

## ***“Complementi di Fisica” Lectures 7-9***

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**Università di Trieste**

**Trieste, 07/09-10-2012**

### **Course Outline - Reminder**

- **Quantum Mechanics: an introduction**
  - **Waves as particles and particles as waves (the crisis of classical physics);** atoms and the Bohr model
  - The Schrödinger equation and its interpretation
  - (1-d) Wave packets, uncertainty relations; barriers and wells
  - (3-d) Hydrogen atom, angular momentum, spin
  - Systems with many particles
- **The physics of semiconductor devices: an introduction**
- **More advanced semiconductor fundamentals**

# The birth of quantum physics

## chronology

### The birth of quantum physics - 1

Year	event	notes
1857	Na absorption/emission lines, blackbody radiation	Kirchhoff
1895	discovery of X-rays	Rontgen, Nobel prize
1897	discovery of the electron	Thomson, Nobel prize
1899	radioactivity (alpha, beta, gamma)	
1901	quantum hypothesis for blackbody spectrum	Planck, Nobel prize
1905	explanation of photoelectric effect	Einstein, Nobel prize
1905	special relativity	Einstein, Nobel prize
1911	electron charge; atomic nucleus	Millikan, Rutherford (both Nobel)
1913	quantum atomic model	Bohr, Nobel prize
1916	conclusive measurements of energy quantization in photoelectric effect	Millikan, Nobel prize
1918	correspondence principle	Bohr, Nobel prize
1919, 1920	discovery of proton and neutron	Rutherford
1923	experimental: Compton effect	Compton, Nobel prize
1923	wavelength of electrons, prediction of diffraction for electrons	DeBroglie, Nobel prize
1924	statistics of light quanta	Bose-Einstein
1925	exclusion principle, electron spin	Pauli, Uhlenbeck
1925	foundation of quantum mechanics	Heisenberg, Nobel prize

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## The birth of quantum physics - 2

Year	event	notes
1925,1926	matrix formalism for quantum mech.	Born
1926	statistics for particles obeying Pauli principle	Fermi
1926	wave mechanics, wave equation, equivalence of wave and quantum mechanics, perturbation theory and applications	Schrodinger, Nobel prize
1926	statistical interpretation of quantum mechanics	Born, Nobel prize
1927, 1928	diffraction of electrons in crystals	Davisson, Thomson, Nobel prize
1927	foundation of quantum field theory ("second quantization") and quantum electrodynamics	Dirac
1927	uncertainty principle	Heisenberg
1928	relativistic wave equation for electrons, prediction of magnetic moment, theory of Zeeman effect	Dirac, Nobel prize
1930	prediction of the existence of anti-particles	Dirac

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## e.m. waves as particles: "photons"

Photoelectric effect

Compton effect

Black-body radiation

## Photons (conclusions...!)

- **Experimental evidence that e.m. radiation (“waves”!) are absorbed and emitted in “quanta” or “photons”**
  - Blackbody spectrum, Photoelectric effect, Compton effect
  - Individual quanta can be detected, i.e. by photomultipliers!
- **Speed  $c$ , momentum  $p$ , energy  $E$  of photons:**
  - From special relativity:
    - Speed of light ( $c \sim 3 \times 10^8$  m/s), “rest mass”  $m_0 = 0$
    - Energy and momentum:  $E = \sqrt{p^2 c^2 + m_0^2 c^4}$   
 $E = |\vec{p}|c \Rightarrow p = E/c$
  - From the interpretation of blackbody spectrum and photoelectric effect: photon energy proportional to the e.m. wave frequency  
 $E = h\nu = \hbar\omega$   

$$\Rightarrow p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda} \quad (\text{waves: } \lambda\nu = c)$$
  - Planck’s constant:  $h \approx 6.63 \times 10^{-34}$  J s     $\hbar = h/2\pi \approx 1.05 \times 10^{-34}$  J s

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## e.m. spectrum

Table 1.3. THE ELECTROMAGNETIC SPECTRUM

Type of Radiation	Frequency	Wavelength	Quantum Energy
“Wave” region	radio waves	$10^9$ Hz and less	300 mm and longer
	microwaves	$10^9$ Hz to $10^{12}$ Hz	300 mm to 0.3 mm
“Optical” region	infrared	$10^{12}$ Hz to $4.3 \times 10^{14}$ Hz	$300 \mu$ to $0.7 \mu$
	visible	$4.3 \times 10^{14}$ Hz to $5.7 \times 10^{14}$ Hz	$0.7 \mu$ to $0.4 \mu$
	ultraviolet	$5.7 \times 10^{14}$ Hz to $10^{16}$ Hz	$0.4 \mu$ to $0.03 \mu$
“Ray” region	x-rays	$10^{16}$ Hz to $10^{19}$ Hz	$300 \text{ \AA}$ to $0.3 \text{ \AA}$
	gamma rays	$10^{19}$ Hz and above	$0.3 \text{ \AA}$ and shorter

Note: The numerical values are only approximate and the division into the various regions are for illustration only. They are quite arbitrary.

Table 4-1 Orders of Magnitudes of Single-Photon Energies Corresponding to Different Parts of the Electromagnetic Spectrum.

	Frequency (s <sup>-1</sup> )	Wavelength (m)	Photon Energy (J)	Photon Energy (eV)
AM radio	$10^6$	300	$7 \times 10^{-28}$	$5 \times 10^{-9}$
FM radio, TV	$10^8$	3	$7 \times 10^{-26}$	$5 \times 10^{-7}$
microwaves	$10^{10}$	$3 \times 10^{-2}$	$7 \times 10^{-24}$	$5 \times 10^{-6}$
visible light	$6 \times 10^{14}$	$5 \times 10^{-7}$	$4 \times 10^{-19}$	2.5
X rays	$10^{18}$	$3 \times 10^{-10}$	$7 \times 10^{-16}$	$5 \times 10^3$
gamma rays from nuclear decay	$10^{21}$	$3 \times 10^{-13}$	$7 \times 10^{-13}$	$5 \times 10^6$

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## Photoelectric effect – experimental facts

- Hertz, 1887; Thomson/Lenard, 1899

- Electron final kinetic energy:

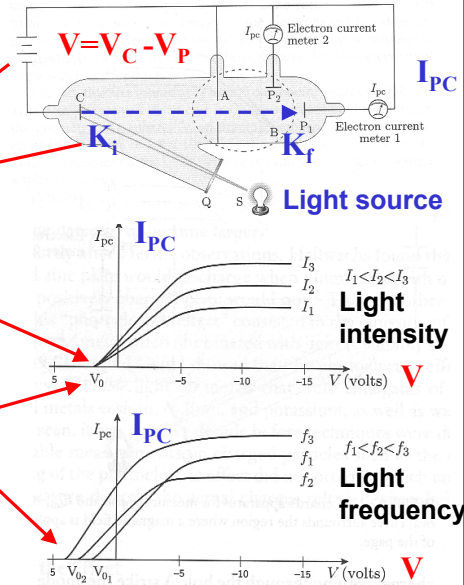
$$K_f = \frac{1}{2}mv^2 = -|q_e|V + K_i$$

- The current  $I_{PC}$  goes to zero if the “stopping potential”  $V_0$  is sufficient to kill the initial  $K_i$

$$-|q_e|V_0 = -K_i \Leftrightarrow V_0 = \frac{K_i}{|q_e|}$$

- $V_0$  depends on radiation frequency, not on intensity !!!

- The electron extraction is immediate, also at very low intensity !!!



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## What is wrong with classical e.m. waves?

- To start with: instantaneous emission, and peculiar behavior of  $V_0$ 
  - (visible) daylight from the Sun as a reference: energy supplied to the cross-sectional area of an atom (radius  $r \approx 0.2$  nm)
$$I \approx 0.049 \text{ J s}^{-1} \text{ m}^{-2} \Rightarrow W_a = I\pi r^2 = 0.049\pi(0.2 \times 10^{-9})^2 \text{ J s}$$

$$\Rightarrow W_a = 0.038 \text{ eV s}^{-1}$$
  - It would take about 76 seconds (over a minute!) before an individual atom could pick up a total of 2.9 eV (typical value of “work function  $W$ ” for a metal)
  - “It is as if one dropped a plank into the sea from a height of 100 feet, and found the spreading ripple was able, after traveling 1000 miles and becoming infinitesimal in comparison with its original amount, to act on a wooden ship in such a way that a plank of that ship flew out of its place to a height of 100 feet.” (Sir William Bragg)

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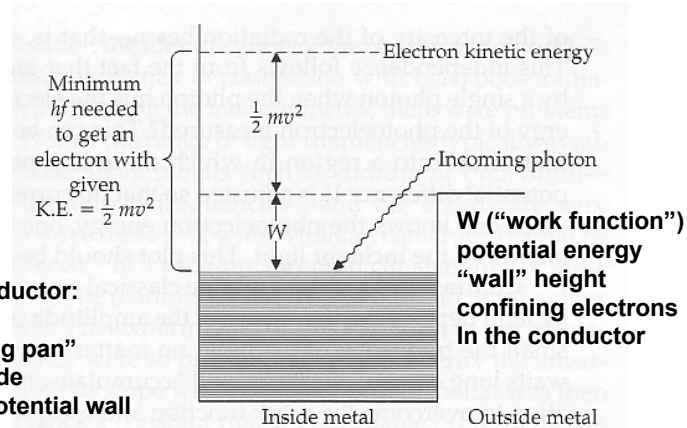
## Photoelectric effect – interpretation (1)

- Einstein

(after Planck, black body):

$$E = h\nu = h \frac{c}{\lambda} = W + \frac{1}{2}mv_{\max}^2$$

Electrons in a conductor:  
similar to  
“marbles in a frying pan”  
- free to move inside  
- contained by a potential wall



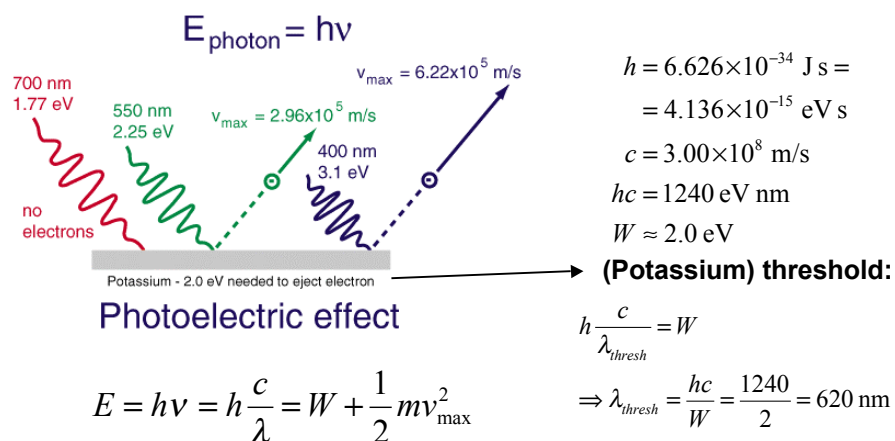
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## Photoelectric effect – interpretation (2)

- numerical examples for extracting electrons from Potassium ( $W = 2.0$  eV) with red, green, blue light



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## Photoelectric effect – decisive tests

- Millikan's experimental tests (up to 1916) of Einstein's interpretation
  - Initial measurements not sufficiently accurate: purity of metals, quality of surfaces (unstable  $W$ )
  - Systematic and accurate measurements with different wavelengths and different metals (Li, Na, ....), and special "tricks"
  - $V_0$  determined by extrapolation for different wavelengths
  - Agreement with Einstein, good determination of  $h$

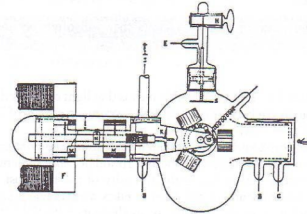


FIGURE 12.3 Diagram of Millikan's photoelectric effect apparatus. Taken with permission from R.A. Millikan, *Phys. Rev.* Vol. 7, 355–388 (1916), ©1916 The American Physics Society

TABLE 12.1 Experimental Values of Photocurrent  $I_{pc}$  vs. Cathode Voltage  $V$  for Sodium Illuminated with Six Different Wavelengths of Light<sup>a</sup>

546.1 nm		433.9 nm		404.7 nm		365.0 nm		312.6 nm		253.5 nm	
$V_0$ (V)	$I_{pc}$ (mm def)	$V_0$ (V)	$I_{pc}$ (mm def)	$V_0$ (V)	$I_{pc}$ (mm def)	$V_0$ (V)	$I_{pc}$ (mm def)	$V_0$ (V)	$I_{pc}$ (mm def)	$V_0$ (V)	$I_{pc}$ (mm def)
0.253	28	0.829	44	0.934	82	1.353	67.5	1.929	52	2.452	68
0.305	14	0.889	20	0.986	55	1.405	36	1.981	29	2.568	38
0.358	7	0.934	10	1.039	36	1.458	19	2.034	12	2.672	26
0.410	3	0.986	4	1.091	24	1.510	11	2.086	5	2.777	16.5
				1.143	10	1.562	4			2.882	8
				1.196	3						
0.46 V		1.03 V		1.21 V		1.59 V		2.13 V		3.03 V	

<sup>a</sup>Adapted from Millikan, A direct photoelectric determination of Planck's " $h$ ," *Phys. Rev.* 7:355–388 (1916). Three entries in his table have been corrected to agree with his graphs, and every entry has been corrected for 2.51 V of contact potential. The bottom row of the table contains the values of  $V_0$  at which  $I_{pc}$  goes to zero as determined by Millikan's extrapolation. The current was read as millimeters of deflection (mm def) on the scale of an electrometer.

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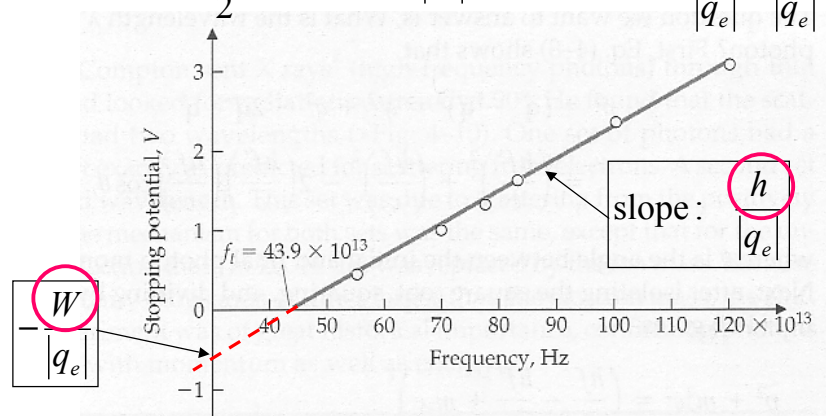
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## Stopping potential $V_0 = \text{max. kinetic energy } K_{\text{max}}$

- Millikan's data for  $V_0$ , plotted against the incident light frequency

$$h\nu = W + \frac{1}{2}mv_{\text{max}}^2 = W + |q_e|V_0 \Rightarrow V_0 = -\frac{W}{|q_e|} + \frac{h}{|q_e|}\nu$$



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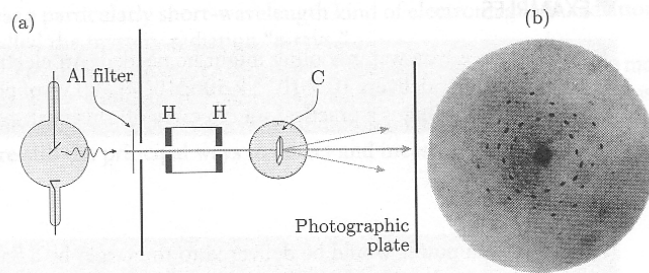
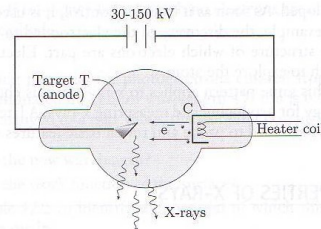
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## X rays – experimental facts

- Production of X-rays ("Coolidge tube")
  - $V = 50 \text{ kV}$     $\lambda > 0.0248 \text{ nm}$
  - $V = 40 \text{ kV}$     $\lambda > 0.031 \text{ nm}$
  - $V = 30 \text{ kV}$     $\lambda > 0.041 \text{ nm}$
- X-rays are waves (Friedrich & Knipping)



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## X rays – experimental facts

- X rays are waves!
- Bragg law of X-rays diffraction on crystals
  - Condition for constructive interference of X-rays in a crystal: difference of optical path related to wavelength!

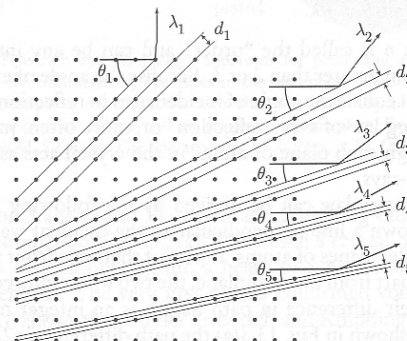
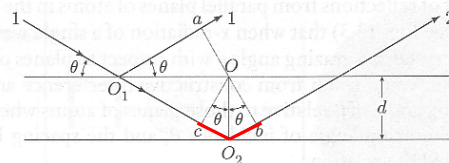
$$2d \sin \theta = n\lambda$$

$d$  atomic planes spacing

$\theta$  grazing angle

$n$  "order"

$\lambda$  wavelength

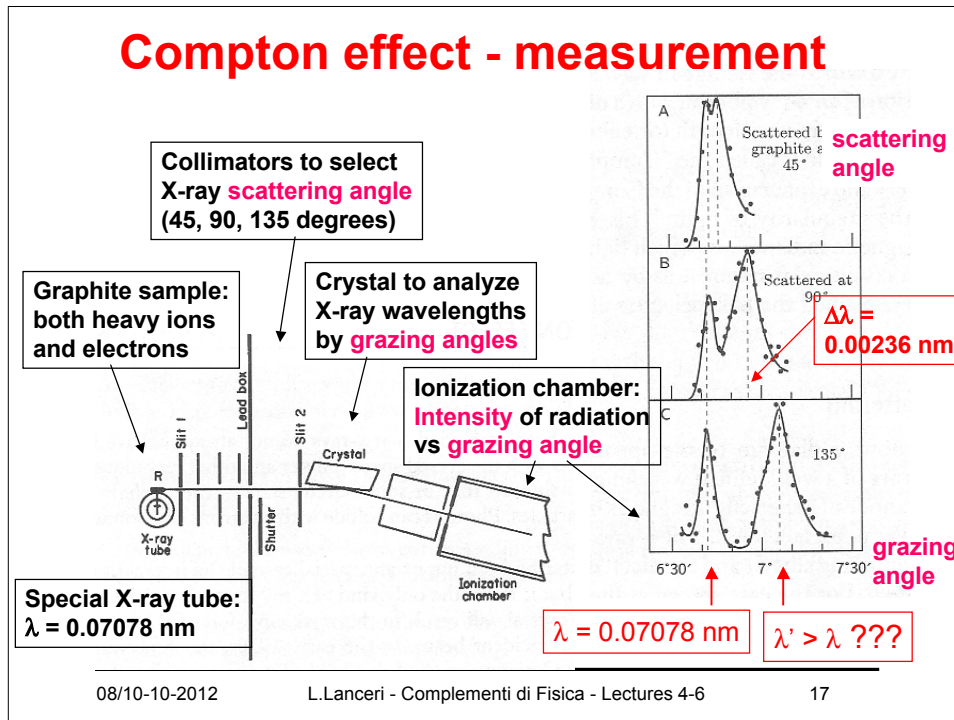


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## Compton effect - interpretation

**Elastic collision between particles:**

- Scattering of photons on heavy ions does not change wavelength significantly
- Scattering of photons on light electrons does!

$$\vec{q} = \vec{q}' + \vec{p}$$

$$hf + m_e c^2 = hf' + \sqrt{p^2 c^2 + m_e^2 c^4}$$

**From conservation of momentum and energy:**

$$2 \left( \frac{hf}{c} \right) \left( \frac{hf'}{c} \right) (1 - \cos \theta) = 2 m_e h c \left( \frac{f}{c} - \frac{f'}{c} \right)$$

$$f = c / \lambda$$

$$\lambda - \lambda' = \frac{h}{m_e c} (1 - \cos \theta)$$

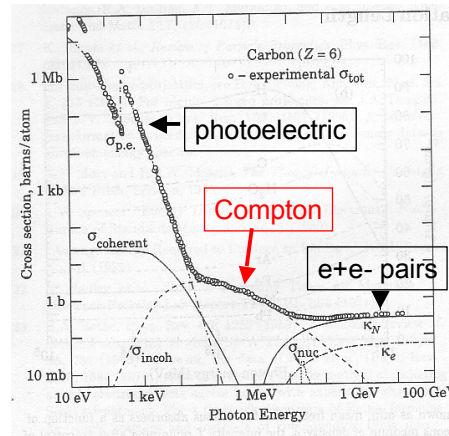
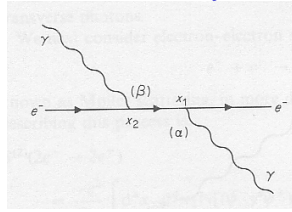
“Compton wavelength of the electron”  
 $h / (m_e c) \approx 2.4 \times 10^{-12} \text{ m}$

The diagram shows an incident photon with momentum  $\vec{q}$  colliding with an electron. The scattered photon has momentum  $\vec{q}'$  and the electron recoils with momentum  $\vec{p}$ . The angle between the incident and scattered photon paths is  $\theta$ .

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## Compton effect - warning

- The previous simple computation proves that:
    - e.m. waves behave also as particles !
  - It is not a full theory of the effect, that should also predict the probability as a function of:
    - Incident radiation energy
    - Scattering angle
- ... “Quantum Electrodynamics”!



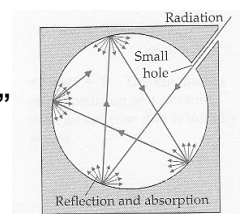
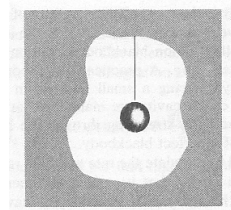
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## “Black-body” radiation

- **Thermodynamics, 2<sup>nd</sup> principle:**
  - all cavities in equilibrium at the same  $T$  have the same radiation density, independently of construction details; for a body  $i$  in the cavity:
    - **Irradiance  $I$**  = incident power per unit surface (a property of the cavity)
    - **Radiance  $H_i$**  = emitted power per unit surface (a property of the body)
    - **Absorption coefficient  $b_i$**  = absorbed fraction of incident energy:
      - at equilibrium:  $I = H_1/b_1 = H_2/b_2 = \dots$
  - A **perfect absorber ( $b = 1$ )** is a “black body” practical realization: a **cavity with a hole!**
    - $b = 1 \Rightarrow H_{max} = I$

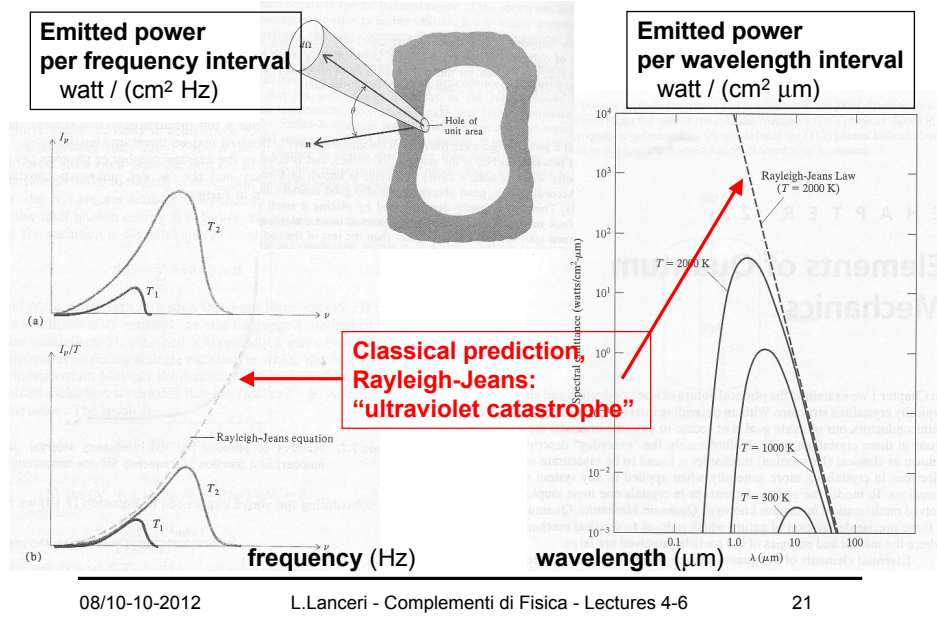


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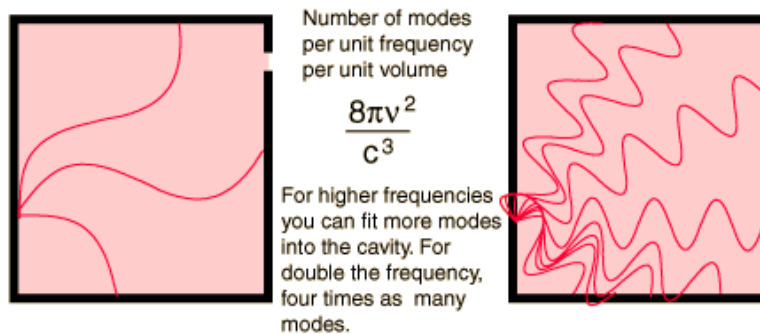
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## Black-body radiation: experiment

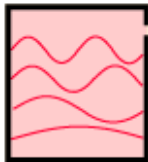


## Theory: cavity "modes"



## Theory: “classical” vs “quantum”

Radiation modes in a hot cavity provide a test of quantum theory



	#Modes per unit frequency per unit volume	Probability of occupying modes	Average energy per mode
CLASSICAL	$\frac{8\pi\nu^2}{c^3}$	Equal for all modes	$kT$
QUANTUM	$\frac{8\pi\nu^2}{c^3}$	Quantized modes: require $h\nu$ energy to excite upper modes, less probable	$\frac{h\nu}{e^{\frac{h\nu}{kT}} - 1}$



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## Black-body radiation: theory

- **Classical expectation: Rayleigh-Jeans law:**
  - Power per unit area per unit frequency interval

$$I_\nu \equiv \frac{dI}{d\nu} = \frac{2\pi\nu^2 kT}{c^2}$$

- Problem: divergence at high frequency!

- **Planck solution: radiation is quantized!**

- at the frequency  $\nu$ :  $n_\nu$  quanta, each one with energy  $E = h\nu$
- Apply statistical mechanics to find the population of each frequency interval (“Bose-Einstein distribution”) and from that the energy density distribution:

$$I_\nu \equiv \frac{dI}{d\nu} = \frac{2\pi h \nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1}$$

- See Fowles (op.cit.), p.204-217; we will come back to this later if we have time, when we will discuss some statistical issues

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## Summary of e.m. radiation as photons

- Experimental evidence that e.m. radiation has also particle-like behavior
- How can we reconcile this with wave-like behavior?
  - Diffraction through two slits:
    - Even attenuating the intensity so that photons are well separated in time and arriving individually, waiting long enough the interference pattern appears on the screen!
    - How do individual photons know that there are two slits?
    - Each photon interferes with itself!?!
  - Polarization:
    - Individual polarized photons are absorbed or transmitted by an analyzer, there is no other possibility
    - On average, they are somehow guided by the expected attenuation factors...

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## (b) particles as “matter waves”

DeBroglie wavelength  
Electron diffraction by crystals  
Two-slit diffraction of electrons

## DeBroglie wavelength

- Bold proposal (PhD thesis...):**

- Since, for photons:  $E = h\nu = \hbar\omega$

$$\Rightarrow p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda} \quad (\text{waves: } \lambda\nu = c)$$

- Idea: generalize to all particles, assuming:

$$\lambda = \frac{h}{p} \quad p = mv \quad (\text{not relativistic})$$

$$p = m_0 v \left(1 - v^2/c^2\right)^{1/2} \quad (\text{relativistic})$$

- Expect wave-like interference effects also for particles, for instance for electrons! This idea can be tested experimentally

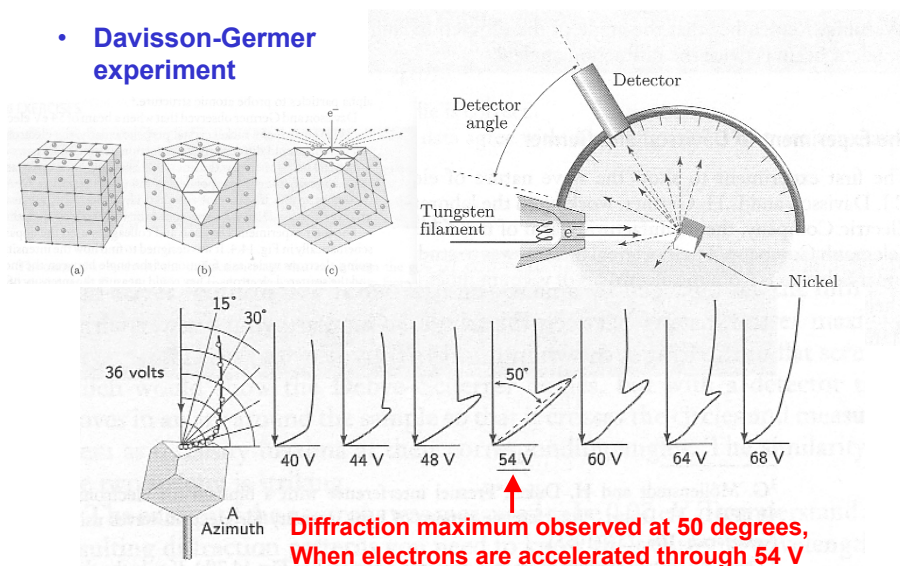
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## Electron diffraction by crystals

- Davisson-Germer experiment**



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## Davisson-Germer: interpretation

**Bragg condition for constructive interference (diffraction maxima)**

$$n\lambda = 2a \sin \theta$$

$a = 0.91 \times 10^{-10} \text{m}$ , measured with X-rays  
First maximum ( $n=1$ ) seen at 50 degrees

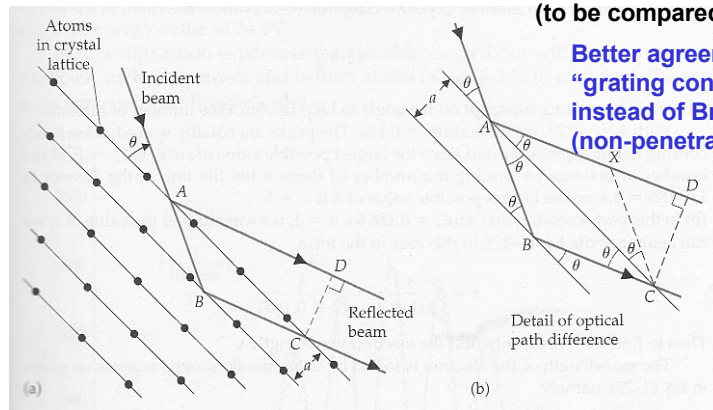
$$\Rightarrow \lambda = 2a \sin \theta = 1.39 \times 10^{-10} \text{m}$$

$$\Rightarrow p = h/\lambda = 4.77 \times 10^{-24} \text{ kg m/s}$$

$$\Rightarrow K = p^2/2m = \dots = 66 \text{ eV,}$$

(to be compared with 54 V)

Better agreement using  
"grating condition"  
instead of Bragg...  
(non-penetrating electrons)



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## Two-slit diffraction of electrons - 1

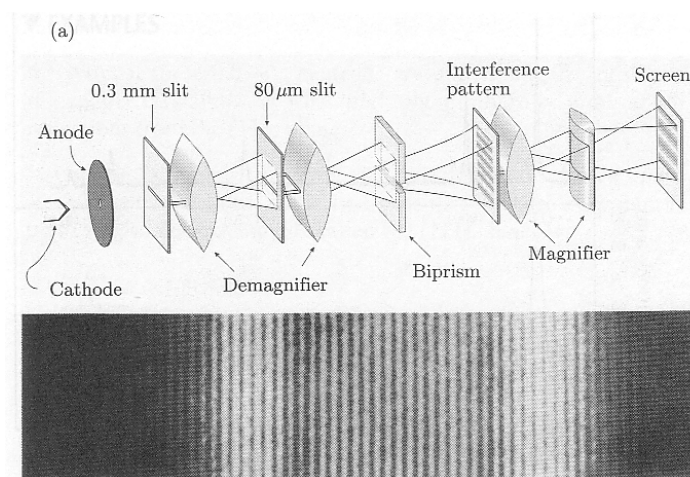


FIGURE 14.7 Double-slit interference of electrons: (a) apparatus; (b) interference pattern.  
Taken from H. Düker, Z. Naturforsch. 10a, 256 (1955) with permission of the publisher

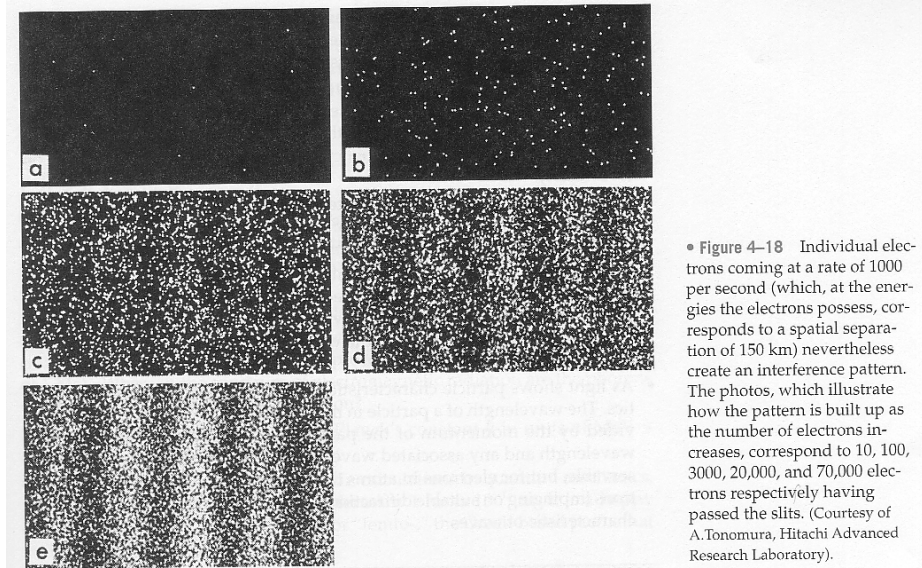
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## Two-slit diffraction of electrons - 2



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## Particles as waves: summary

- **Experimental evidence that particles (electrons, but also neutrons, etc.) show also wave-like behavior**
- **Far-reaching consequences!**
  - **Example: two-slit diffraction:**
    - Individual electrons, coming one by one through a “two-slit” arrangement, build up an interference pattern
    - Each electron interferes with itself !?!
    - Each electron “goes simultaneously through two different slits” !?!,
    - Crisis of localization in space (trajectory not well defined)
    - Any attempt to localize the slit through which the electron goes destroys the interference pattern!!!

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## Lecture 3 - summary

- Blackbody spectra in conflict with classical expectation; require light quanta carrying both energy ( $E=h\nu$ ) and momentum, moving at the speed of light
- The quantum nature of light is confirmed for instance by the photoelectric and Compton effects
- The classical expressions are obtained in the limit  $h \rightarrow 0$  (macroscopic world)
- Like e.m. radiation, also matter particles show wave-like behavior, expressed by the DeBroglie relation
- A new theory is needed for microscopic phenomena...

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## Lecture 3 - exercises

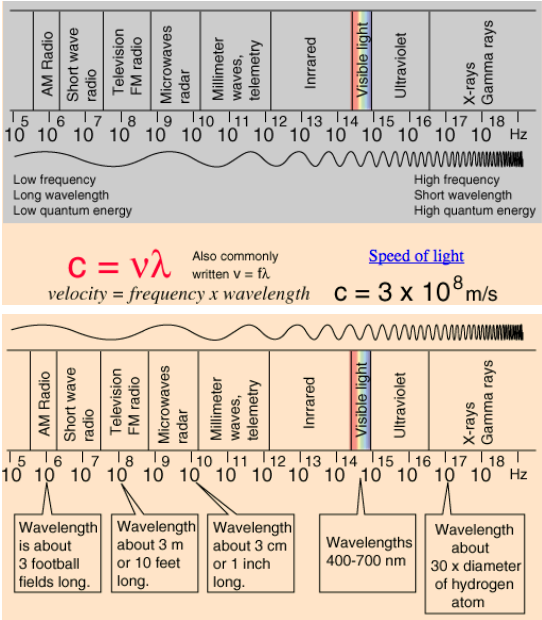
- **Exercise 3.1:** Suppose that a 60 W light-bulb radiates primarily at a wavelength of about 1000 nm. Find the number of photons emitted per second.
- **Exercise 3.2:** When electromagnetic radiation of wavelength 270 nm falls on an aluminum surface, photoelectrons are emitted. The most energetic are stopped by a potential difference of 0.406 volts. Find the work function of aluminum in electronvolts.
- **Exercise 3.4:** Find the DeBroglie wavelengths of an electron with kinetic energy of 1 eV, 1 keV, 10 MeV; of a neutron with kinetic energy  $kT$ , where  $T=300K$ ; a neutron with kinetic energy of 10 MeV
- **Exercise 3.5:** Find the DeBroglie wavelength of an electron with kinetic energy of 100 eV. Supposing a beam of such electrons is sent into a crystal with spacing between atomic planes  $a = 1.0$  nm, at what scattering angle would you expect the first diffraction maximum? (assume the Bragg condition for constructive interference)

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Back-up slides



Electro-magnetic Radiation Spectrum

<http://hyperphysics.phy-astr.gsu.edu>

## Matter

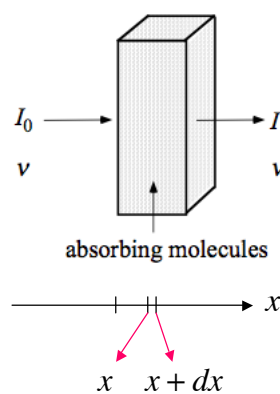
- Individually *free charged particles* (negative electrons, positive nuclei: “plasma”)
  - All energy values allowed
  - “Direct” interaction with e.m. fields (photons)
- Neutral composite objects (molecules, atoms; crystals, ...), made of *bound charged particles*
  - Discrete energy values
  - “Indirect” interaction with e.m. fields (for instance via electric or magnetic dipole moments)

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## Radiation-Matter Interactions



Each additional layer  $dx$   
absorbs the same fraction  
of the incident intensity  $I(x)$

$$I(x + dx) = I(x) + dI$$

$$dI = -(1/\lambda) I(x) dx$$

$$\frac{dI}{dx} = -(1/\lambda) I(x)$$

result: exponential absorption law

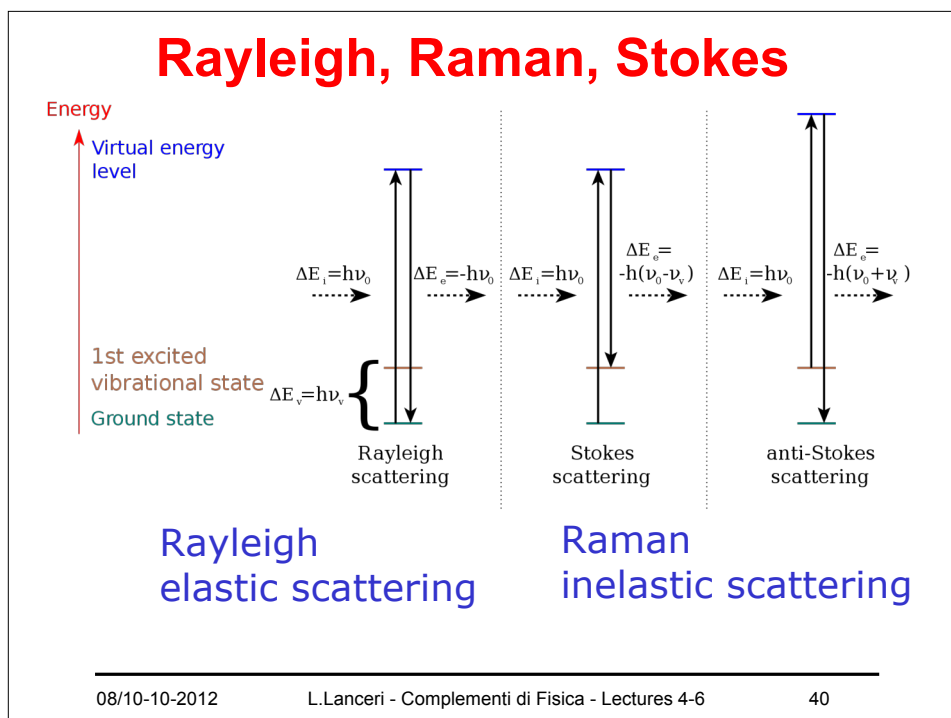
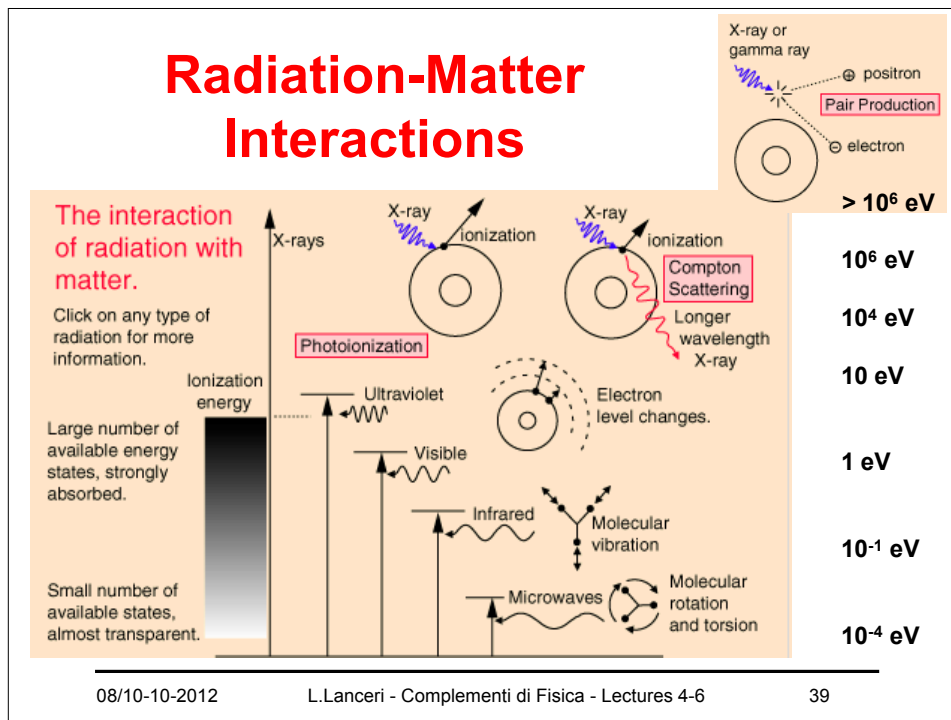
$$\Rightarrow I = I_0 \exp(-x/\lambda)$$

Several different processes contribute to the disappearance of photons from the incident beam, depending on the photon energy (frequency) range

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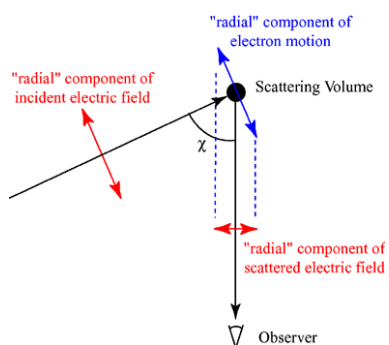
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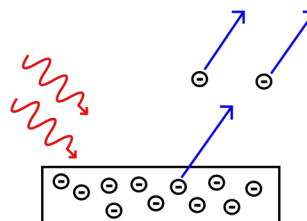


## Light-matter interaction

Classical Rayleigh  
(elastic) scattering



Quantum Photoelectric  
effect



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