Physics of Condensed Matter I

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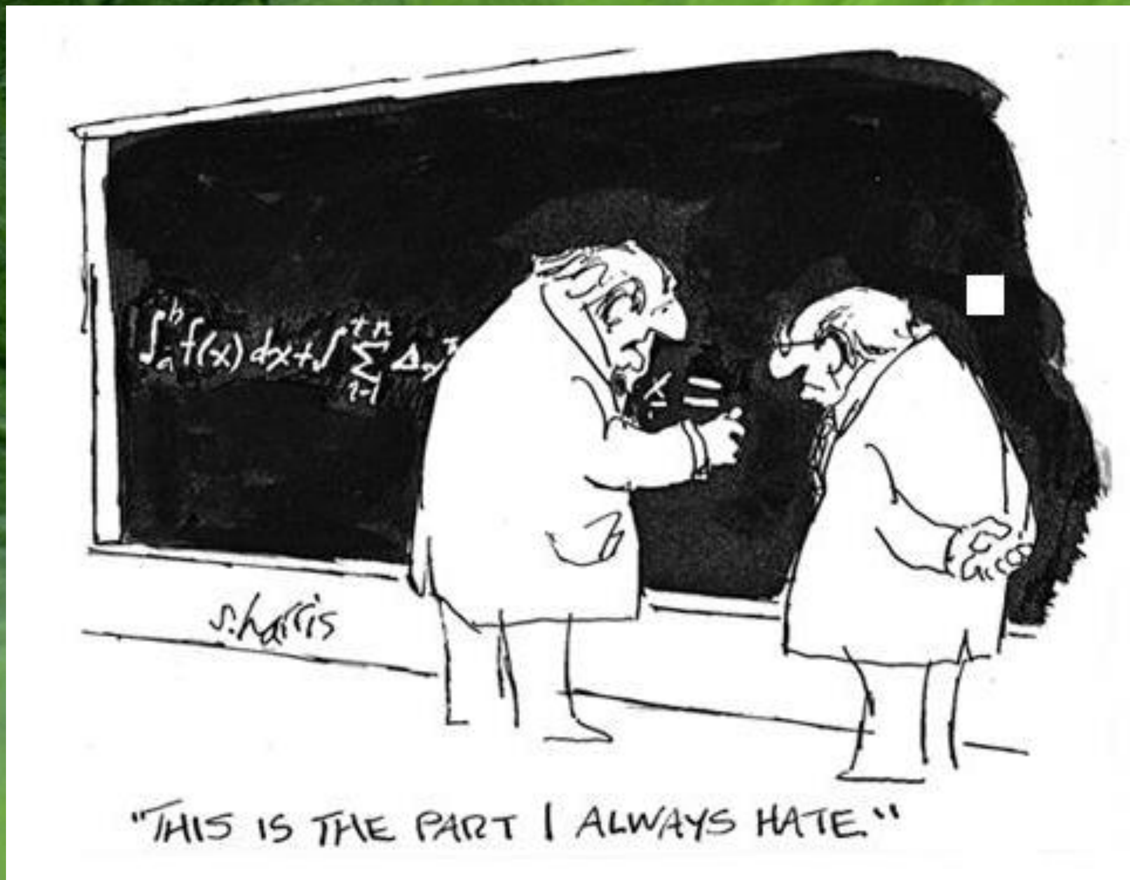


Faculty of Physics UW

Jacek.Szczytko@fuw.edu.pl

inżynieria nanostruktur

Dictionary

$$\vec{D} = \varepsilon \vec{E}$$

ε_0 **vacuum permittivity, permittivity of free space** (przenikalność elektryczna próżni)
ε_r relative permittivity (względna przenikalność elektryczna)
$\varepsilon = \varepsilon_0 \varepsilon_r$ permittivity (przenikalność elektryczna)

$$\vec{B} = \mu \vec{H}$$

μ_0 **vacuum permeability, permeability of free space** (przenikalność magnetyczna)

$$\mu_0 = 4\pi \cdot 10^{-7}\text{H/m}$$

μ_r relative permeability (względna przenikalność magnetyczna)
$\mu = \mu_0 \mu_r$ permeability (przenikalność magnetyczna)

magnetic susceptibility $\chi_m = \mu_r - 1$

electric field $\vec{E}$ and the magnetic field $\vec{B}$
displacement field $\vec{D}$ and the magnetizing field $\vec{H}$

Fine structure

The fine structure means the splitting of the spectral lines of atoms due to electron spin and relativistic corrections to the Schrödinger equation. We got corrections to the value of energy levels.

- Kinetic energy relativistic correction
- Spin-orbit coupling
- Darwin term

$$\Delta E_n' = -\frac{E_n^2}{2mc^2}\left[\frac{4n}{l+\frac{1}{2}} - 3\right] = -\frac{\alpha^2 Z^2}{2n^4} E_n \left[\frac{n}{l+\frac{1}{2}} - \frac{3}{4}\right]$$

$$E_{SO} = \frac{Z^4}{2(137)^2 a_0^3 n^3}\left(\frac{j(j+1) - l(l+1) - s(s+1)}{2l(l+1/2)(l+1)}\right)$$

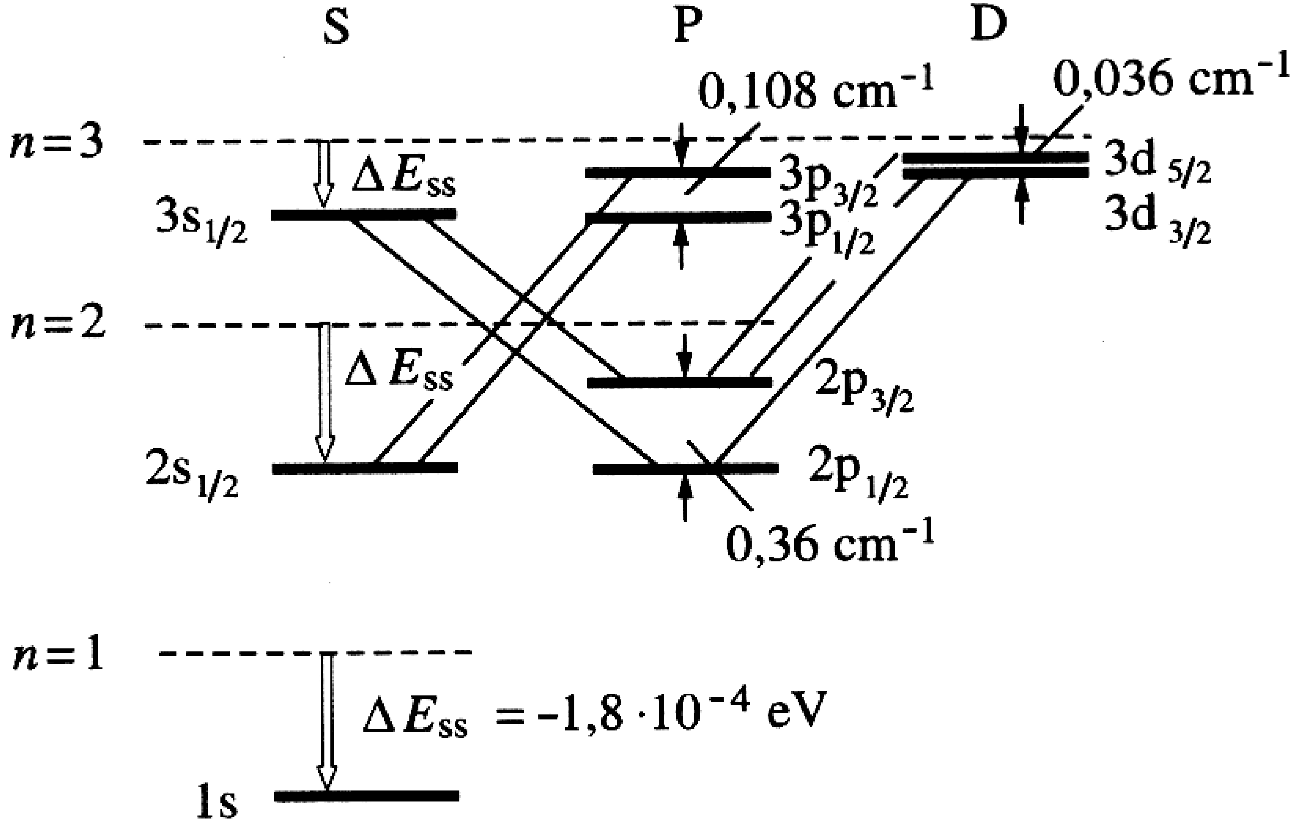
$$E_{Darwin} = \frac{\hbar^2}{8m^2c^2} 4\pi \left(\frac{Ze^2}{4\pi\epsilon_0}\right) |\psi(\vec{r} = 0)|^2$$

Total effect:

$$\boxed{\Delta E_n' = -\frac{\alpha^2 Z^2}{n^2} E_n \left[\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right]}$$

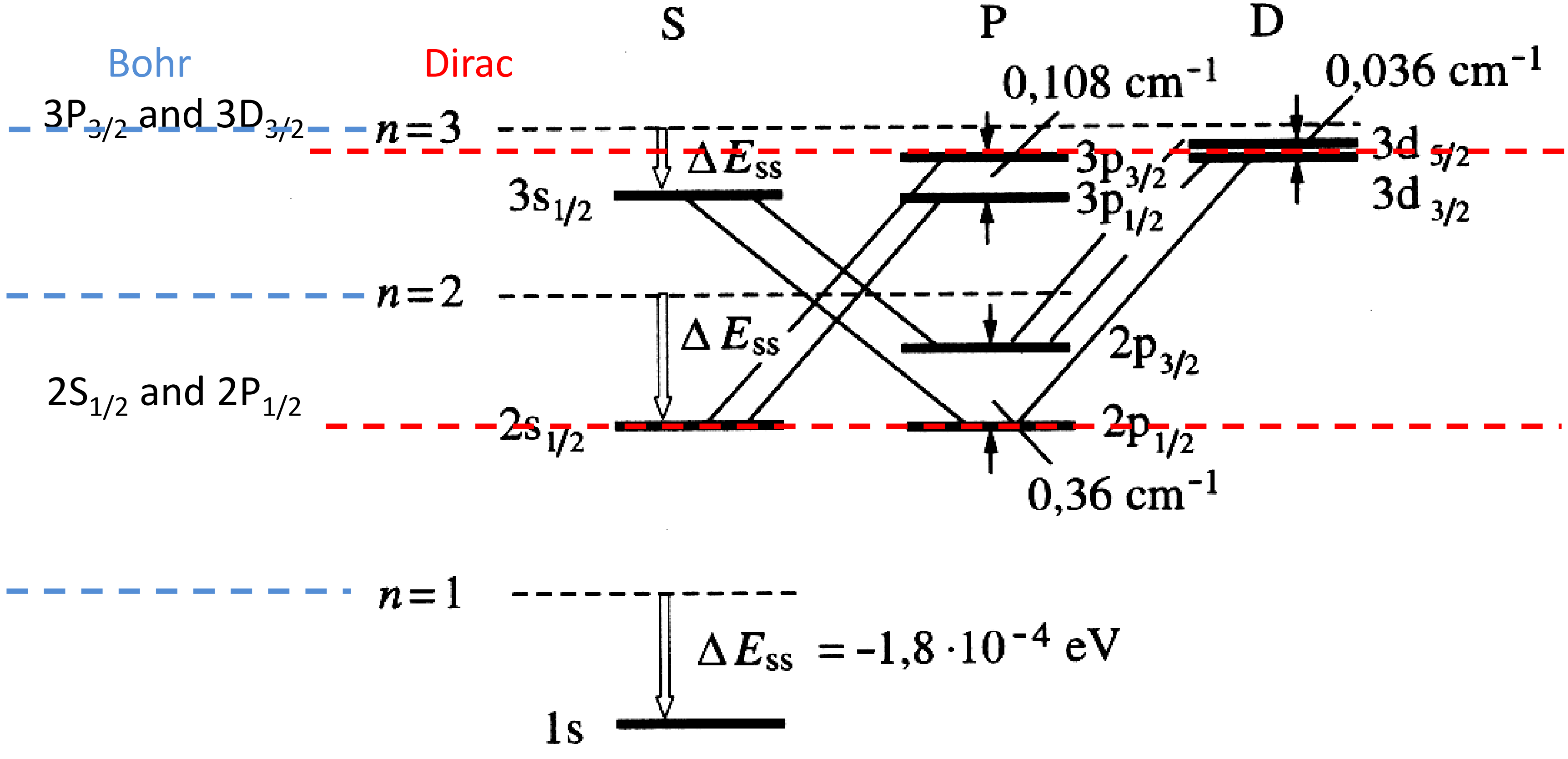
Fine structure

Paul Dirac calculations:



Fine structure

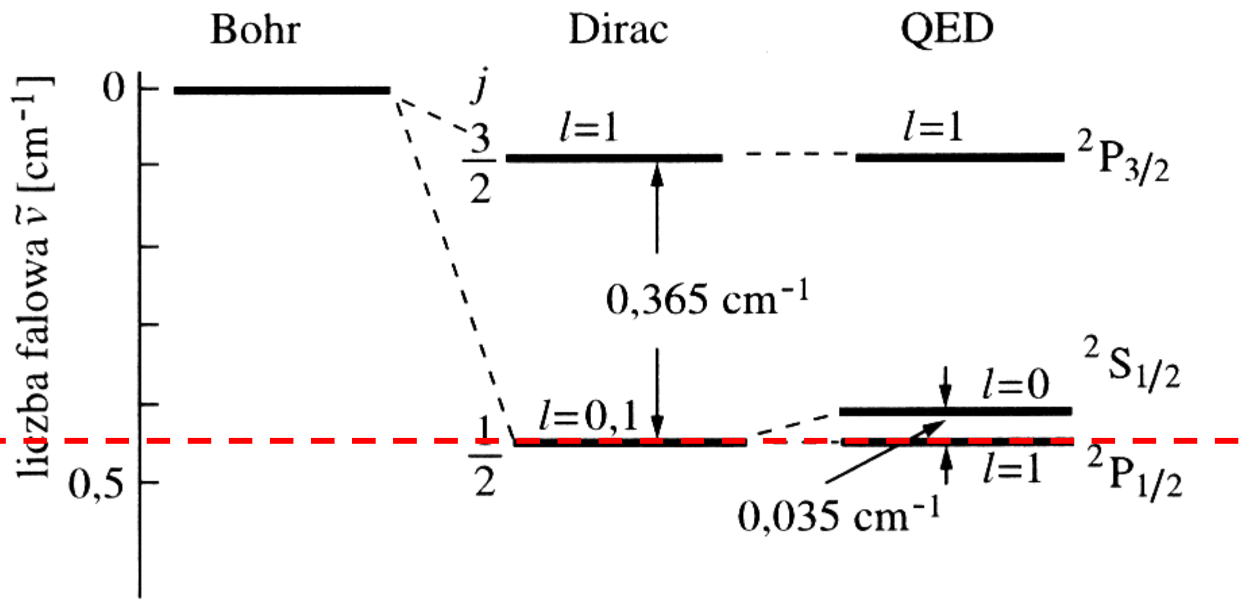
Paul Dirac (Nobel 1933) calculations:



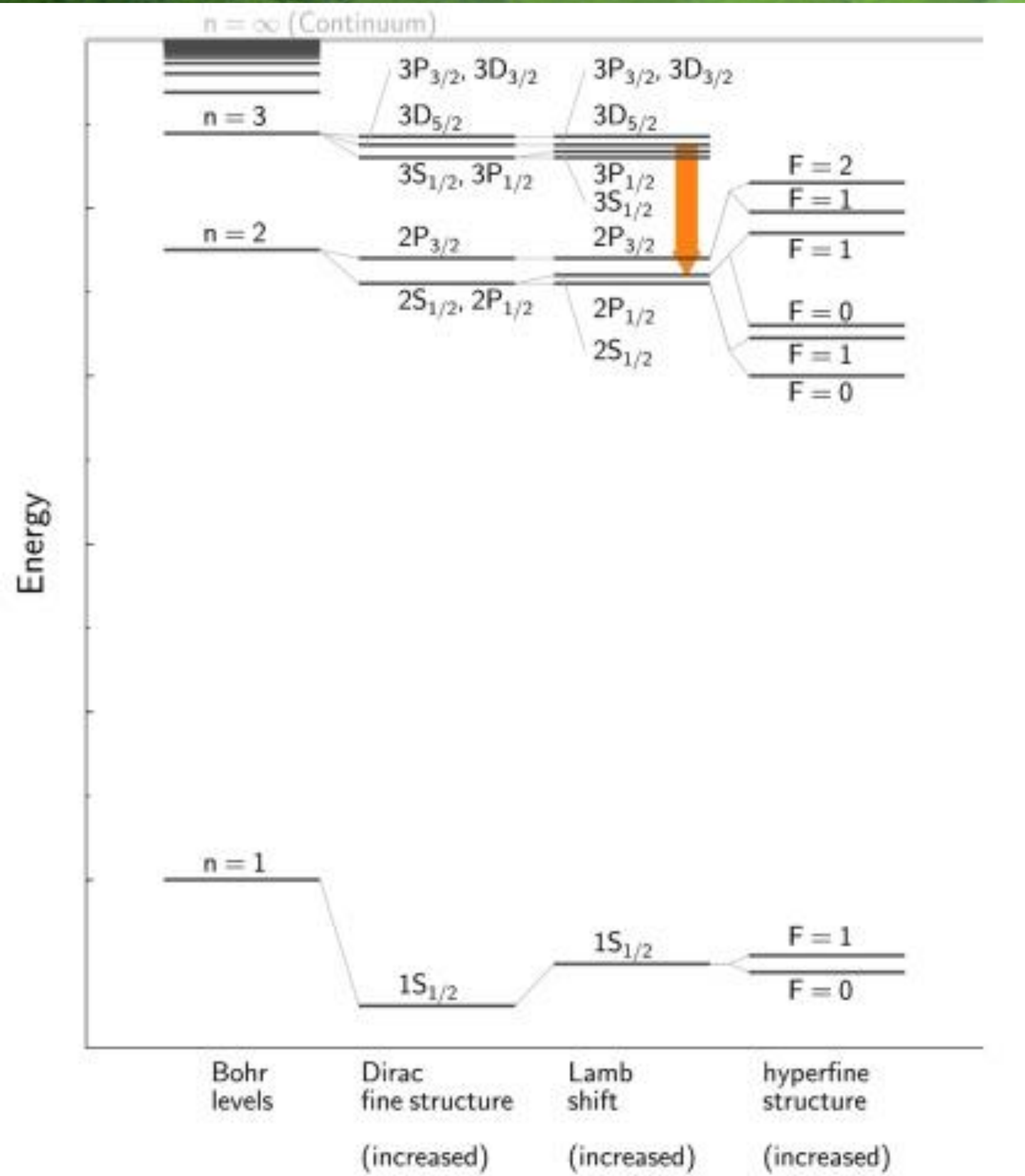
Fine structure

Willis Lamb (Nobel 1955) calculations:

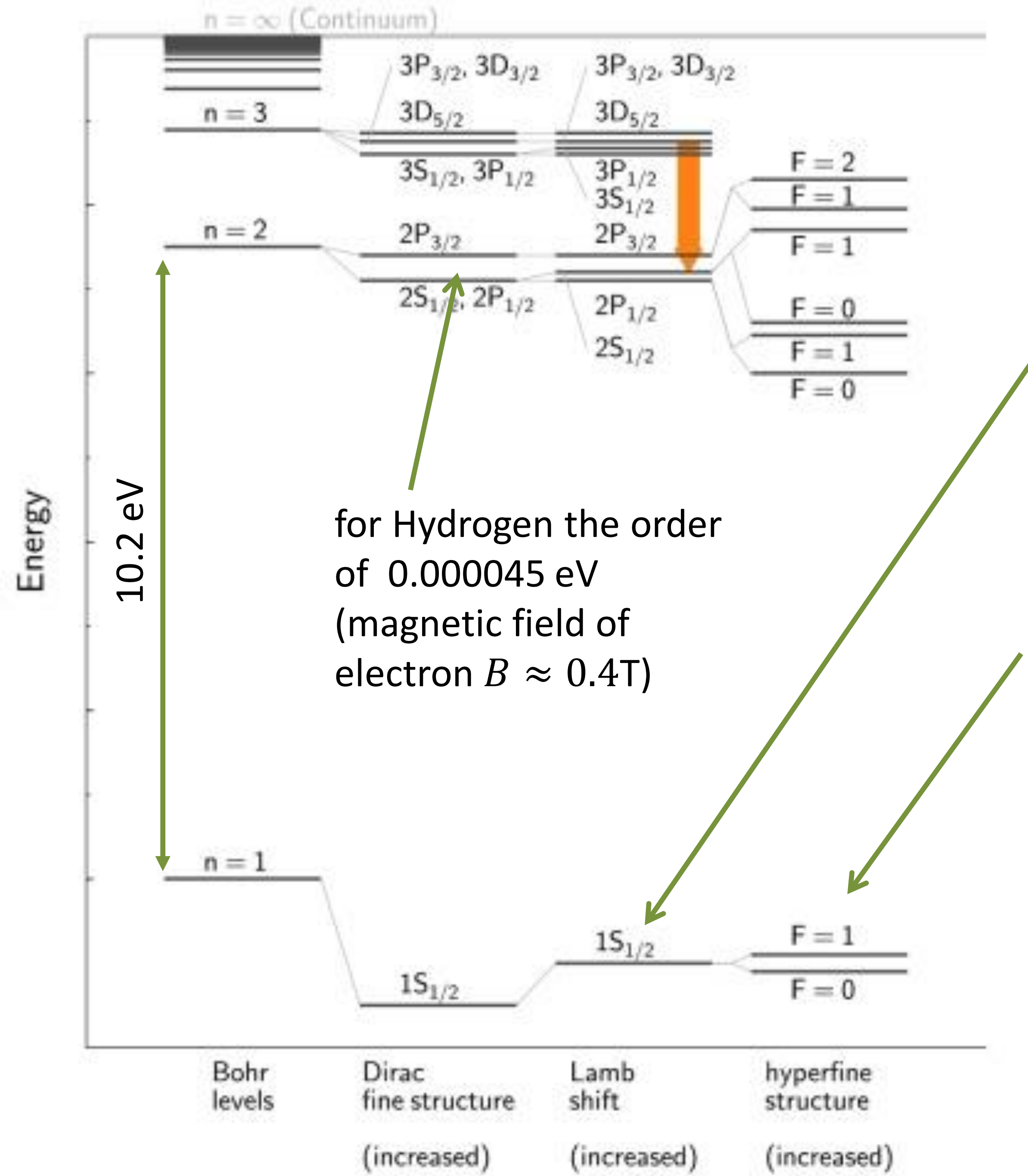
$2S_{1/2}$ and $2P_{1/2}$



QED – Quantum ElectroDynamics – Lamb shift due to the interaction of the atom with virtual photons emitted and absorbed by it. In quantum electrodynamics the electromagnetic field is quantized and therefore its lowest state cannot be zero ($E_{min} = \frac{\hbar\omega}{2}$), which perturbs Coulomb potential.



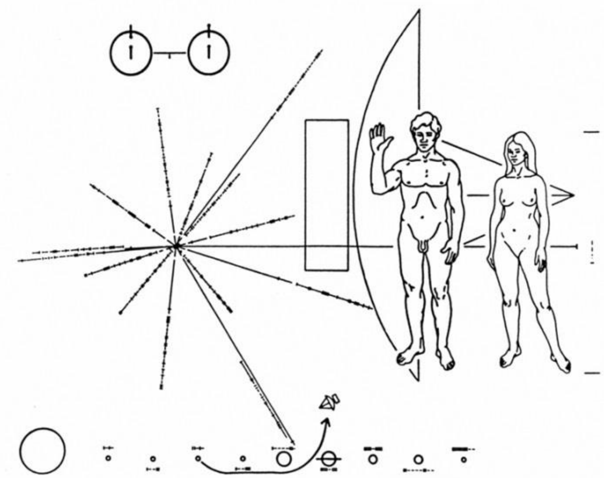
http://backreaction.blogspot.com/2007/12/hydrogen-spectrum-and-its-fine.html



for Hydrogen the order of 0.000045 eV (magnetic field of electron $B \approx 0.4$T)

Lamb shift – (Willis Lamb) QED
size of the proton!
(hydrogen vs muonic hydrogen)
[about 1 GHz]

Hyperfine interaction: interaction with nuclear moment
[21 cm (1420 MHz) for atomic H]



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Fine structure

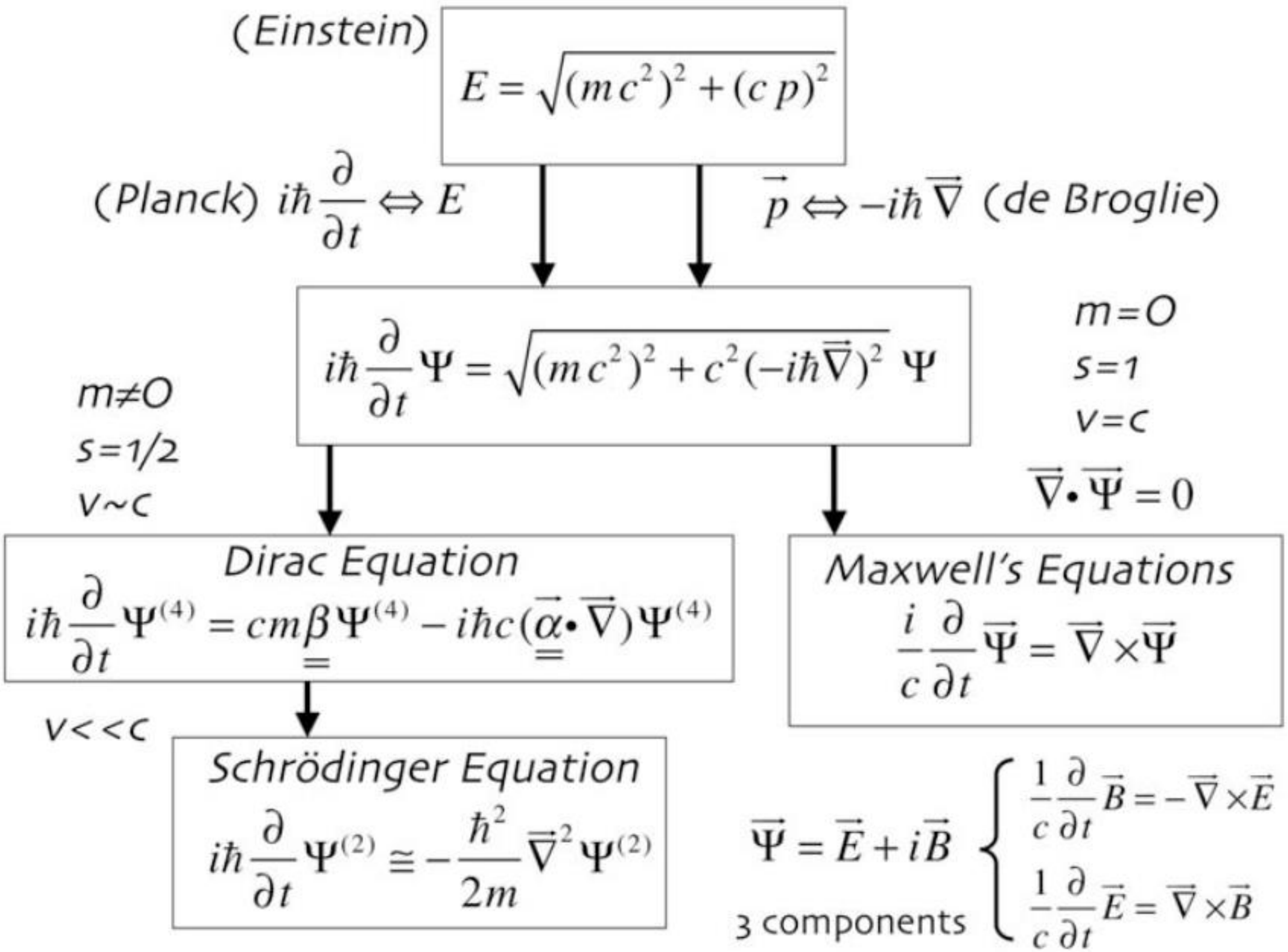


Fig.1 Flow chart for derivations of electron and photon wave equations, m = rest mass, s = spin, v = velocity.

The Maxwell wave function of the photon M. G. Raymer and Brian J. Smith, SPIE conf. Optics and Photonics 2005

Time-dependent perturbation theory

General solution of Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\,\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\,\nabla^2\psi(\vec{r},t) + V(\vec{r},t)\psi(\vec{r},t)$$

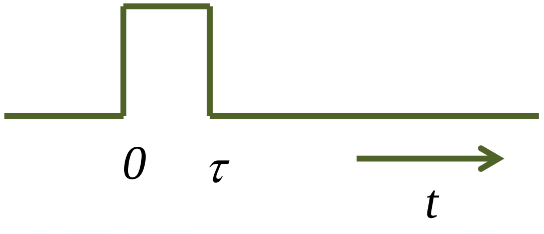
Time-independent potential

$$H_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x) \qquad \psi(x,t) = A\varphi(x)e^{-iEt/\hbar}$$

Time-~~in~~dependent potential $H = H_0 + V(t)$

The simplest case:

$$V(t) = \begin{cases} W(t) & \text{dla } 0 \le t \le \tau \\ 0 & \text{dla } t < 0 \text{ i } t > \tau \end{cases}$$



Time-dependent perturbation theory

Time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi = H_0 + V(t)$$

$$\psi(x,t) = \sum_n A_n(t)\varphi_n(x)e^{-iE_nt/\hbar}$$

By analogy

Time-independent potential

$$H_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x) \qquad \psi(x,t) = A\varphi(x)e^{-iEt/\hbar}$$

Time-~~in~~dependent potential $\quad H = H_0 + V(t)$

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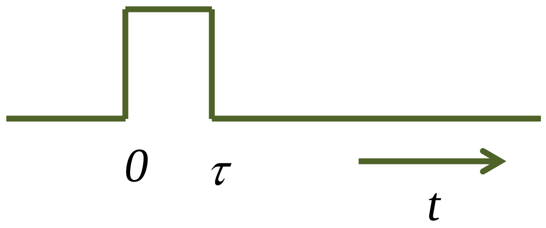

Fast track → 28

Time-dependent perturbation theory

Time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}\psi = H_0 + V(t) \qquad \psi(x,t) = \sum_n A_n(t)\varphi_n(x)e^{-iE_n t/\hbar}$$

For $t < 0$ the system was in the initial state m $\quad \psi(x, t<0) = \varphi_m(x)e^{-iE_m t/\hbar}$

For $t > \tau$ the system will be in a different state $\quad \psi(x, t>\tau) = \sum_n A_{nm}(\tau)\varphi_n(x)e^{-iE_n t/\hbar}$

wherein the probability that the system will be in a steady state of energy E_n is given by the transition probability at time τ from an initial state m to a state n.

$$w_{mn} = |A_{mn}(\tau)|^2$$

Functions $\varphi_n(x)$ are eigenstates of the Hamiltonian, i.e.: $H_0\varphi_n(x) = E_n^0\varphi_n(x)$

i.e. $H_0|n\rangle = E_n^0|n\rangle$

We have to compute: $i\hbar\frac{\partial}{\partial t}\psi(x,t)$

Time-dependent perturbation theory

Time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi = H_0 + V(t) \qquad \psi(x,t) = \sum_n A_n(t)\varphi_n(x)e^{-iE_nt/\hbar}$$

For $t < 0$ the system was in the initial state m $\qquad \psi(x,t<0) = \varphi_m(x)e^{-iE_mt/\hbar}$

For $t > \tau$ the system will be in a different state $\qquad \psi(x,t>\tau) = \sum_n A_{nm}(\tau)\varphi_n(x)e^{-iE_nt/\hbar}$

wherein the probability that the system will be in a steady state of energy E_n is given by the transition probability at time τ from an initial state m to a state n.

$$w_{mn} = |A_{mn}(\tau)|^2 \qquad \text{i.e. } H_0|n\rangle = E_n^0|n\rangle$$

We calculate coefficients A_{mn}.

$$i\hbar\frac{d}{dt}A_{ml}(t) = \sum_n \langle l|W(t)|n\rangle A_{mn}e^{+i\omega_{ln}t}$$

$$\langle l|W(t)|n\rangle = \int \varphi_l{}^* W(t)\varphi_n dx$$

$$\hbar\omega_{ln} = E_l - E_n$$

Time-dependent perturbation theory

Unfortunately, the exact solution of the equation is not possible

$$i\hbar \frac{d}{dt} A_{ml}(t) = \sum_n \langle l|W(t)|n\rangle A_{mn} e^{+i\omega_{ln}t} \qquad \langle l|W(t)|n\rangle = \int \varphi_l{}^* W(t) \varphi_n dx$$

We calculate coefficents A_{mn} iteratively $\qquad \hbar\omega_{ln} = E_l - E_n$

$$A_{ml}^{(0)}(t) = \langle l|\varphi_m(x)\rangle = \langle l|m\rangle = \delta_{lm}$$

$$i\hbar \frac{d}{dt} A_{ml}^{(j)}(t) = \sum_n \langle l|W(t)|n\rangle A_{mn}^{(j-1)} e^{+i\omega_{ln}t}$$

New solution

Previous solution

Odcałkowywujewujemy:

$$A_{ml}^{(1)}(t) = A_{ml}^{(0)}(0) + \frac{1}{i\hbar} \int_0^\tau \sum_n \langle l|W(t)|n\rangle A_{mn}^{(0)} e^{+i\omega_{ln}t}\, dt$$

$W(t)$ Is in the range of 0 to τ

Time-dependent perturbation theory

Unfortunately, the exact solution of the equation is not possible

$$i\hbar\frac{d}{dt}A_{ml}(t) = \sum_n \langle l|W(t)|n\rangle A_{mn}e^{+i\omega_{ln}t} \qquad \langle l|W(t)|n\rangle = \int \varphi_l{}^* W(t)\varphi_n dx$$

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$$= \delta_{lm} + \frac{1}{i\hbar}\int_0^\tau \sum_n \langle l|W(t)|n\rangle \delta_{mn}e^{+i\omega_{ln}t}\,dt = \delta_{lm} + \frac{1}{i\hbar}\int_0^\tau \langle l|W(t)|m\rangle e^{+i\omega_{lm}t}\,dt$$

Time-dependent perturbation theory

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$$i\hbar\frac{d}{dt}A_{ml}(t) = \sum_n \langle l|W(t)|n\rangle A_{mn}e^{+i\omega_{ln}t}$$

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$$i\hbar\frac{d}{dt}A_{ml}^{(j)}(t) = \sum_n \langle l|W(t)|n\rangle A_{mn}^{(j-1)}e^{+i\omega_{ln}t}$$

New solution

Only when the initial and final are the same. And we calculate the probability of transition to another state.

Odcałkowywujewujemy:

$$A_{ml}^{(1)}(t) = A_{ml}^{(0)}(0) + \frac{1}{i\hbar}\int_0^{\tau}\sum_n \langle l|W(t)|n\rangle A_{mn}^{(0)}e^{+i\omega_{ln}t}\,dt =$$

$$= \delta_{lm} + \frac{1}{i\hbar}\int_0^{\tau}\sum_n \langle l|W(t)|n\rangle \delta_{mn}e^{+i\omega_{ln}t}\,dt = \delta_{lm} + \frac{1}{i\hbar}\int_0^{\tau}\langle l|W(t)|m\rangle e^{+i\omega_{lm}t}\,dt$$

Time-dependent perturbation theory

Substitute into the equation, we consider the initial condition (see *Quantum Mechanics* S.A Dawydov)

$$w_{mn} = |A_{mn}(\tau)|^2 = \frac{1}{\hbar^2}\left|\int_0^\tau \langle m|W(t)|n\rangle e^{+i\omega_{mn}t}dt\right|^2$$

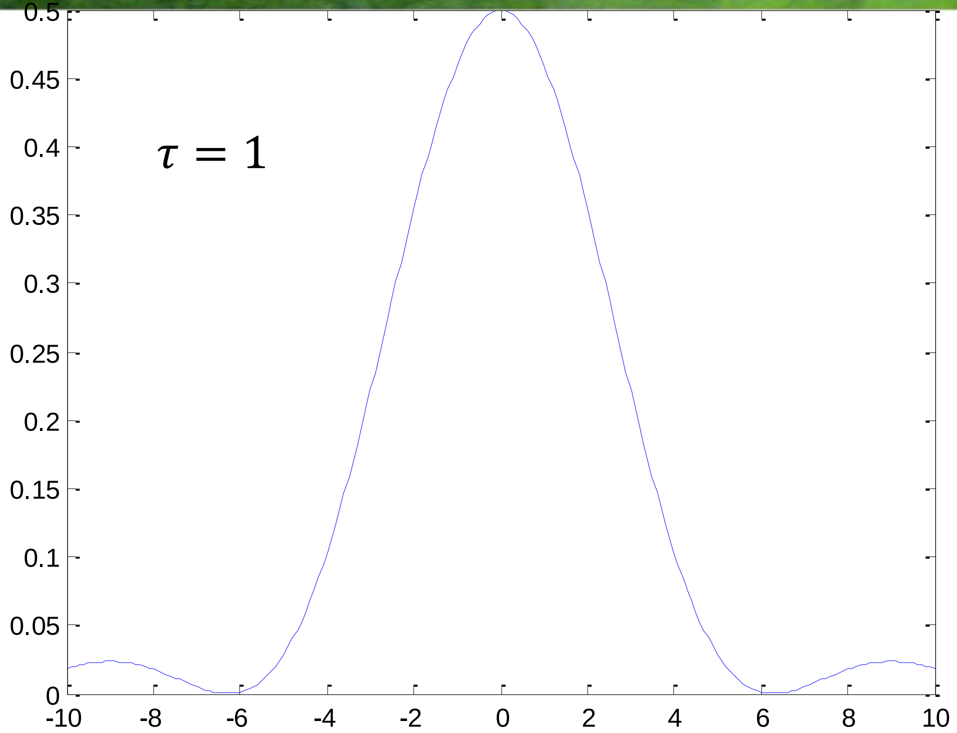
When $W(t) = const = W$ for $0 \le t \le \tau$ it is easy to obtain:

$$\int_0^\tau \langle n|W(t)|l\rangle e^{i\omega_{nl}t}dt = \frac{e^{i\omega_{nl}\tau} - 1}{i\omega_{nl}}\langle n|W|l\rangle$$

Then the corresponding probability of transition under perturbation is given by

$$w_{mn} = |A_{mn}(\tau)|^2 = \frac{2}{\hbar^2}|\langle m|W|n\rangle|^2 \; \frac{1 - \cos\left[(E_n - E_m)\frac{\tau}{\hbar}\right]}{\left[(E_n - E_m)\frac{1}{\hbar}\right]^2}$$

Time-dependent perturbation theory



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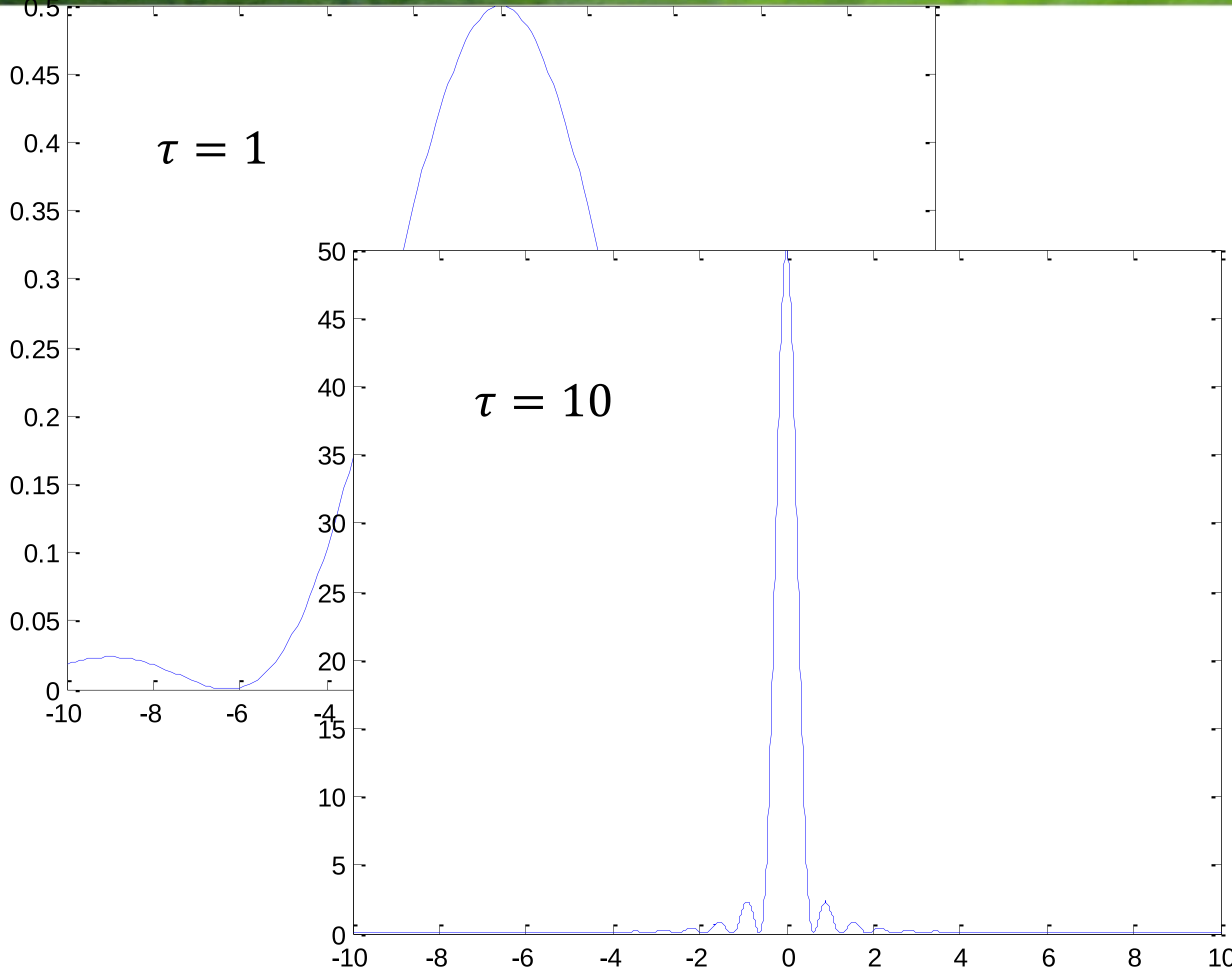
Time-dependent perturbation theory



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Time-dependent perturbation theory

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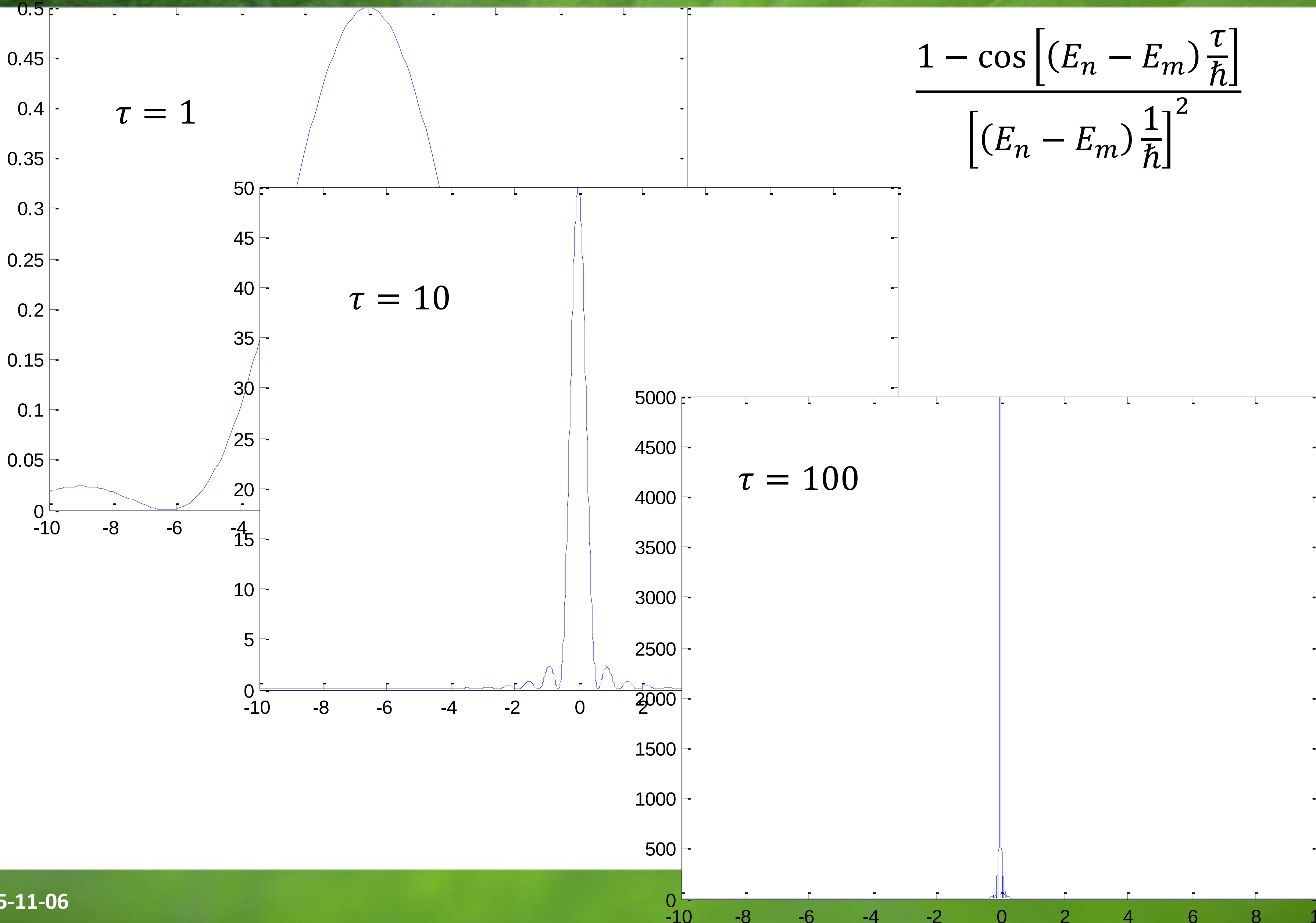

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$$w_{mn} = |A_{mn}(\tau)|^2 = \frac{1}{\hbar^2}\left|\int_0^{\tau} \langle m|W(t)|n\rangle e^{+i\omega_{mn}t} dt\right|^2$$

When $W(t) = const = W$ for $0 \leq t \leq \tau$ it is easy to obtain:

$$\int_0^{\tau} \langle n|W(t)|l\rangle e^{i\omega_{nl}t} dt = \frac{e^{i\omega_{nl}\tau} - 1}{i\omega_{nl}} \langle n|W|l\rangle$$

Then the corresponding probability of transition under perturbation is given by

$$w_{mn} = |A_{mn}(\tau)|^2 = \frac{2}{\hbar^2} |\langle m|W|n\rangle|^2 \; \frac{1 - \cos\left[(E_n - E_m)\frac{\tau}{\hbar}\right]}{\left[(E_n - E_m)\frac{1}{\hbar}\right]^2}$$

For $\tau \gg \dfrac{\hbar}{E_n - E_m}$

$$\frac{1 - \cos\left[(E_n - E_m)\frac{\tau}{\hbar}\right]}{\left[(E_n - E_m)\frac{1}{\hbar}\right]^2} \approx \tau\pi\hbar\delta(E_n - E_m)$$

Time-dependent perturbation theory

Finally, the probability of transition

$$w_{mn} = \frac{2\pi}{\hbar} |\langle m|W|n\rangle|^2 \tau \delta(E_m - E_n)$$

The probability of transitions is proportional to the perturbation time, so the probability of transition per unit time is given by:

$$P_{mn} = \frac{w_{mn}}{\tau} = \frac{2\pi}{\hbar} |\langle m|W|n\rangle|^2 \delta(E_m - E_n)$$

Time-dependent perturbation theory

If the perturbation is in the form of a **periodic wave** we back to the general formula:

$$w_{nm} = |A_{nm}(\tau)|^2 = \frac{1}{\hbar^2}\left|\int_0^\tau \langle n|W(t)|m\rangle e^{+i\omega_{nm}t}dt\right|^2$$

for the case where $W(t) = w^{\pm}e^{\pm i\omega t}$ for $0 \le t \le \tau$ it is easy to calculate:

$$\int_0^\tau \langle n|w^{\pm}|l\rangle e^{i(\omega_{nl}\pm\omega)t}dt = \frac{e^{i(\omega_{nl}\pm\omega)\tau} - 1}{i(\omega_{nl}\pm\omega)}\langle n|w^{\pm}|l\rangle$$

Transition probability:

$$w_{nm} = \frac{2\pi}{\hbar}\left|\langle n|w^{\pm}|m\rangle\right|^2 \tau\delta(E_n - E_m \pm \hbar\omega)$$

Transition probability per unit time:

$$P_{nm} = \frac{w_{nm}}{\tau} = \frac{2\pi}{\hbar}\left|\langle n|w^{\pm}|m\rangle\right|^2 \delta(E_n - E_m \pm \hbar\omega)$$

Time-dependent perturbation theory

Conclusions:

$$W(t) = w^{\pm} e^{\pm i\omega t}$$
$$0 \leq t \leq \tau$$

$$\boxed{P_{nm} = \frac{w_{nm}}{\tau} = \frac{2\pi}{\hbar} \left| \langle n | w^{\pm} | m \rangle \right|^2 \delta(E_n - E_m \pm \hbar\omega)}$$

The transitions are possible only for states $E_m = E_n \pm \hbar\omega$

The system can either gain energy (absorbs) or lose (emits).

Electromagnetic wave

The perturbation in a form of an electromagnetic wave.

$$\boxed{P_{nm} = \frac{w_{nm}}{\tau} = \frac{2\pi}{\hbar}\left|\langle n|w^{\pm}|m\rangle\right|^2 \delta(E_n - E_m \pm \hbar\omega)}$$

General form of the hamiltonian in the electromagnetic field is given by tha vector potential A and scalar φ:

$$H = \frac{1}{2m}\left(\vec{p} + e\vec{A}\right)^2 - e\varphi + V$$

Assuming suitable gauging (pol: „cechowanie”) $\varphi = 0$, div$A=0$ and neglecting terms with A^2 (low radiation, etc.)

$$H \approx \frac{e}{m}\vec{A}\vec{p}$$

Vector potential for an electromagnetic wave may be introduced in the form :

$$\vec{A} = \overrightarrow{A_0}\left\{e^{-i(\omega t - \vec{k}\vec{r})} + e^{i(\omega t - \vec{k}\vec{r})}\right\}$$

$$\vec{E} = -\nabla\varphi - \frac{\partial\vec{A}}{\partial t} \qquad \vec{E} = 2\omega\overrightarrow{A_0}\sin(\omega t - \vec{k}\vec{r})$$

$$\vec{B} = \nabla \times \vec{A} \qquad \vec{B} = 2(\vec{k} \times \overrightarrow{A_0})\sin(\omega t - \vec{k}\vec{r})$$

Electromagnetic wave

The perturbation in a form of an electromagnetic wave.

$$H \approx \frac{e}{m}\vec{A}\vec{p}$$

$$\boxed{P_{nm} = \frac{w_{nm}}{\tau} = \frac{2\pi}{\hbar}\left|\langle n|w^{\pm}|m\rangle\right|^2 \delta(E_n - E_m \pm \hbar\omega)}$$

$$\vec{A} = \overrightarrow{A_0}\left\{e^{-i(\omega t - \vec{k}\vec{r})} + e^{i(\omega t - \vec{k}\vec{r})}\right\}$$

expanding a series $\quad \vec{p}\, e^{-i(\vec{k}\vec{r})} \approx \vec{p}\left[1 + \left(-i\vec{k}\vec{r}\right) + \frac{\left(-i\vec{k}\vec{r}\right)^2}{2!} + \cdots\right]$

We use the commutation rules $\quad [\vec{r}, H_0\,] = \vec{r}H_0 - H_0\vec{r} = \frac{i\hbar}{m}\vec{p}$

we get $\quad \langle n|\vec{p}|m\rangle = im\omega_{nm}\langle n|\vec{r}|m\rangle$

Subsequent terms in this expansion give: dipole magnetic transitions, quadrupole electric transitions etc.

Electromagnetic wave

The perturbation in a form of an electromagnetic wave.

$$H \approx \frac{e}{m}\vec{A}\vec{p}$$

$$\boxed{P_{nm} = \frac{w_{nm}}{\tau} = \frac{2\pi}{\hbar}\left|\langle n|w^{\pm}|m\rangle\right|^{2}\delta(E_n - E_m \pm \hbar\omega)}$$

$$\vec{A} = \overrightarrow{A_0}\left\{e^{-i(\omega t-\vec{k}\vec{r})} + e^{i(\omega t-\vec{k}\vec{r})}\right\}$$

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after laborious calculations we get the probability of emission of electromagnetic radiation dipole (described by the operator $e\vec{r}$)

$$\boxed{A_{nm} = \frac{w_{nm}}{\tau} = \frac{{\omega_{nm}}^3 e^2}{3\pi\varepsilon_0\hbar c^3}|\langle n|\vec{r}|m\rangle|^2 = \frac{4\alpha}{3}\frac{{\omega_{nm}}^3}{c^2}|\langle n|\vec{r}|m\rangle|^2} \qquad \alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx \frac{1}{137}$$

It is one of the **Einstein coefficients** (lasers, etc. - next week!) for nondegenerated states.

Electromagnetic wave

The perturbation in a form of an electromagnetic wave.

$$\boxed{A_{nm} = \frac{{\omega_{nm}}^3 e^2}{3\pi\varepsilon_0 \hbar c^3} |\langle m|\vec{r}|n\rangle|^2 = \frac{4\alpha}{3}\frac{{\omega_{nm}}^3}{c^2} |\langle m|\vec{r}|n\rangle|^2}$$

In the case o degenerated states we introduce „oscillator strength”

$$A_{nm} = \frac{4\alpha}{3}\frac{{\omega_{nm}}^3}{c^2}\frac{S_{mn}}{g_m} \qquad S_{nm} = \sum_i \sum_j \left|\langle n_i|\vec{r}|m_j\rangle\right|^2$$

the degeneracy of the initial state

In the case of the hydrogen atom states it is convenient to represent operator $\vec{r}$ in the circular form:

$$\left|\langle n_i|\vec{r}|m_j\rangle\right|^2 = \left|\langle n_i|z|m_j\rangle\right|^2 + \frac{1}{2}\left|\langle n_i|x+iy|m_j\rangle\right|^2 + \frac{1}{2}\left|\langle n_i|x-iy|m_j\rangle\right|^2$$

it is easy to then integrate spherical harmonics, because:

$$z = r\cos\vartheta$$

$$x \pm iy = re^{\pm i\varphi}\sin\vartheta$$

Check it!

Electromagnetic wave

Some final remarks

$$A_{nm} = \frac{4\alpha}{3}\frac{{\omega_{nm}}^3}{c^2}\frac{S_{mn}}{g_m} \qquad\qquad S_{nm} = \sum_i \sum_j \left|\langle n_i|\vec{r}|m_j\rangle\right|^2$$

By calculating the Einstein coefficients of eg. the hydrogen atom, we can get the so called **optical transitions selection rules** , eg. for hydrogen:

$\Delta l = \pm 1$ momentum conservation rule – the photon has an integer spin

$\Delta m = \pm 1$ transition in circular polarization σ

$\Delta m = 0$ transition in linear polarization π

Optical transitions are possible only between atomic levels of **different symmetry**, since the operator $\vec{r}$ is antisymmetric

Electromagnetic wave

Some final remarks

$$A_{nm} = \frac{4\alpha}{3}\frac{{\omega_{nm}}^3}{c^2}\frac{S_{mn}}{g_m}$$

$$S_{nm} = \sum_i \sum_j \left|\langle n_i|\vec{r}|m_j\rangle\right|^2$$

We can introduce *radiative recombination rate* (recombination lifetime) τ_{mn}

$$\tau_{nm} = \frac{1}{A_{nm}}$$

czas życia

In the case of dipole optical transition this lifetime is of the order of nanoseconds.

The power of the optical transition $P_{nm} = A_{nm}\hbar\,\omega_{nm}$

Summary –Fermi golden rule

The probability of transition per unit time:

$$W(t) = W$$
$$0 \leq t \leq \tau$$

$$\boxed{P_{mn} = \frac{w_{mn}}{\tau} = \frac{2\pi}{\hbar}|\langle m|W|n\rangle|^2 \delta(E_m - E_n)}$$

Transitions are possible only for states, for which $E_m = E_n$

$$W(t) = w^{\pm}e^{\pm i\omega t}$$
$$0 \leq t \leq \tau$$

$$\boxed{P_{nm} = \frac{w_{nm}}{\tau} = \frac{2\pi}{\hbar}\left|\langle n|w^{\pm}|m\rangle\right|^2 \delta(E_n - E_m \pm \hbar\omega)}$$

Transitions are possible only for states, for which $E_m = E_n \pm \hbar\omega$

The perturbation in a form of an electromagnetic wave:

$$\boxed{A_{nm} = \frac{{\omega_{nm}}^3 e^2}{3\pi\varepsilon_0\hbar c^3}|\langle m|\vec{r}|n\rangle|^2 = \frac{4\alpha}{3}\frac{{\omega_{nm}}^3}{c^2}|\langle m|\vec{r}|n\rangle|^2}$$

$$\boxed{P_{nm} = A_{nm}\delta(E_n - E_m \pm \hbar\omega)}$$

Summary –Fermi golden rule

The transition rate – the probability of transition per unit time – from the initial state $|i\rangle$ to final $|f\rangle$ is given by:

Szybkość zmian – czyli prawdopodobieństwo przejścia na jednostkę czasu – ze stanu początkowego $|i\rangle$ do końcowego $|f\rangle$ dane jest wzorem:

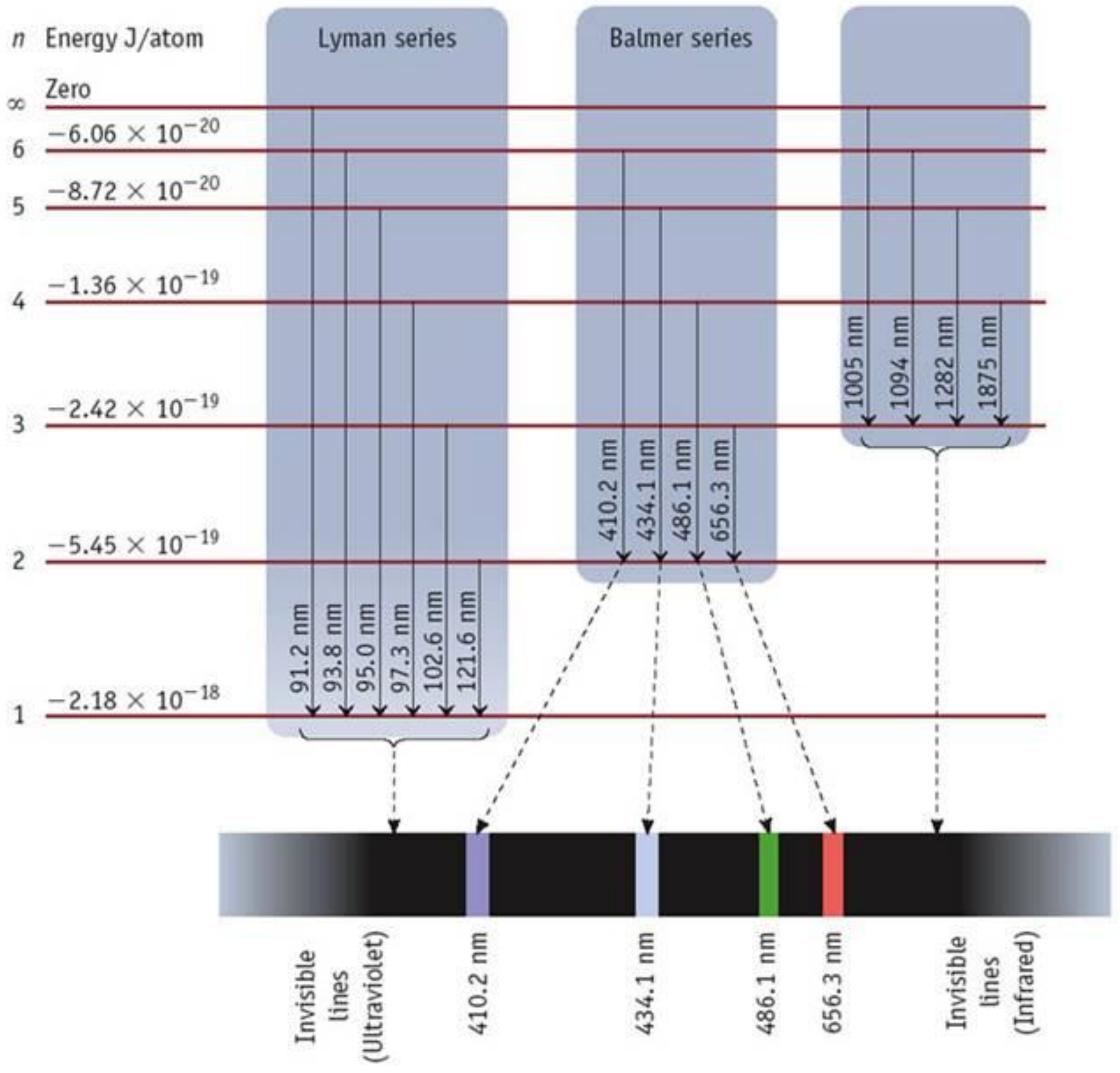
$$\boxed{P_{mn} = \frac{2\pi}{\hbar}|\langle f|W|i\rangle|^2 \rho(E_f)}$$

W - interaction with the field

$\rho(E_f)$ - the density of final states

Perturbation W does not have to be in the form of an electromagnetic wave.

Summary –Fermi golden rule



Hydrogen

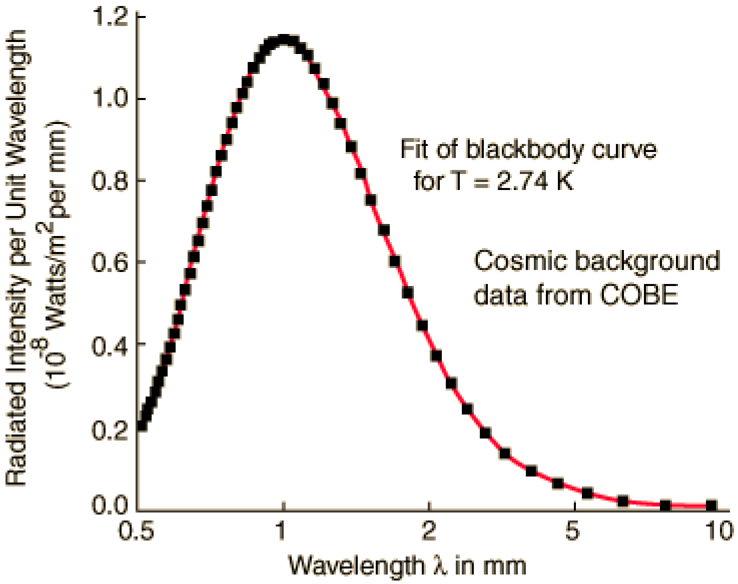
$$A_{nm} = \frac{4\alpha}{3}\frac{{\omega_{nm}}^3}{c^2}|\langle m|\vec{r}|n\rangle|^2$$

$$P_{nm} = A_{nm}\delta(E_n - E_m \pm \hbar\omega)$$

The history

- In the XIX century: the matter is granular, the energy (mostly e-m) is a wave

- Problems NOT solved
  - Black body radiation
  - Photoelectric effect
  - Origin of spectral lines of atoms



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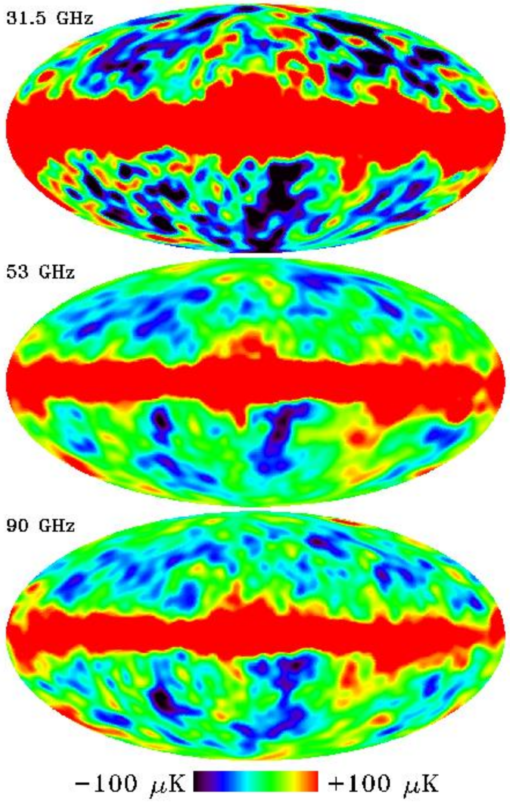
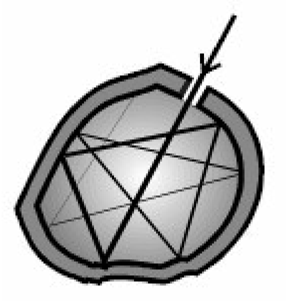


Ultraviolet catastrophe

Rayleigh–Jeans law



Rozkład widmowy ciała doskonale czarnego:

Classically – The theorem of equipartition of energy: average energy of the standing wave is independent of frequency $\langle E \rangle = kT$
Energy density ρ amount waves of a particular frequency range $\nu \, d\nu$ times the average energy $\langle E \rangle$, divided by the volume of the cavity:

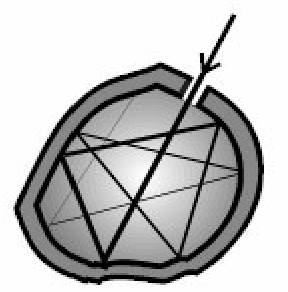
$$\rho(\nu, T)d\nu = \frac{8\pi\nu^2}{c^3} kTd\nu$$

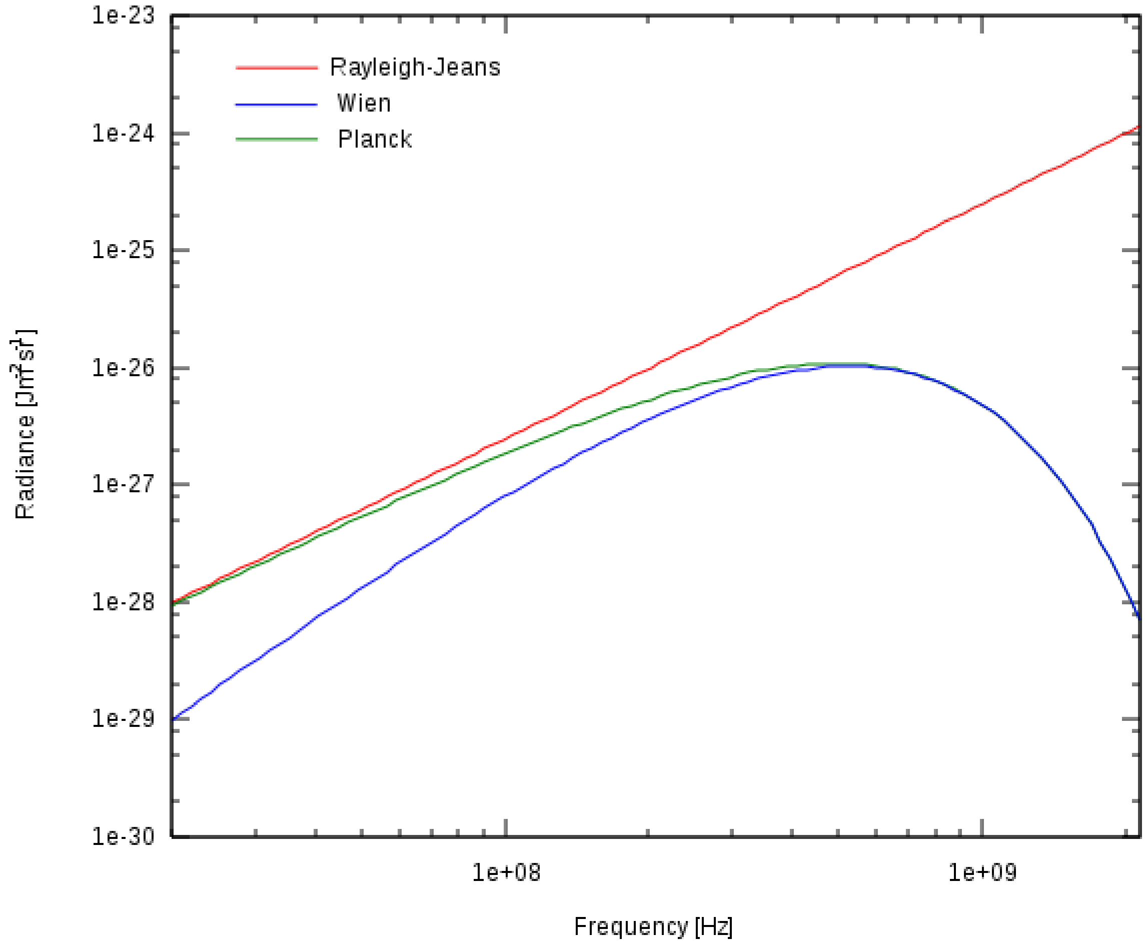
The total radiation energy density at a given temperature is given by the sum of all frequencies:

$$\rho(T) = \int_0^\infty \rho(\nu, T)d\nu = \frac{8\pi}{c^3} kT \int_0^\infty \nu^2 \, d\nu = \infty$$

Ultraviolet catastrophe

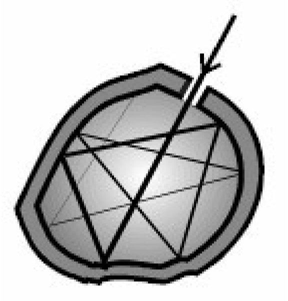
Rayleigh–Jeans law

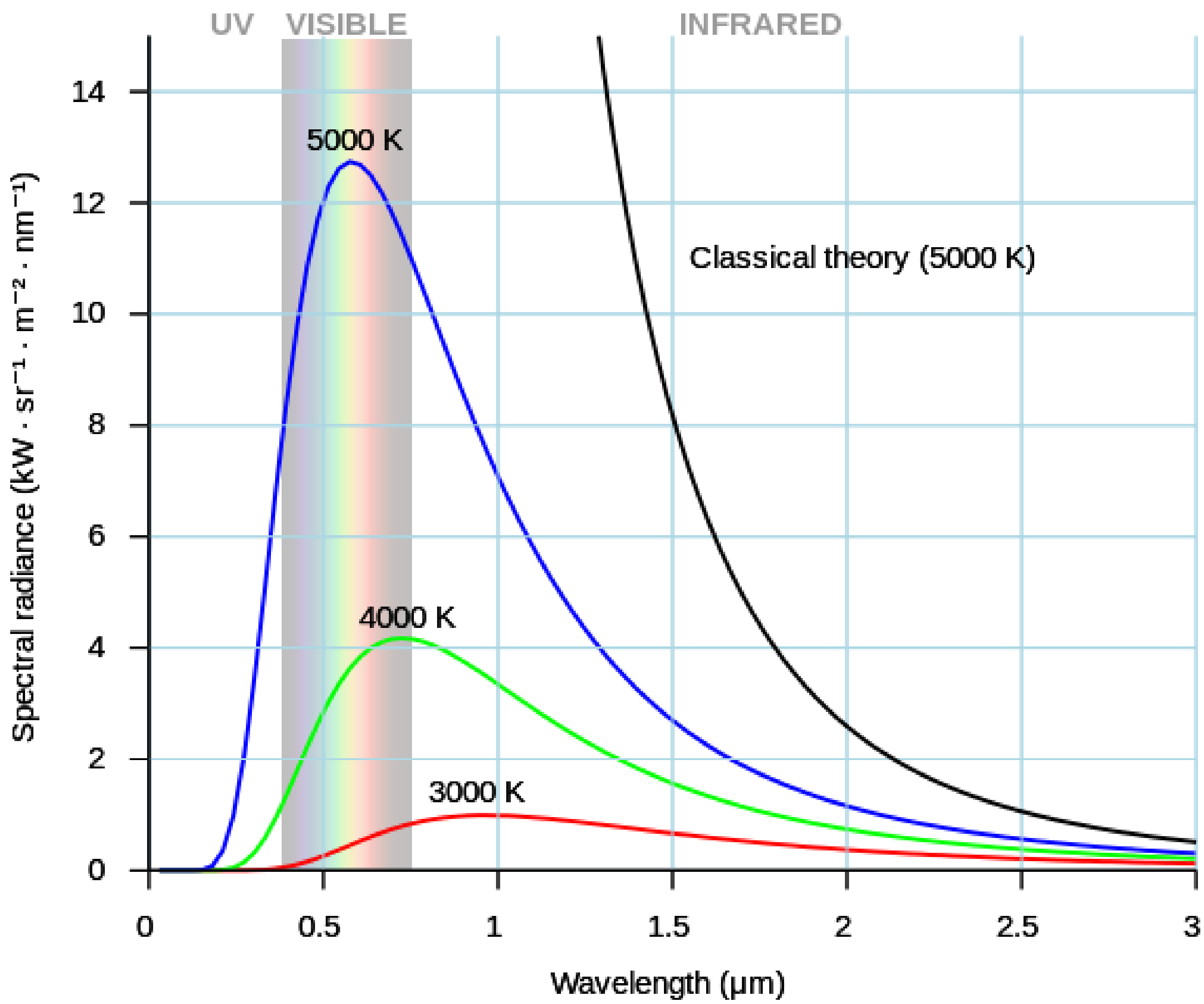




Ultraviolet catastrophe

Rayleigh–Jeans law





https://en.wikipedia.org/wiki/Ultraviolet_catastrophe#/media/File:Black_body.svg

The history

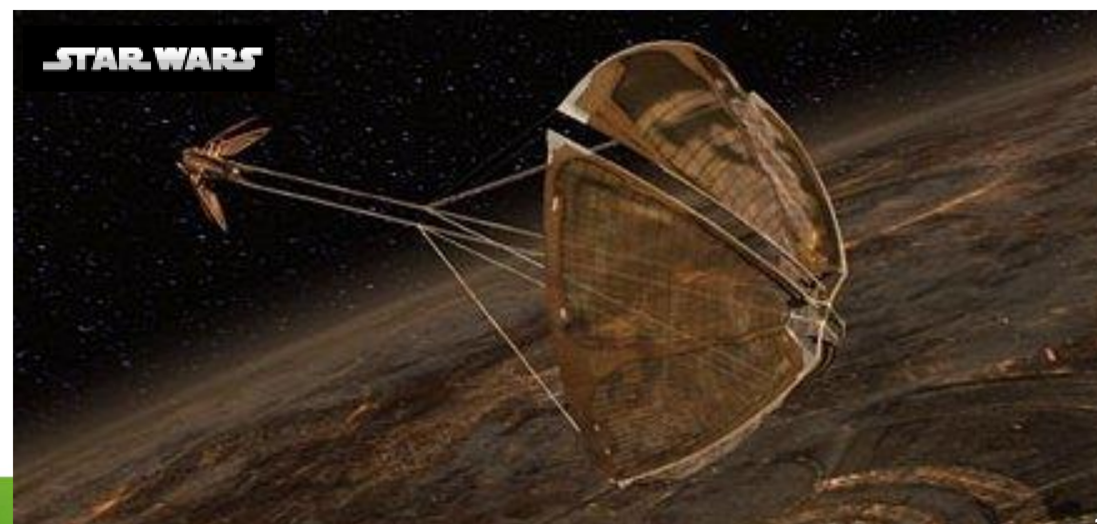
- In the XX century: the matter is (also) a wave and the energy is (also) granular (corpuscular)
- Solved problems:
  - Black body radiation spectrum (Planck 1900, Nobel 1918)
  - Photoelectric effect (Einstein 1905, Nobel 1922)
  - Origin of spectral lines of atoms (Bohr 1913, Nobel 1922)

$\boxed{p = h / \lambda}$

- *Photons* – *energy:* $E = h\nu$ (h = 6.626×10^{-32} J s = 4.136×10^{-15} eV s)

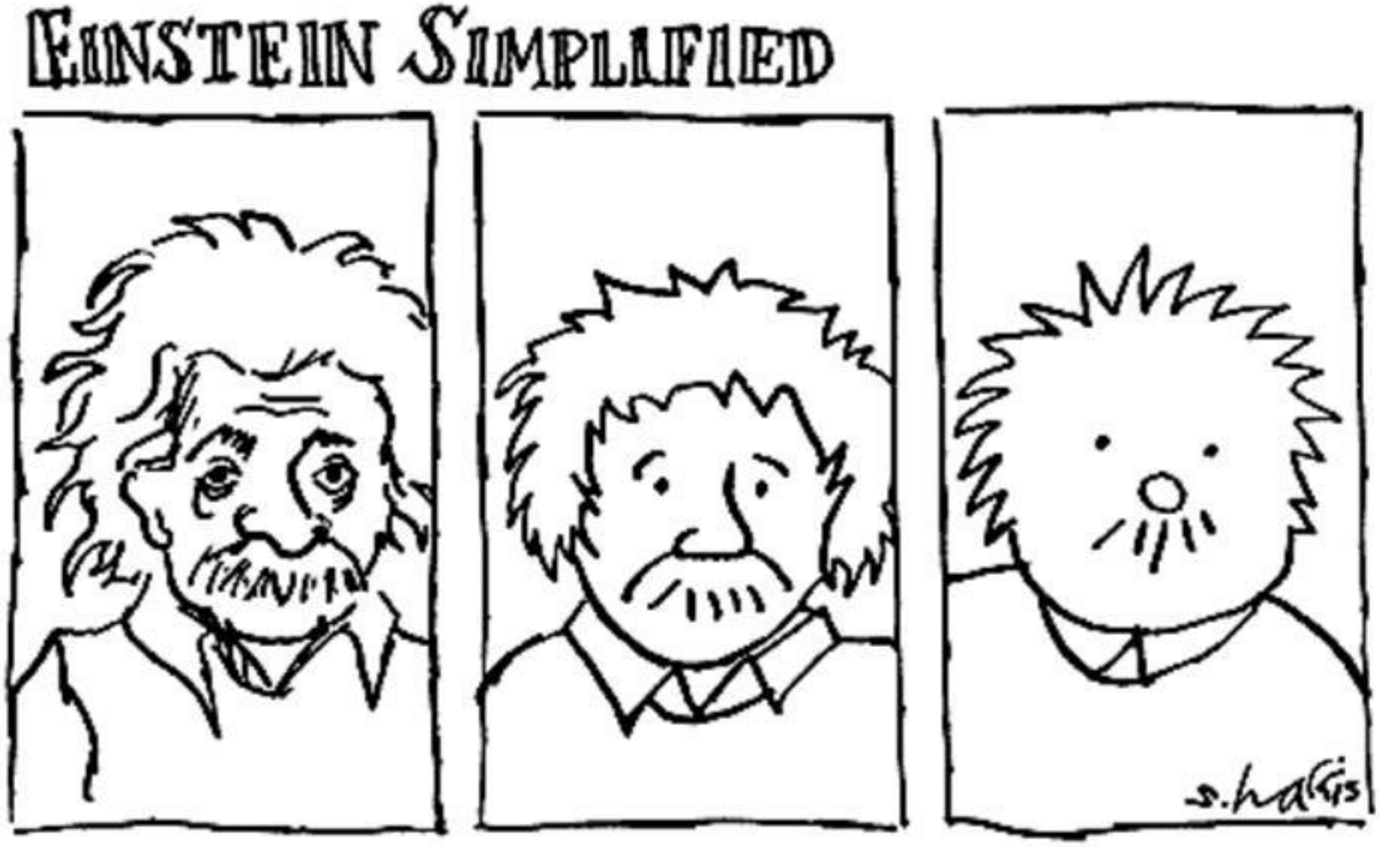
  – momentum: $p = E / c = h / \lambda$

Count Dooku's Geonosian solar sailer



light mill - **Crookes radiometer**

Derivation of Planck's law. Lasers.



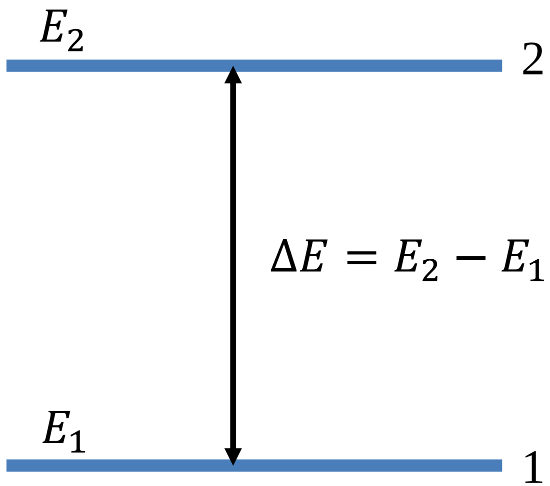
S. Harris

Everything should be made as simple as possible, but not simpler

Albert Einstein

The spontaneous and stimulated emission

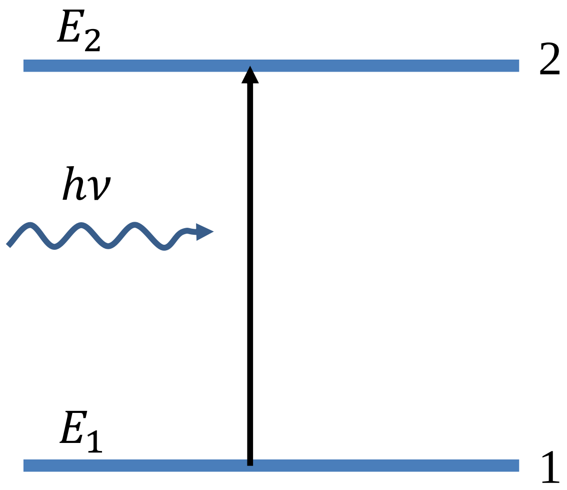
Let's consider the transition between two states



What are the parameters describing the number of transitions from the state 1 to 2 and vice versa?

The spontaneous and stimulated emission

Let's consider the transition between two states



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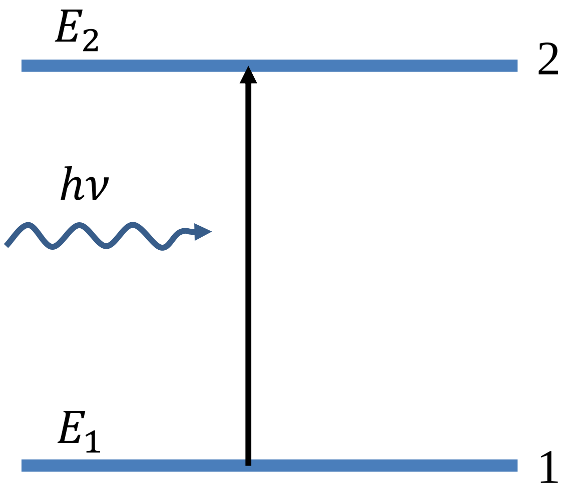
$\hbar\omega = h\nu = E_2 - E_1$

1. Absorption

The spontaneous and stimulated emission

Let's consider the transition between two states



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$$\hbar\omega = h\nu = E_2 - E_1$$

1. Absorption

the number of transitions

$$\left(\frac{dN}{dt}\right)_{abs} = N_1 B_{12} \rho$$

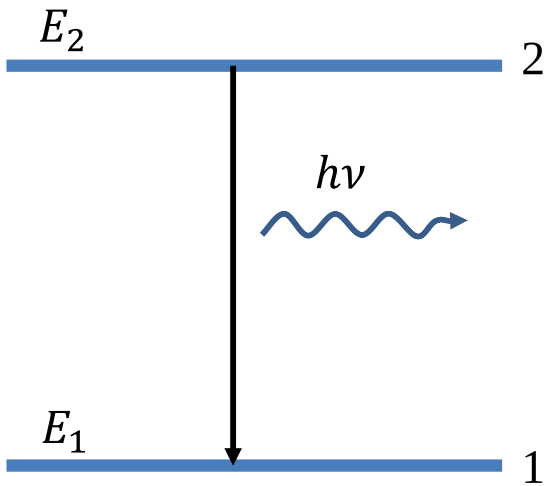
The number of availabale states

The proportionality factor

Radiation energy density

The spontaneous and stimulated emission

Let's consider the transition between two states



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The spontaneous and stimulated emission

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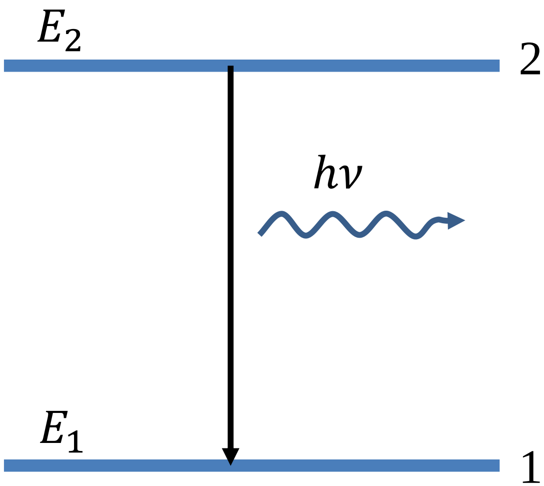

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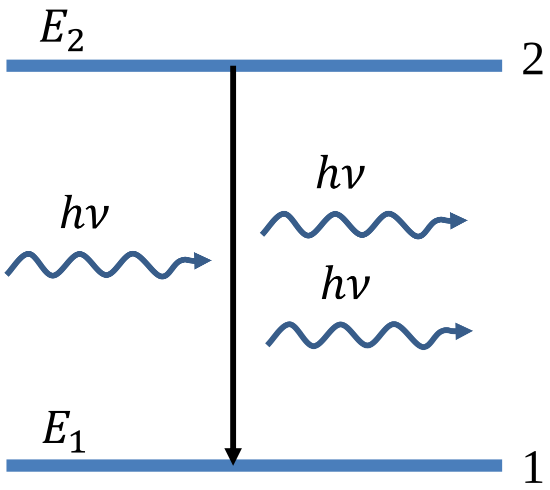

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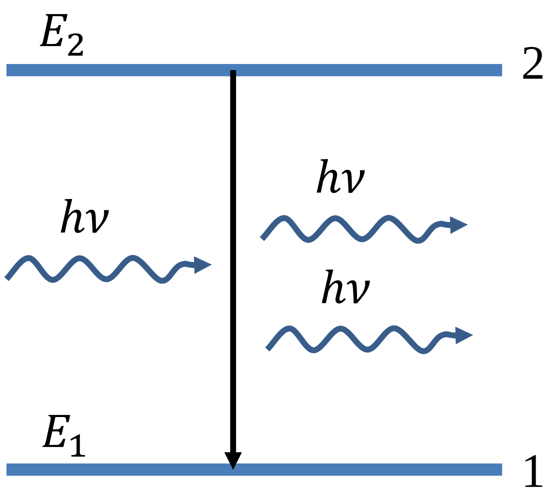
3. Stimulated emission

The spontaneous and stimulated emission

Let's consider the transition between two states



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1. Absorption

$$\left(\frac{dN}{dt}\right)_{abs} = N_1 B_{12}\rho$$

2. Spontaneous emission

$$\left(\frac{dN}{dt}\right)_{spon} = AN_2$$

3. Stimulated emission

$$\left(\frac{dN}{dt}\right)_{wym} = N_2 B_{21}\rho$$

the number of transitions

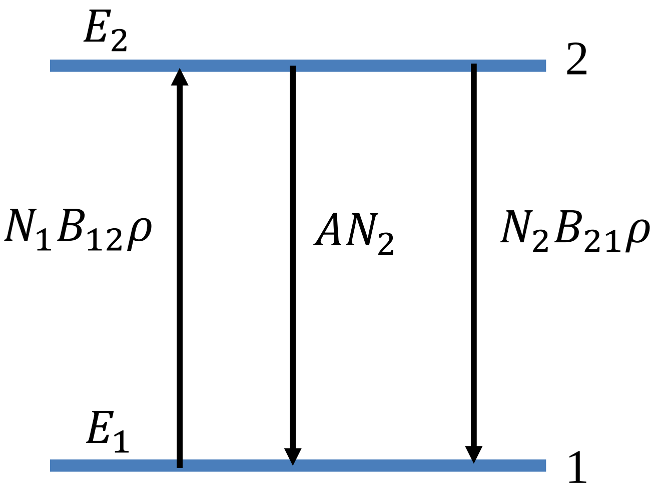
The number of availabale states

The proportionality factor

Radiation energy density

The spontaneous and stimulated emission

Let's consider the transition between two states



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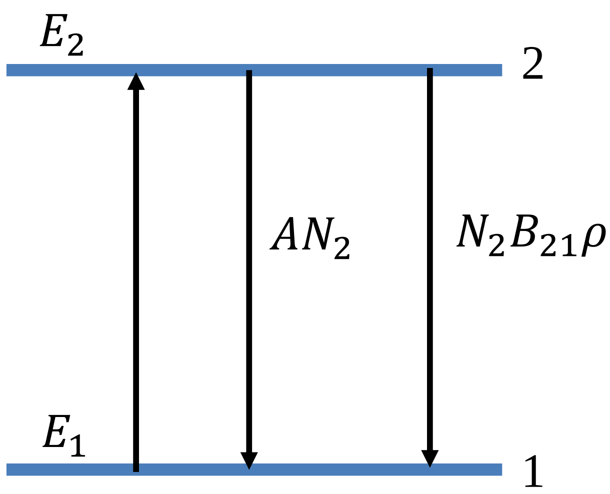


$$\left(\frac{dN}{dt}\right)_{abs} = N_1 B_{12} \rho$$

$$\left(\frac{dN}{dt}\right)_{spon} = AN_2$$

$$\left(\frac{dN}{dt}\right)_{wym} = N_2 B_{21} \rho$$

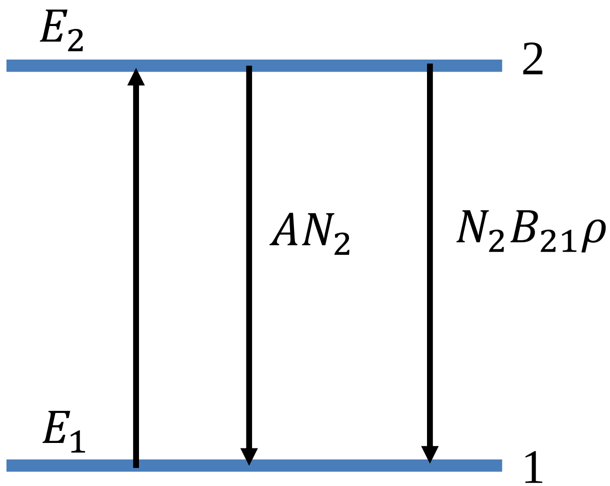
In thermal equilibrium conditions (a necessary condition, but it is also true in states far from equilibrium, eg. in lasers!)

$$\left(\frac{dN}{dt}\right)_{abs} = \left(\frac{dN}{dt}\right)_{spon} + \left(\frac{dN}{dt}\right)_{wym}$$

$$N_1 B_{12} \rho = AN_2 + N_2 B_{21} \rho$$

The spontaneous and stimulated emission

Let's consider the transition between two states



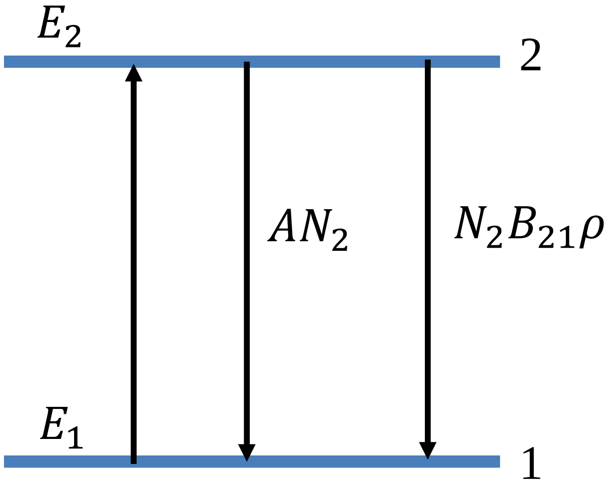
$$N_1B_{12}\rho = AN_2 + N_2B_{21}\rho$$

$$\rho = \frac{A}{B_{21}} \times \frac{1}{\frac{N_1B_{12}}{N_2B_{21}} - 1}$$

The occupations of N_1 and N_2 in thermal equilibrium conditions are given by Boltzman distribution

The spontaneous and stimulated emission

Let's consider the transition between two states



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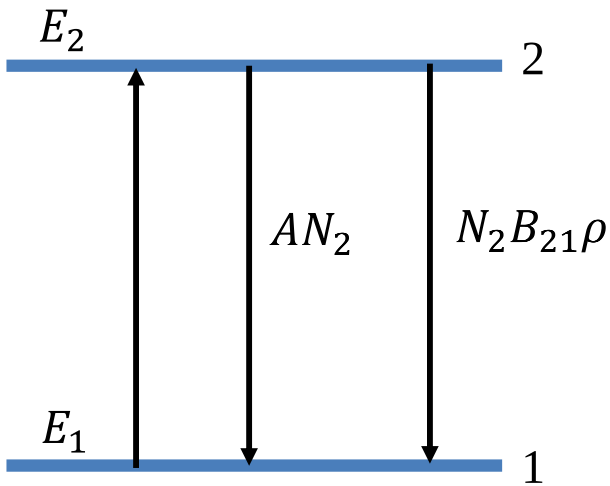
$$N_1 = \mathrm{const}\, e^{-\frac{E_1}{kT}} \qquad N_2 = \mathrm{const}\, e^{-\frac{E_2}{kT}} \qquad \frac{N_1}{N_2} = e^{-\frac{(E_1 - E_2)}{kT}} = e^{\frac{h\nu}{kT}}$$

What happens with ρ when $T \to \infty$?

The spontaneous and stimulated emission

Let's consider the transition between two states



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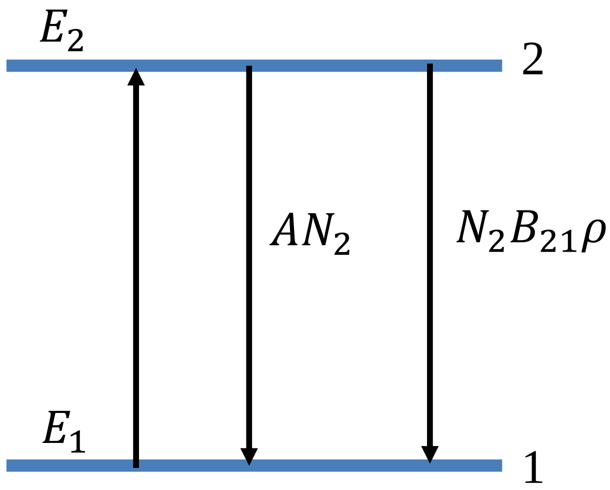
What happens with ρ when $T \to \infty$? $\quad B_{12} = B_{21}$

Considering the degree of the degeneracy of levels $\quad g_{12}B_{12} = g_{21}B_{21}$

The spontaneous and stimulated emission

Let's consider the transition between two states



$$\rho(\nu,T) = \frac{A}{B_{21}} \times \frac{1}{\frac{N_1B_{12}}{N_2B_{21}} - 1} = \frac{A}{B} \times \frac{1}{\exp\left(\frac{h\nu}{kT}\right) - 1}$$

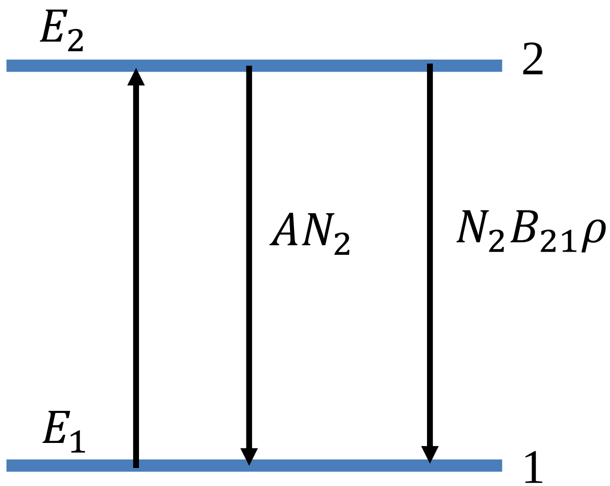
In turn, for $h\nu \ll kT$ we have Reileigh-Jeans law

$$\rho(\nu,T)d\nu = \frac{8\pi\nu^2}{c^3}kTd\nu$$

Expanding the exponential function

The spontaneous and stimulated emission

Let’s consider the transition between two states



$$\rho(\nu,T)=\frac{A}{B_{21}}\times\frac{1}{\frac{N_1B_{12}}{N_2B_{21}}-1}=\frac{A}{B}\times\frac{1}{\exp\left(\frac{h\nu}{kT}\right)-1}$$

In turn, for $h\nu \ll kT$ we have Reileigh-Jeans law

$$\rho(\nu,T)d\nu=\frac{8\pi\nu^2}{c^3}kTd\nu$$

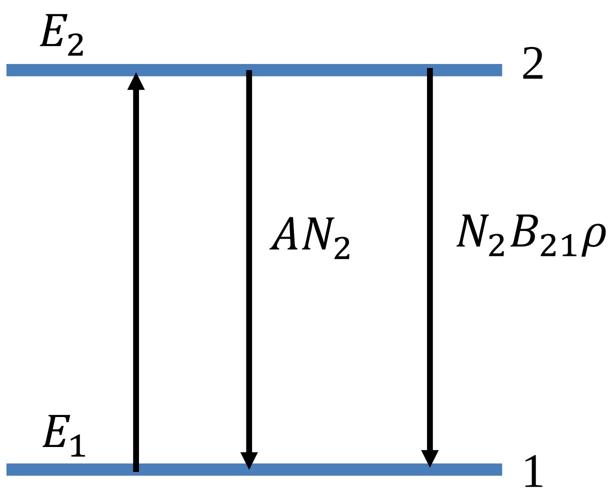
Expanding the exponential function $\rho(\nu,T)\approx\frac{A}{B}kT/h\nu$

Thus: $$\frac{A}{B}=\frac{8\pi}{c^3}h\nu^3=D(\nu)h\nu$$

The amount of radiation modes in a given volume

The spontaneous and stimulated emission

Let's consider the transition between two states



$$\rho(\nu, T) = \frac{1}{\exp\left(\frac{h\nu}{kT}\right) - 1} \frac{8\pi\nu^2}{c^3} h\nu$$

Planck equation

A and B are **Einstein coefficients**. Units of A:

$$\left(\frac{dN}{dt}\right)_{spon} = AN_2 \Rightarrow A = \frac{1}{\tau}$$

and: $B = [\tau D(\nu) h\nu]^{-1}$

Electromagnetic wave

The perturbation in a form of an electromagnetic wave.

$$H \approx \frac{e}{m}\vec{A}\vec{p}$$

$$\boxed{P_{nm} = \frac{w_{nm}}{\tau} = \frac{2\pi}{\hbar}\left|\langle n|w^{\pm}|m\rangle\right|^2 \delta(E_n - E_m \pm \hbar\omega)}$$

$$\vec{A} = \overrightarrow{A_0}\left\{e^{-i(\omega t - \vec{k}\vec{r})} + e^{i(\omega t - \vec{k}\vec{r})}\right\}$$

expanding a series $\vec{p}\, e^{-i(\vec{k}\vec{r})} \approx \vec{p}\left[1 + \left(-i\vec{k}\vec{r}\right) + \frac{\left(-i\vec{k}\vec{r}\right)^2}{2!} + \cdots\right]$

after laborious calculations we get the probability of emission of electromagnetic radiation dipole (described by the operator $e\vec{r}$)

$$\boxed{A_{nm} = \frac{w_{nm}}{\tau} = \frac{{\omega_{nm}}^3 e^2}{3\pi\varepsilon_0\hbar c^3}|\langle n|\vec{r}|m\rangle|^2 = \frac{4\alpha}{3}\frac{{\omega_{nm}}^3}{c^2}|\langle n|\vec{r}|m\rangle|^2} \qquad \alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx \frac{1}{137}$$

It is one of the **Einstein coefficients** (lasers, etc. - next week!) for nondegenerated states.

Fala elektromagnetyczna

The perturbation in a form of an electromagnetic wave.

$$\boxed{A_{nm} = \frac{{\omega_{nm}}^3 e^2}{3\pi\varepsilon_0 \hbar c^3} |\langle m|\vec{r}|n\rangle|^2 = \frac{4\alpha}{3}\frac{{\omega_{nm}}^3}{c^2} |\langle m|\vec{r}|n\rangle|^2}$$

In the case o degenerated states we introduce „oscillator strength”

$$A_{nm} = \frac{4\alpha}{3}\frac{{\omega_{nm}}^3}{c^2}\frac{S_{mn}}{g_m} \qquad S_{nm} = \sum_i \sum_j \left|\langle n_i|\vec{r}|m_j\rangle\right|^2$$

the degeneracy of the initial state

In the case of the hydrogen atom states it is convenient to represent operator $\vec{r}$ in the circular form:

$$\left|\langle n_i|\vec{r}|m_j\rangle\right|^2 = \left|\langle n_i|z|m_j\rangle\right|^2 + \frac{1}{2}\left|\langle n_i|x+iy|m_j\rangle\right|^2 + \frac{1}{2}\left|\langle n_i|x-iy|m_j\rangle\right|^2$$

it is easy to then integrate spherical harmonics, because:

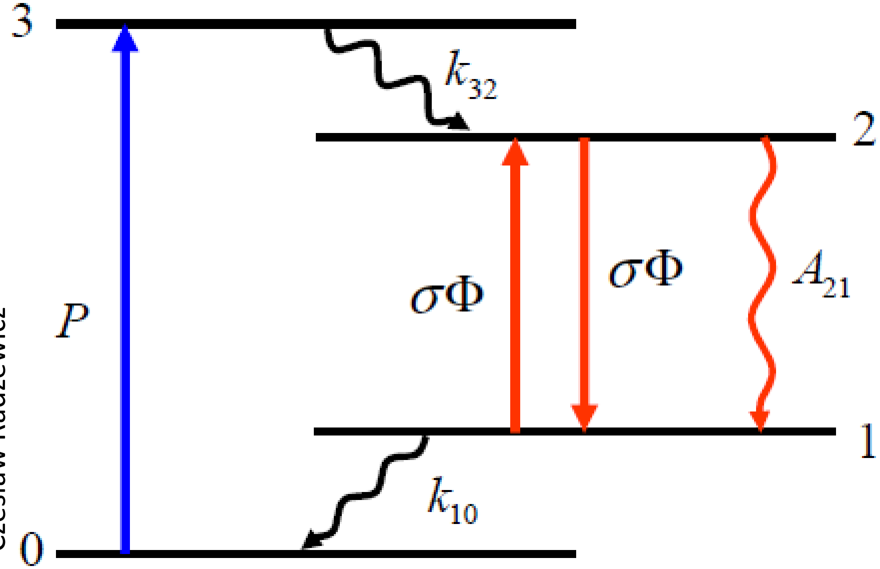
$$z = r\cos\vartheta$$

$$x \pm iy = re^{\pm i\varphi}\sin\vartheta$$

Check it!

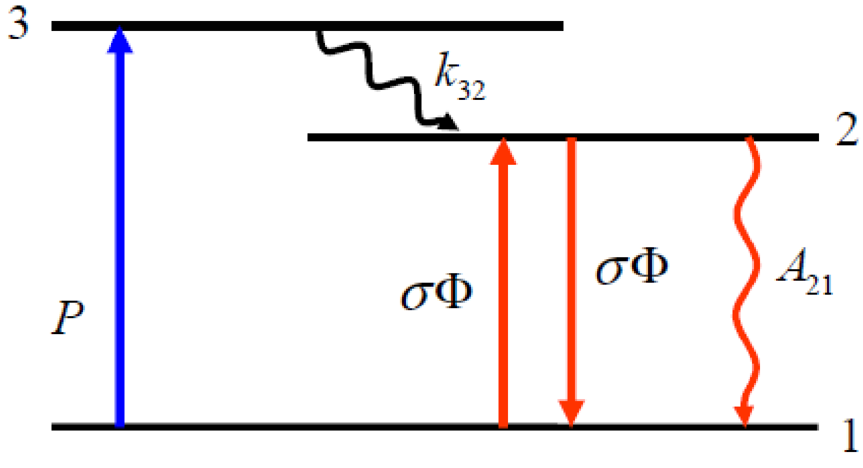
Fala elektromagnetyczna

Laser needs minimum 3 states



Czesław Radzewicz

Rzadko stosowany laser 3-poziomowy



Derivation of Planck's law. Lasers.

S. Harris