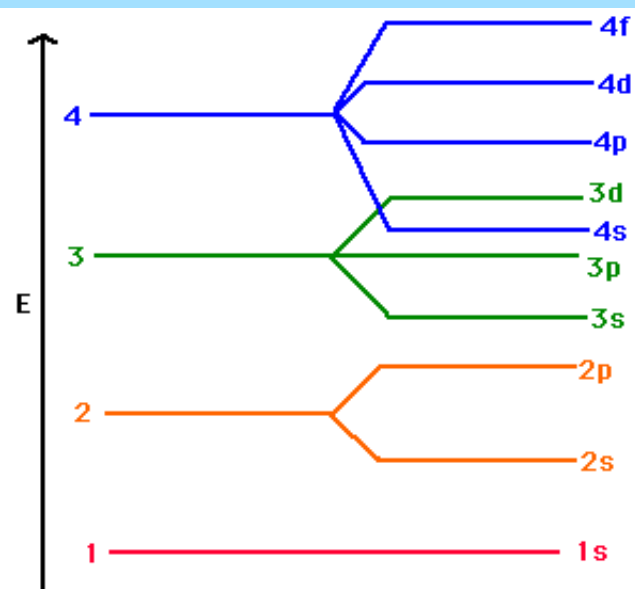
$2n^2$ states are allowed on each level

4f
4d
4p
3d
4s
3p
3s
2p
2s
1s

E

4
3
2
1

Aurora August 21,1990 by Gary Boyles

X-ray spectra

Electrons

Target

High voltage
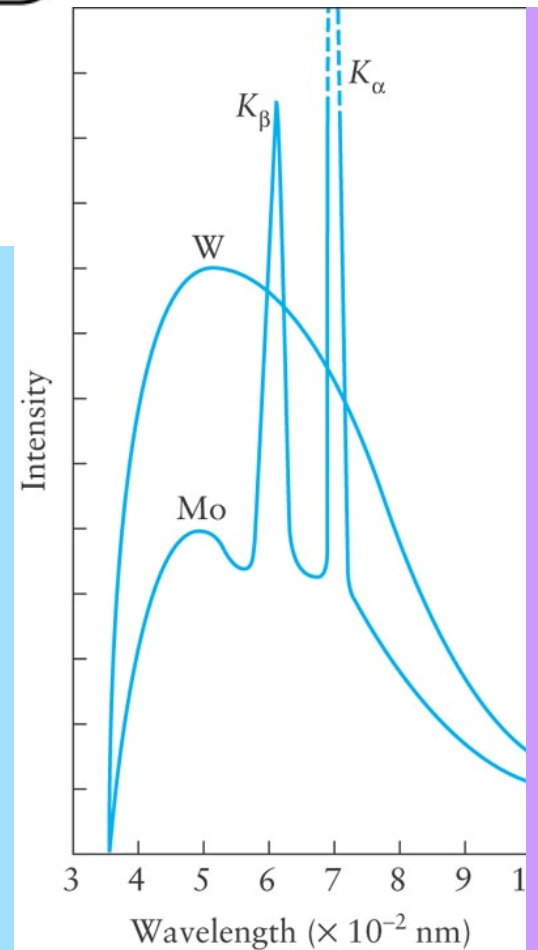
© 2005 Brooks/Cole - Thomson

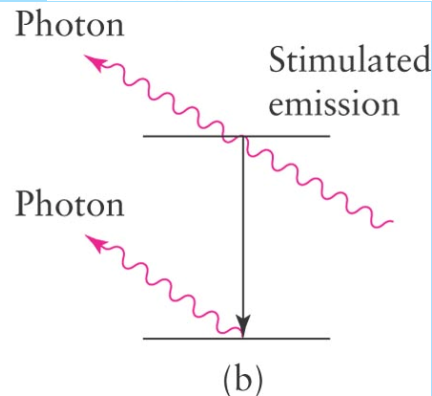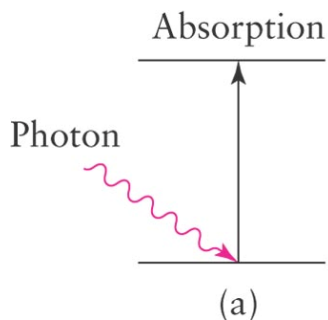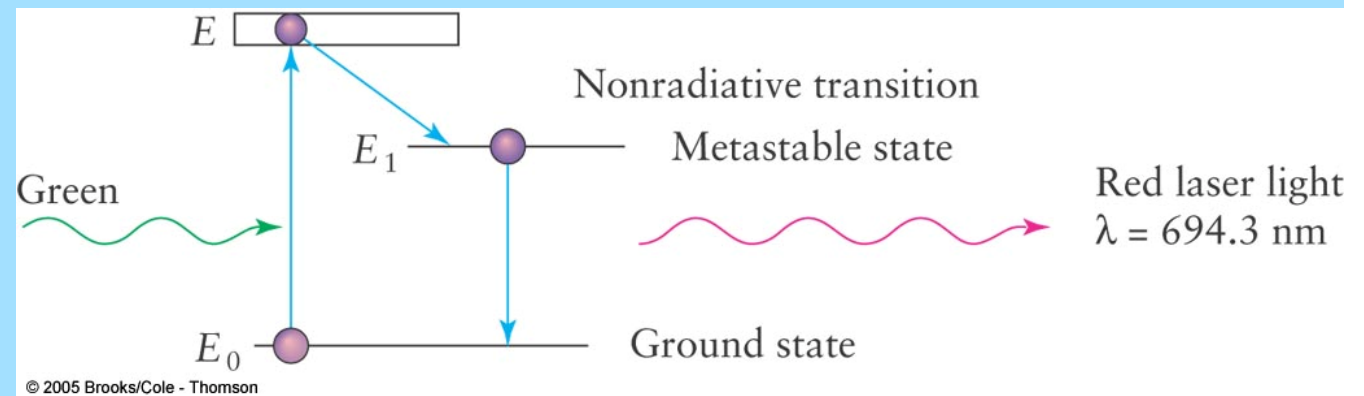Broad background from fast slow down of electrons – bremsstrahlung radiation

Peaks due to electronic transitions within atom – if the internal electron on n=1 level (ground state) is kicked out, another electron from "above" (n=2,3) jumps down causing the emission of an X-ray photon. It is called K_α and K_β correspondingly.

K_β

K_α

W

Mo

Intensity

3 4 5 6 7 8 9 1
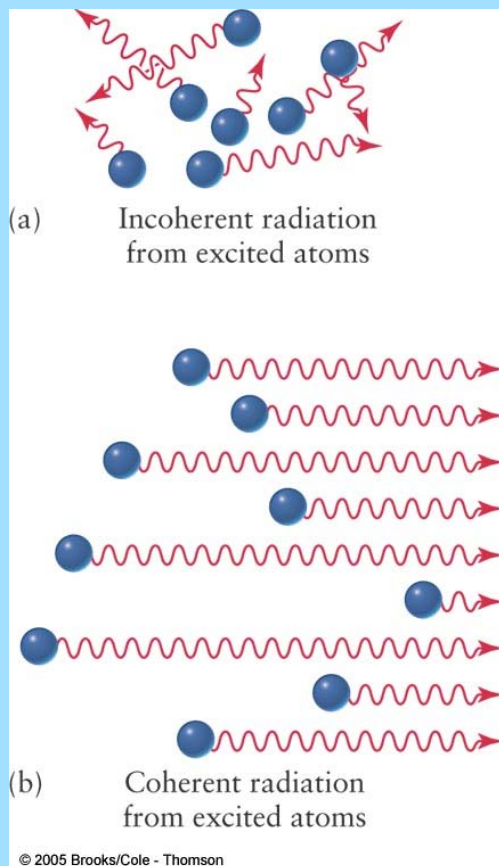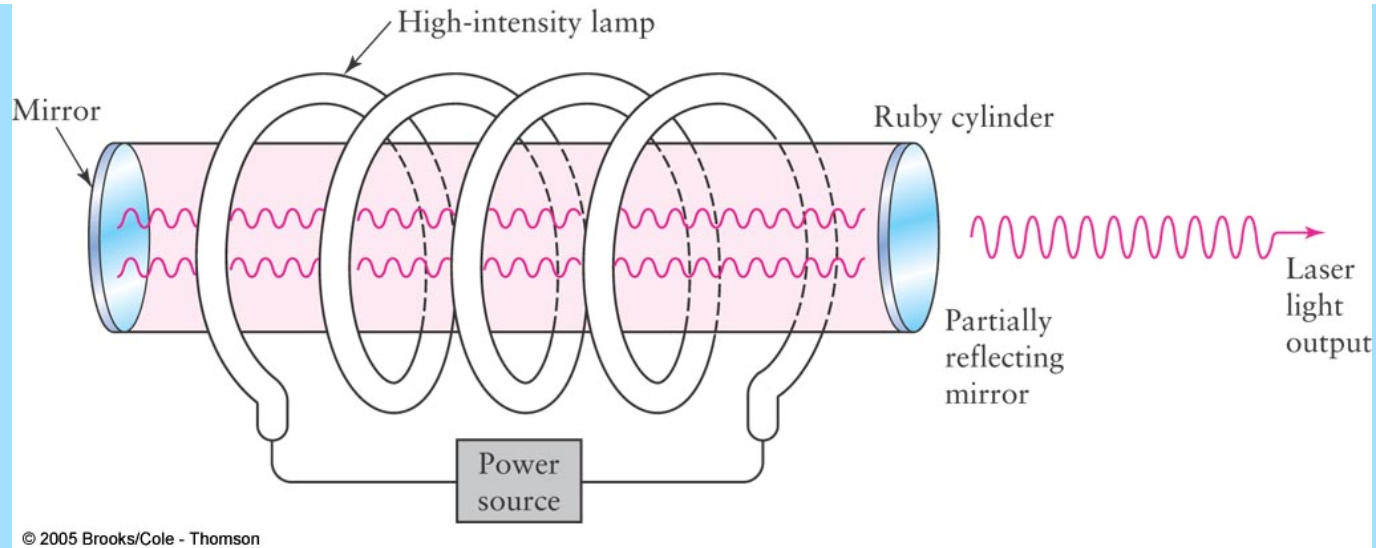
Wavelength ($\times 10^{-2}$ nm)

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Lasers = "Light Amplification by Stimulated Emission of Photons"

- Excite majority of atoms into a specific excited state – population inversion

- Specific state can be "stimulated" into emission when the atom gets hit by another photon

- "Chain reaction"

  - Amplification

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(a) Incoherent radiation from excited atoms

(b) Coherent radiation from excited atoms

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Radiation – stimulated and spontaneous – A. Einstein

"Coherent" – all waves are in the same phase – far order

Inverse population – a system with a negative temperature

Other coherent systems:

- Electrons in a superconductor

- Electrons in a white dwarf

- Neutrons in a neutron star

- Condensed systems at extremely low temperatures

Main features: ultra high pressure or ultra low temperature
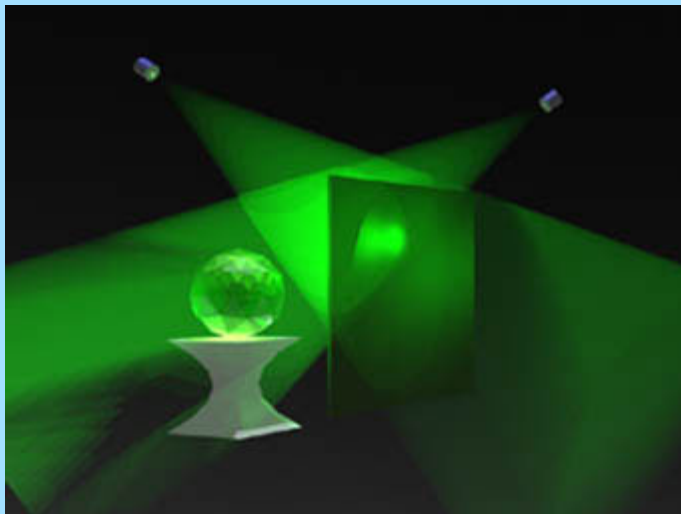
Holographic image – a result of interference of two coherent beams – a phase image – 3D

Dennis Gabor, 1947