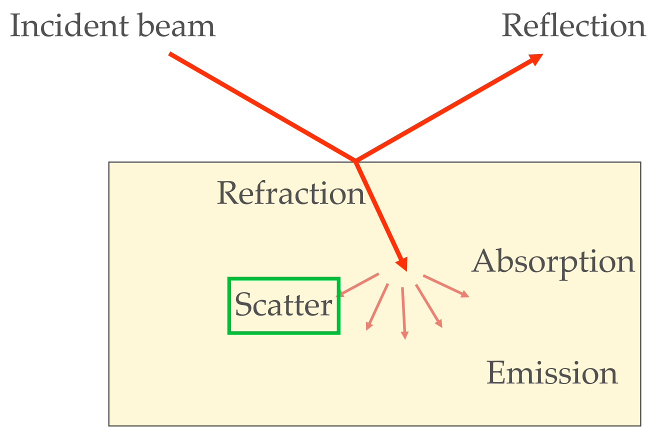
# Interaction of light with matter:

## Scatter, absorption

Miklós Kellermayer

# Interaction of light with matter




# Scattering of light

What are these days?
Crepuscular rays
(St. Peter's basilica)

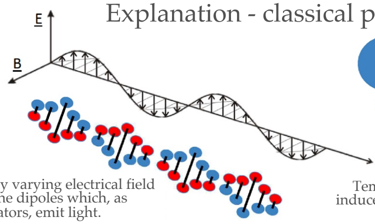
Why is the sky blue?

What makes the sunset red?

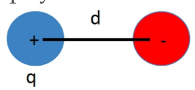
# Scattering of light

## Explanation - classical physics

Light is an electromagnetic wave ($E$, $B$: electric and magnetic fields)




The temporally varying electrical field vibrates the dipoles which, as oscillators, emit light.




Molecule as a dipole
Dipole moment ($p_0$):

$$p_0 = Qd$$

Temporally varying dipole moment induced by the varying electrical field: $p = p_0 \sin \omega t$

Dimension: $Qdt^{-1}$

How large is the scattered ("re-radiated") light's power? ($P_{scatt}$; dimension $W = Fdt^{-1}$)

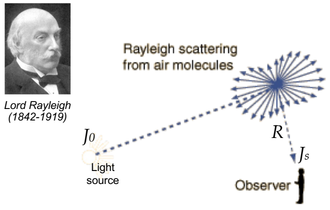
N.B. - Coulomb's law: $F \sim \dfrac{Q_1 Q_2}{r^2}$ (dimension $Q^2 d^{-2}$)

Dimensional derivation

| Physical parameter | Dimension | Operation |
|---|---|---|
| $p_0^2$ | $Q^2d^2$ | Square |
| $p_0^2$ | $Q^2d^{-2}d^4 = Fd^4$ | Expand with $d^2d^{-2}$ |
| $p_0^2/c^3$ | $Fdt^3$ | Divide by $c^3$ ($d^3t^{-3}$) |
| $(p_0^2/c^3)\omega^4$ | $Fdt^{-1} = W$ | Multiply by $\omega^4$ ($t^{-4}$) |

$$P_{scatt} = \frac{p_0^2}{c^3}\omega^4$$

# Light scattering




- Elastic collision: photon energy (wavelength) does not change
- Emission by resonating dipoles
- Scattering particles far from each other

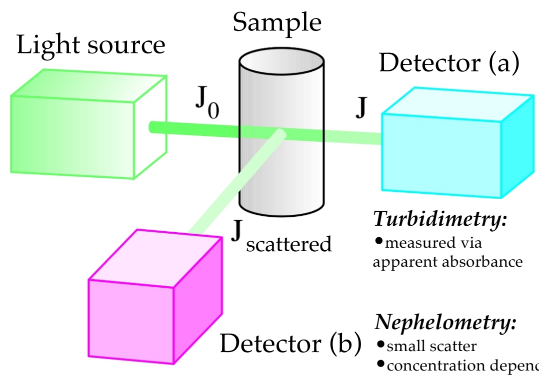
$$J_s = J_0 \frac{8\pi^4 N \alpha^2}{\lambda^4 R^2}\left(1+\cos^2\Theta\right)$$

$J_s$=intensity of scattered light
$J_0$=intensity of incident light
$N$=number of scattering particles
$\alpha$=polarizability (dipole moment per electric field)
$\lambda$=wavelength of light
$R$=distance between scatterer and observer
$\Theta$=angle between light source and observer

Strong wavelength dependence ➛ enhancement of short wavelengths ➛ blue sky

If scatterers are interacting particles the the overall size of which is comparable to the wavelength ➛ interference, cancellation ➛ gray clouds

# Biomedical applications of light scattering

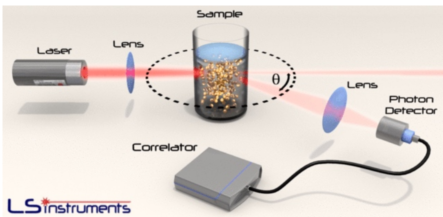



***Turbidimetry:***
- measured via apparent absorbance

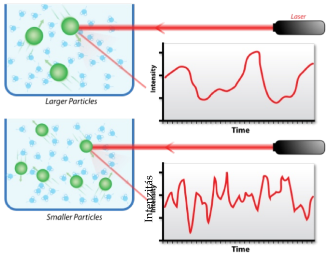
***Nephelometry:***
- small scatter
- concentration dependence
- concentration measurement of immune complexes

# Dynamic Light Scattering (DLS)

Diffusing nm-scale particles



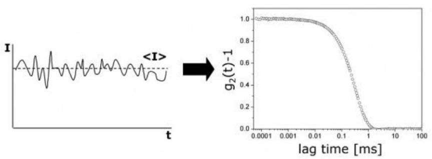

Intensity of scattered light fluctuates in time



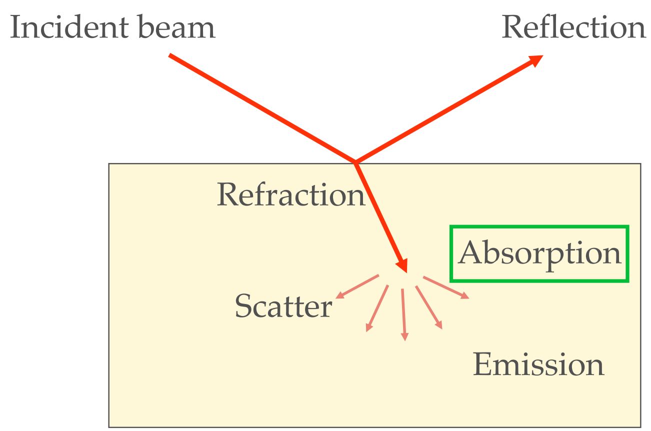

Fluctuation rate depends on particle size

- From the autocorrelation function ("self-similarity") of temporal intensity fluctuation the diffusion constant ($D$) can be calculated.
- From the diffusion constant the radius ($r$) of the spherical particle can be calculated (Stokes-Einstein):

$$D = \frac{k_B T}{6\pi\eta r}$$

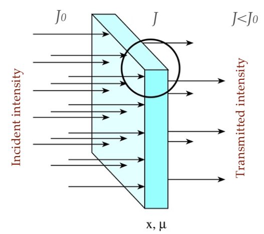


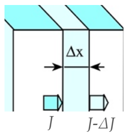

# Interaction of light with matter




**Absorption** - *absorbere, lat.*, swallow

# General absorption (attenuation) law



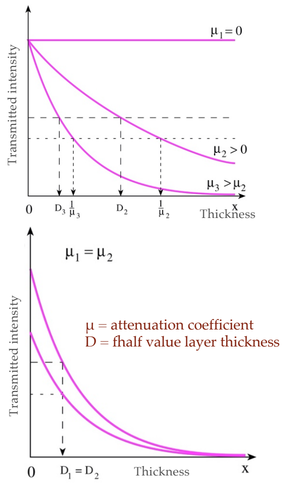




A given quantity ($J$) and its change ($\Delta J$) are proportional:

$$\Delta J = -\mu \Delta x J$$

Exponential function:

$$J = J_0 e^{-\mu x}$$

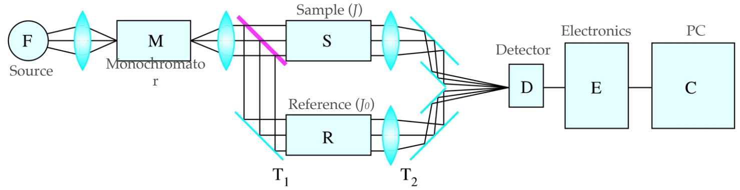



# Parameters and measurement of absorption

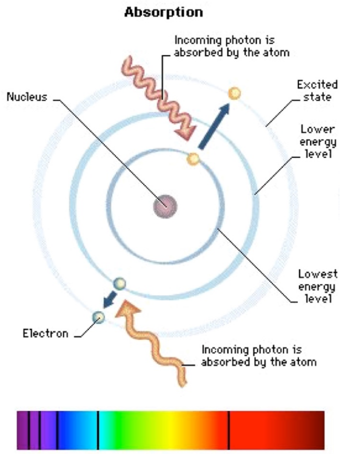
Absorbance (A): $A = \lg \frac{J_0}{J} = \lg e \cdot \mu \cdot x$ — Dimensionless number. *Synonyms*: extinction, optical density (OD)

Transmittance (T): $T = \frac{J}{J_0} \cdot 100$ — Expressed in percent (%). *Synonym*: transmission coefficient

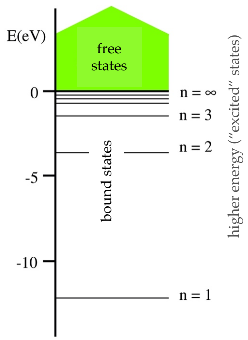
Photometry
("measurement of light"):




# Light absorption by an atom

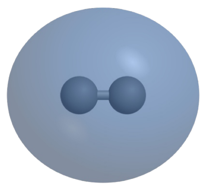



Absorption line spectrum




# State of a molecule is affected by its motional modes

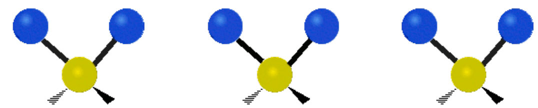
Molecule: atoms connected by chemical bonds
Simplest case: diatomic molecule (e.g., hydrogen molecule)



Molecules ***vibrate*** and ***rotate***!

***Vibration***: periodic motion ***along*** the axis of the covalent bond
***Rotation***: periodic motion ***around*** the axis of the covalent bond

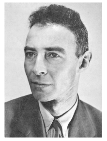
Examples of vibrational motion in the triatomic methylene group ($-CH_2-$):



*Asymmetric stretching* — *Symmetric stretching* — *Scissoring*

# Energy of a molecule

Max Born
(1882-1970)



J. Robert Oppenheimer
(1904-1967)

Born-Oppenheimer approximation:

$$E_{total} = E_e + E_v + E_r$$

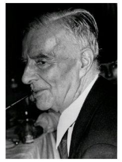
***Iportant notions:***
Types of energy states are independent (not coupled)
Energy states are non-continuous, but discrete
Transition between states involves packets (quanta) of energy
Scales of transition energies between different states are different:

$$E_e \overset{\sim 100x}{>} E_v \overset{\sim 100x}{>} E_r$$

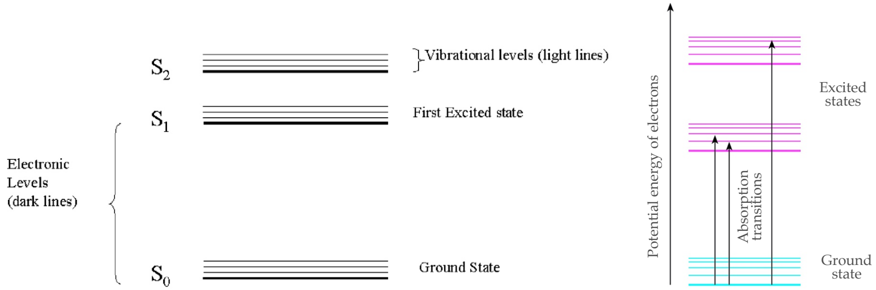
~3x10$^{-19}$ J (~2 eV) > ~3x10$^{-21}$ J > ~3x10$^{-23}$ J

# Representation of energy states

Jabłoński diagram:
illustrates the electronic states of a molecule and the transitions between them (with arrows)

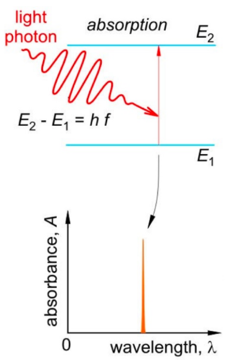


Alexander Jabłoński
(1898-1980)

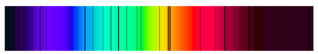



# Origin of the band spectrum

Individual atoms

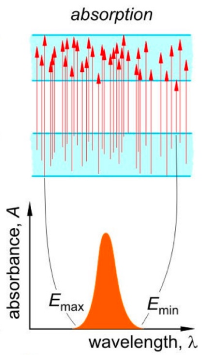



Line absorption spectrum



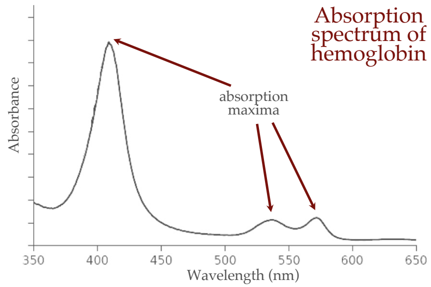
Narrow black lines ("missing colors") appear in the spectrum of the light source: absorption lines

Molecules




**Band spectrum** - origin:
- chemically identical molecules are in different energy states
- thermal motion
- solvent conditions

# Molecules have band absorption spectra




General attenuation law:

$$A = \lg \frac{J_0}{J} = \lg e \cdot \mu \cdot x$$

For dilute solutions - Lambert-Beer law:

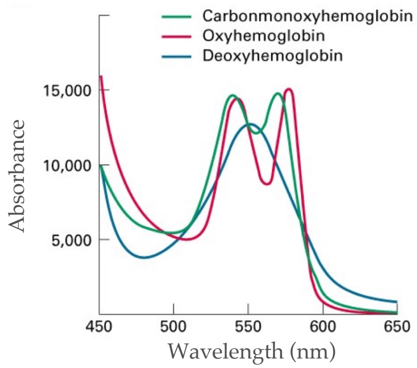
$$A_\lambda = \lg \frac{J_0}{J} = \varepsilon_\lambda \cdot c \cdot x$$

$\varepsilon_\lambda$ = molar extinction coefficient
$c$ = concentration

- SI unit of molar extinction coefficient ($\varepsilon_\lambda$) : m$^2$mol$^{-1}$
- Method ideal for concentration measurement
- Based on the wavelength (at maximum) the transition energy may be calculated:

$$E_2 - E_1 = E_{foton} = h \cdot f = h \cdot \frac{c}{\lambda}$$

# Absorption spectroscopy

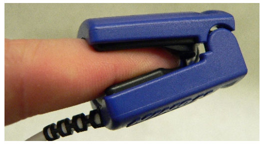


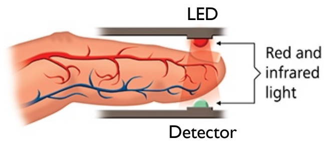

- *Spectrum*: intensity (or its derived units, e.g., OD) as a function of photon energy (or its derived units, e.g., frequency, wavelength).
- *Spectroscopy*: qualitative analysis of the spectrum.
- *Spectrometry, spectrophotometry*: quantitative analysis of the spectrum.
- *Applications*: analysis of chemical structure, concentration measurement, etc.

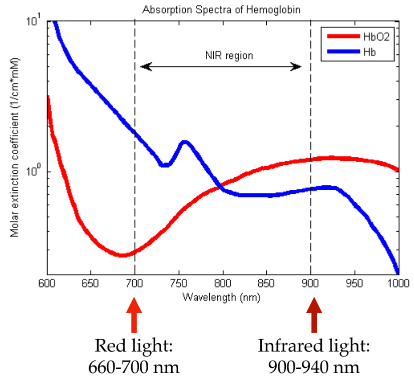
# Pulse oxymetry

Non-invasive meaurement of oxygen saturation ($SO_2$)

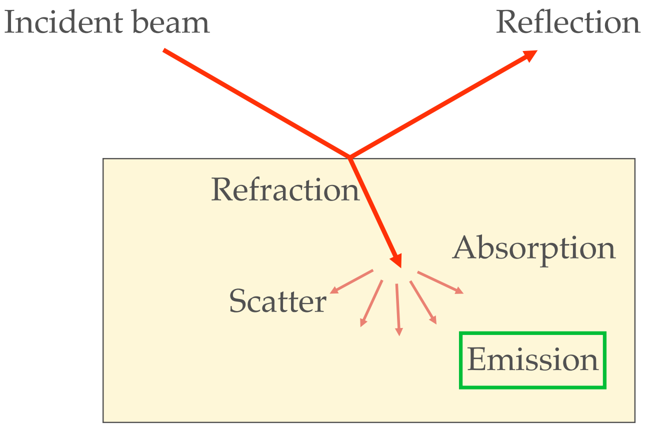
- % of HgB that carries $O_2$ is measured
- Arterial oxygen saturation ($SaO_2$) is estimated from the peripheral ($SpO_2$)
- Normal value: 95-99%
- Ratio measurement is carried out (red/IR)






# Interaction of light with matter




# Feedback

http://report.semmelweis.hu/linkreport.php?qr=1S82J6QA50OSG5N4

pin: S9S