Plan of lectures

- 1   15.04.2015   Preliminary Discussion / Introduction

- 2   22.04.2015   Experiments (discovery of the positron, formation of antihydrogen, ...)
- 3   29.04.2015   Experiments (Lamb shift, hyperfine structure, quasimolecules and MO spectra)
- 4   06.05.2015   Theory (from Schrödinger to Dirac equation, solutions with negative energy)
- 5   13.05.2015   Theory (bound-state solutions of Dirac equation, quantum numbers)
- 6   20.05.2015   Theory (bound-state Dirac wavefunctions, QED corrections)

- 7   27.05.2015   Experiment (photoionization, radiative recombination, ATI, HHG...)
- 8   03.06.2015   Theory (description of the light-matter interaction)
- 9   10.06.2015   Experiment (Kamiokande, cancer therapy, ….)

- 10   17.06.2015   Experiment (Auger decay, dielectronic recombination, double ionization)
- 11   24.06.2015   Theory (interelectronic interactions, extension of Dirac (and Schrödinger) theory for the description of many-electron systems, approximate methods)

- 12   01.07.2015   Theory (atomic-physics tests of the Standard Model, search for a new physics)
- 13   08.07.2015   Experiment (Atomic physics PNC experiments (Cs,...), heavy ion PV research)
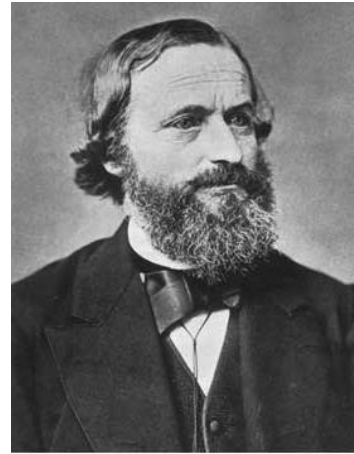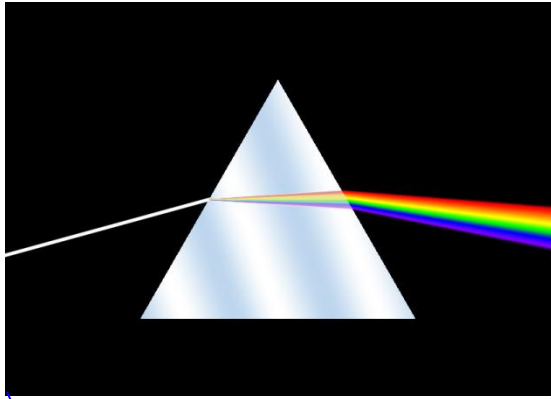
Interaction of ions with electromagnetic field

(One-photon absorption and emission)

Plan of lecture

♦ **Spectral analysis: Basic ideas and a little bit history**

♦ **Transition rates for bound-bound transitions**

  ♦ **Electromagnetic field**

  ♦ **Interaction of EM field with hydrogen-like ions**

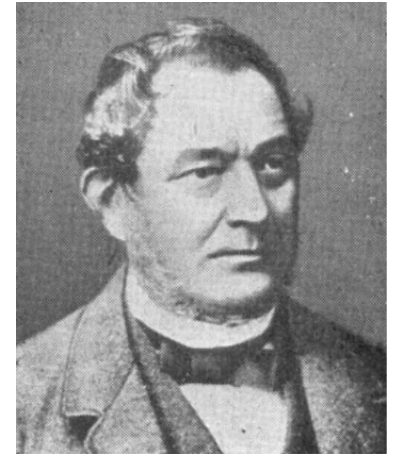 ♦ **Transition matrix elements and their evaluation**

  ♦ **Selection rules**

Spectral analysis in atomic physics
(brief reminder from experimental lectures)

Gustav Kirchhoff   Robert Bunsen

- **The basic ideas of spectral analysis in modern atomic physics have been given by Kirchhoff and Bunsen in 1859 in Heidelberg.**

Spectral analysis in atomic physics
(brief reminder from experimental lectures)

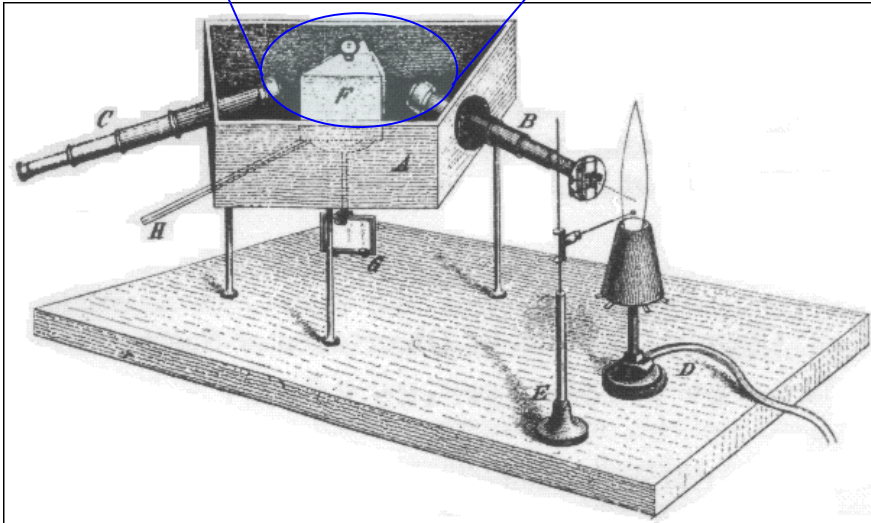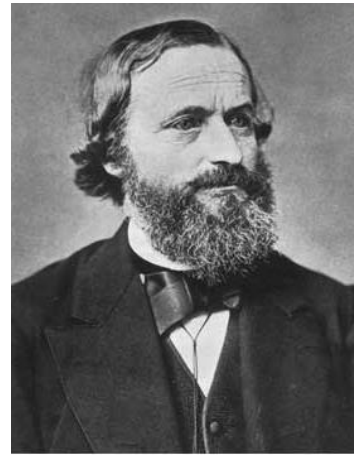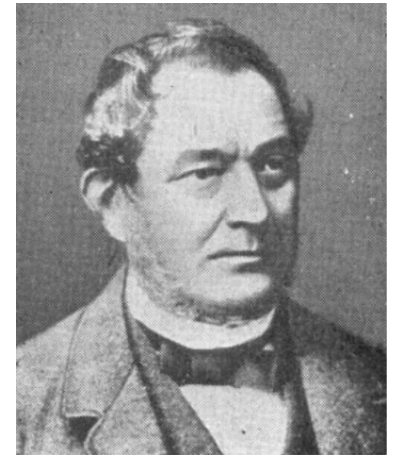Haus zum Riesen, Hauptstrasse 52

Library of Congress

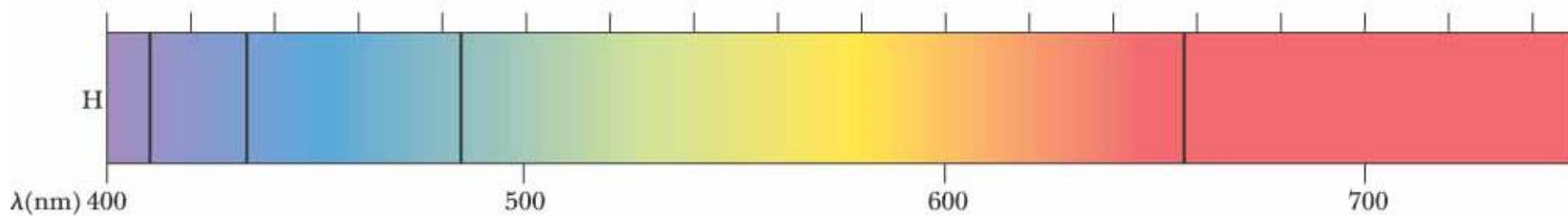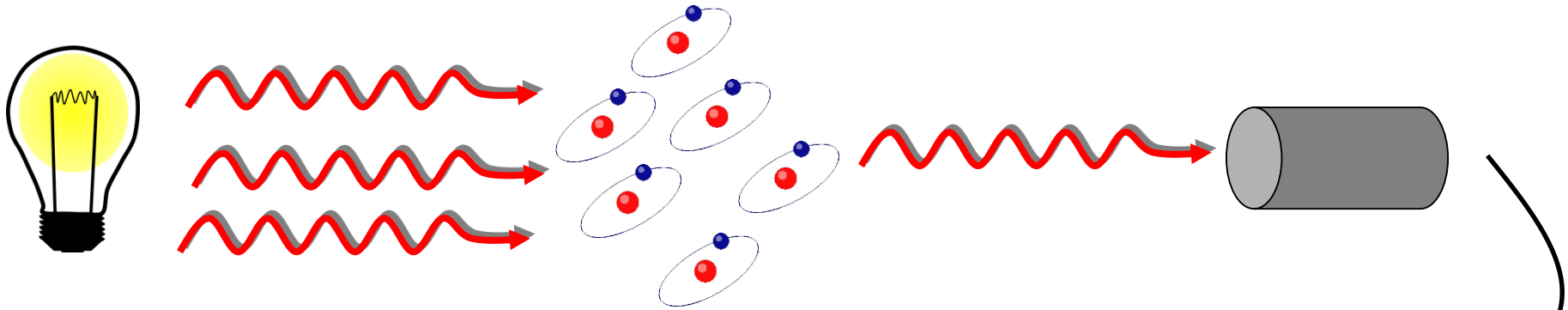Gustav Kirchhoff   Robert Bunsen

- **The basic ideas of spectral analysis in modern atomic physics have been given by Kirchhoff and Bunsen in 1859 in Heidelberg.**

Absorption spectrum

- **Let us consider for the moment absorption of light by hydrogen atoms.**

H

λ(nm) 400   500   600   700

(b)

©2004 Thomson - Brooks/Cole

- **Can we understand observed spectrum?**

Absorption spectrum: Theoretical explanation

- We may consider absorption of light by hydrogen atoms.

- The spectrum (positions of absorption lines) can be understood from our knowledge on the energy levels of H atom.

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

H

λ(nm) 400   500   600

5 → 2   4 → 2   3 → 2

(b)

©2004 Thomson - Brooks/Cole

n=6
n=5
n=4
n=3
n=2
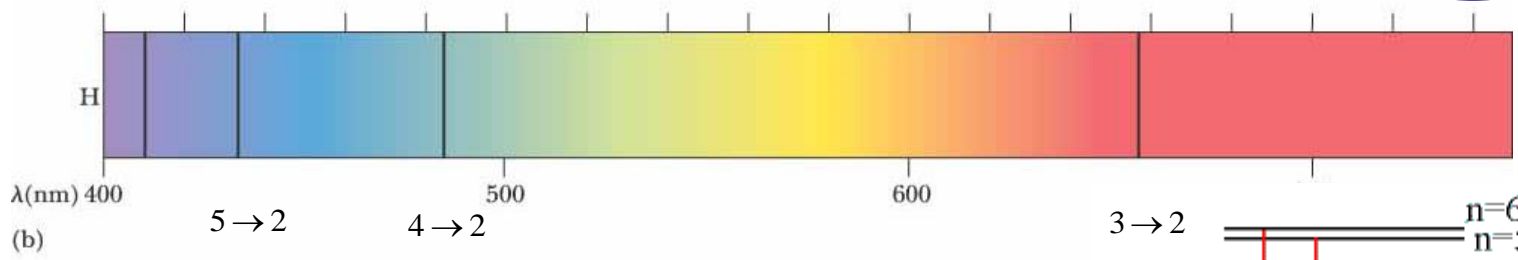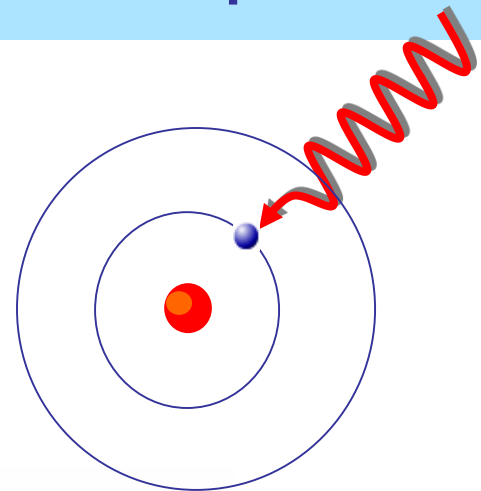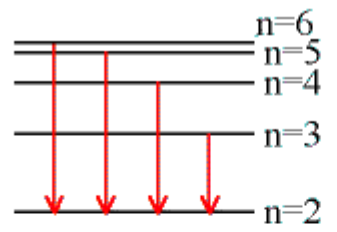
- Bound-state energies (for neutral hydrogen relativistic effects are small):

$$E_{nj} \approx -\frac{\varepsilon_0 Z^2}{2n^2}$$

n=1 (Ground State)

Absorption spectrum: Problems

● **Let us analyze absorption spectrum in more details:**
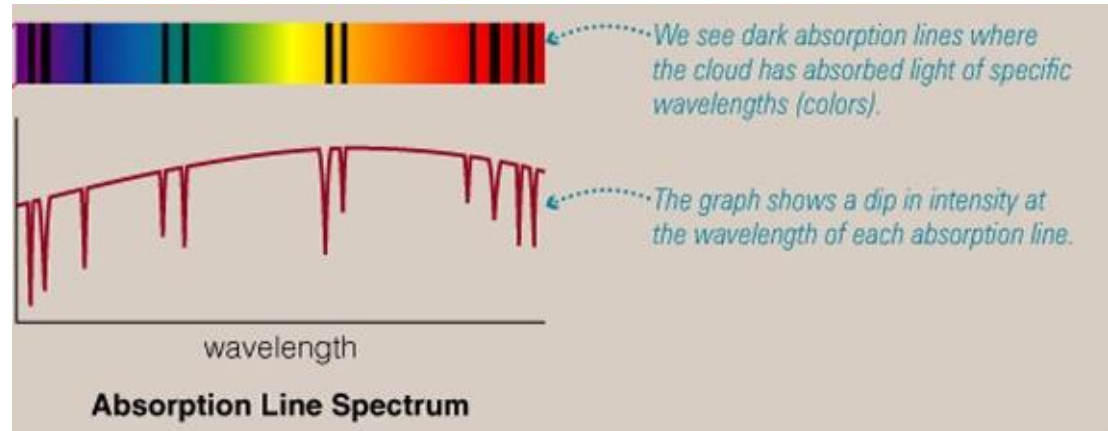
We see dark absorption lines where the cloud has absorbed light of specific wavelengths (colors).

The graph shows a dip in intensity at the wavelength of each absorption line.

wavelength

Absorption Line Spectrum

● **The spectrum (positions of absorption lines) can be understood from our knowledge on the energy levels of H atom.**
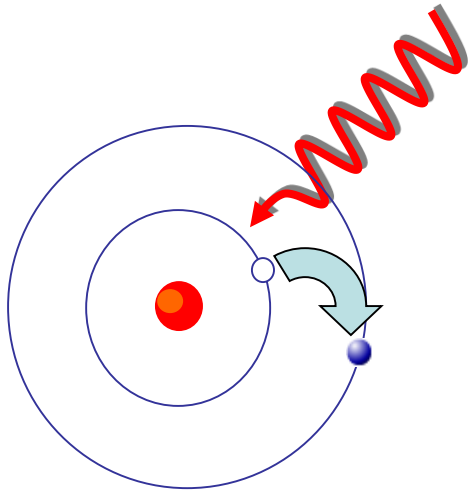
● **But why some dips in intensity are deeper than the other ones?**

→ **Different atomic transitions have different probabilities!**

Emission spectrum: Problems

Niels Bohr

From Bohr model:

$$\Delta E = h\nu = 13.6 \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] eV$$

$$\lambda = \frac{c}{\nu}$$

Lyman Series (Ultraviolet)

Balmer Series (Visible)
410.2 nm violet

434.1 nm violet

n=2

n=4

n=5

n=1

656.3 nm red

Paschen Series (Infrared)

n=3

486.1 nm bluegreen
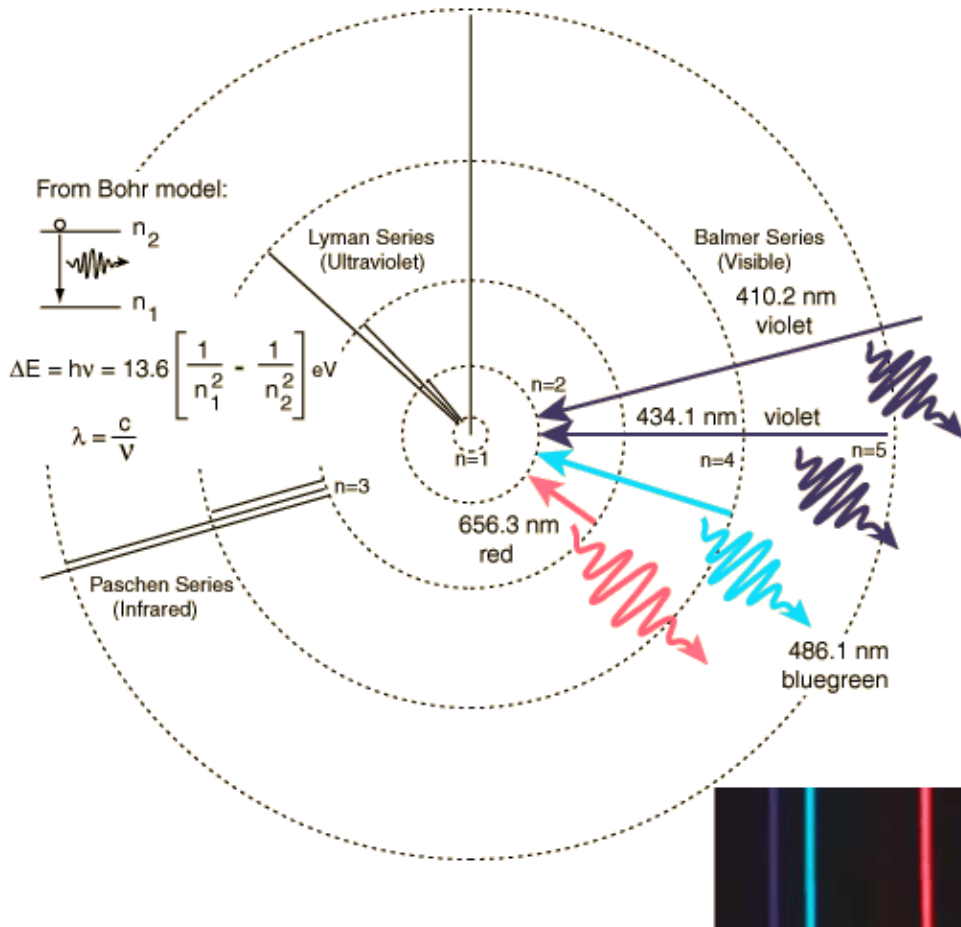
◆ **Similar effect can be observed in emission spectrum: some spectral lines are brighter than the others!**

◆ **That was the main problem of "old" Bohr model (1913): it could explain positions of the lines but not their relative intensities.**
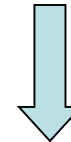
Efforts to resolve this problem finally lead to a creation of Quantum Mechanics!

Emission spectrum: Problems

Niels Bohr

From Bohr model:

$\Delta E = h\nu = 13.$

$\lambda = \dfrac{c}{\nu}$

Lyman Series

Balmer Series

Pasche
(Infra
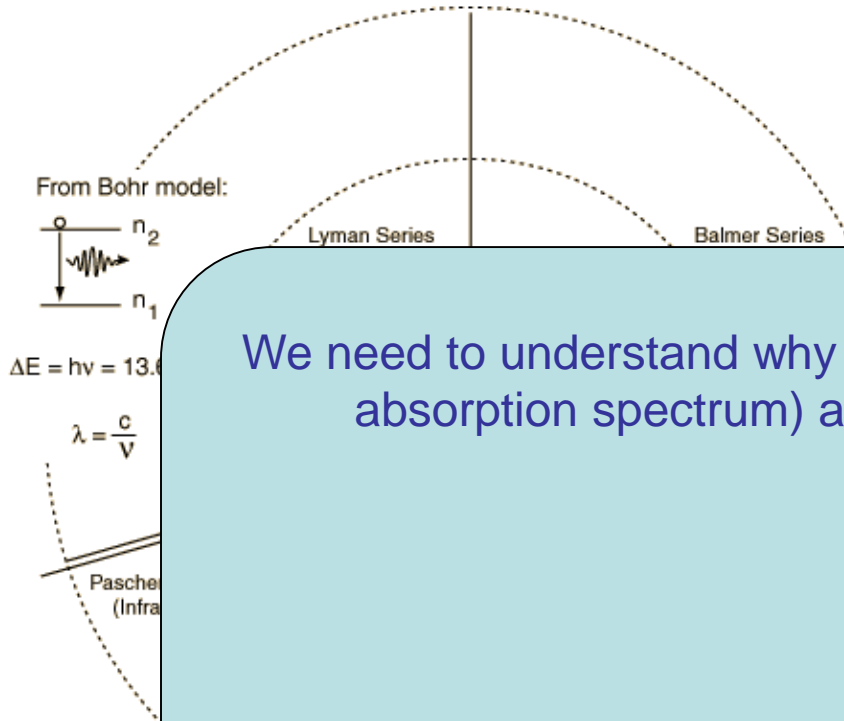
We need to understand why some transitions (either is emission or absorption spectrum) are more probable than the others.
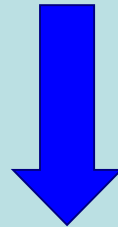
We shall learn how to calculate <u>probabilities</u> for atomic transition!

Efforts to resolve this problem finally lead to a creation of Quantum Mechanics!

Plan of lecture

◆ **Spectral analysis: Basic ideas and a little bit history**

◆ **Transition rates for bound-bound transitions**

> ⊕ **Electromagnetic field**

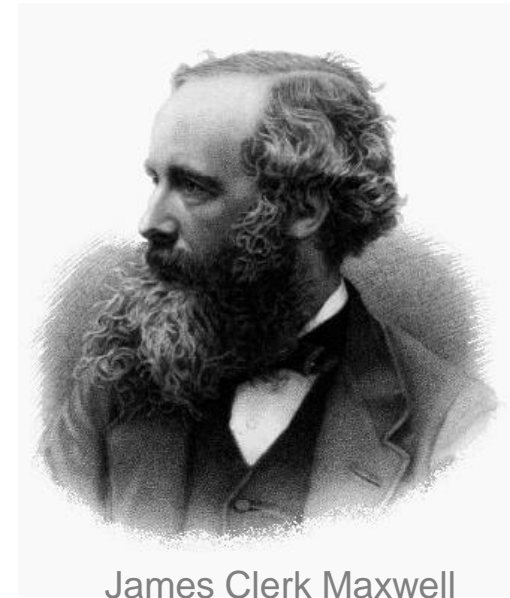> ⊕ **Interaction of EM field with hydrogen-like ions**

> ⊕ **Transition matrix elements and their evaluation**

> ⊕ **Selection rules**

Electromagnetic fields
(classical theory)

- **The classical electromagnetic field is described by electric and magnetic field vectors which satisfy Maxwell's equation (here written in SI units).**

Gauss' Law	$\nabla \cdot \mathbf{D} = \rho_F$
Gauss' Law for Magnetism	$\nabla \cdot \mathbf{B} = 0$
Faraday' Law	$\nabla \times \mathbf{E} = -\dfrac{\partial \mathbf{B}}{\partial t}$
Ampere-Maxwell Law	$\nabla \times \mathbf{H} = \mathbf{J}_F + \dfrac{\partial \mathbf{D}}{\partial t}$

James Clerk Maxwell

$$\boldsymbol{D} = \varepsilon\, \boldsymbol{E}$$

electric displacement

electric field

permitivity

$$\boldsymbol{B} = \mu\, \boldsymbol{H}$$

magnetic field

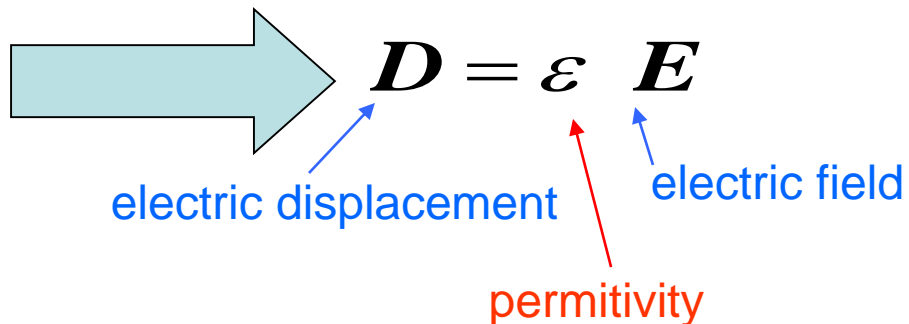magnetic field strength

permeability

Electromagnetic fields
(classical theory)

- **The classical electromagnetic field is described by electric and magnetic field vectors which satisfy Maxwell's equation (here written in units).**

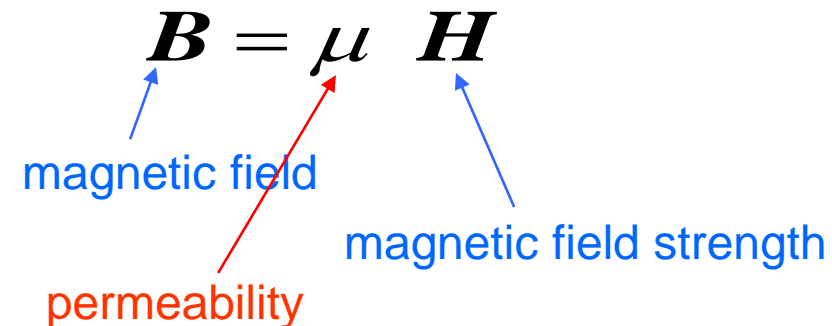|		
Gauss' Law	$\nabla \cdot \mathbf{D} = \rho_F$	
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Ampere-Maxwell Law	$\nabla \times \mathbf{H} = \mathbf{J}_F + \dfrac{\partial \mathbf{D}}{\partial t}$	

$$\boldsymbol{D} = \varepsilon \; \boldsymbol{E}$$

electric displacement

electric field

permitivity

$\Delta\Phi = E\Delta A$

$\Phi_{electric} = \dfrac{Q}{\varepsilon_0}$

The sum of the flux is proportional to the total charge enclosed.

ΔA perpendicular

Moving magnet toward coil

$\dfrac{\Delta B}{\Delta t} = 0.4$ T/s

$B = \mu n I$

From: http://hyperphysics.phy-astr.gsu.edu/

magnetic field strength
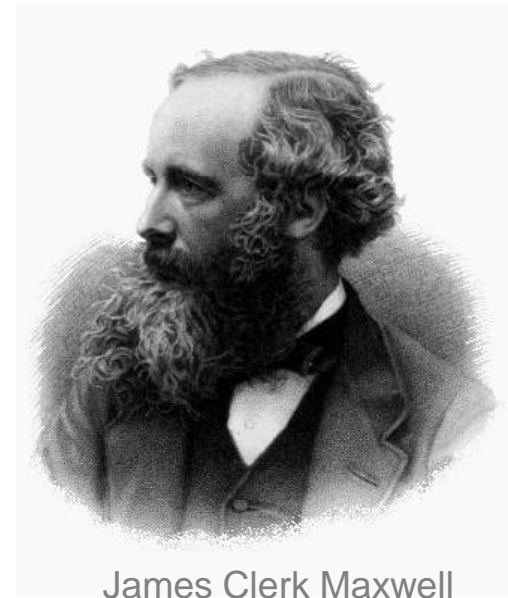
permeability

Scalar and vector potentials
(classical theory)

- **The classical electromagnetic field is described by electric and magnetic field vectors which satisfy Maxwell's equation (here written in SI units).**

Gauss' Law	$\nabla \cdot \mathbf{D} = \rho_F$
Gauss' Law for Magnetism	$\nabla \cdot \mathbf{B} = 0$
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Ampere-Maxwell Law	$\nabla \times \mathbf{H} = \mathbf{J}_F + \dfrac{\partial \mathbf{D}}{\partial t}$

James Clerk Maxwell

- **The electric field *E* and magnetic field *B* can be generated from scalar and vector potentials by:**

$$\mathbf{E}(\mathbf{r},t) = -\nabla \phi(\mathbf{r},t) - \frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t}$$

$$\mathbf{B}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t)$$

Potentials are not directly observable - only the fields they describe may be measured.

Gauge invariance
(classical theory)

- **The electric field *E* and magnetic field *B* can be generated from scalar and vector potentials by:**

$$\mathbf{E}(\mathbf{r},t) = -\nabla\phi(\mathbf{r},t) - \frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t}$$
$$\mathbf{B}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t)$$

- **These potentials are not completely defined! If we substitute:**

$$A \to A + \nabla\chi \qquad \varphi \to \varphi - \frac{\partial\chi}{\partial t}$$

- **The electric and magnetic fields will be unaltered (gauge invariance).**
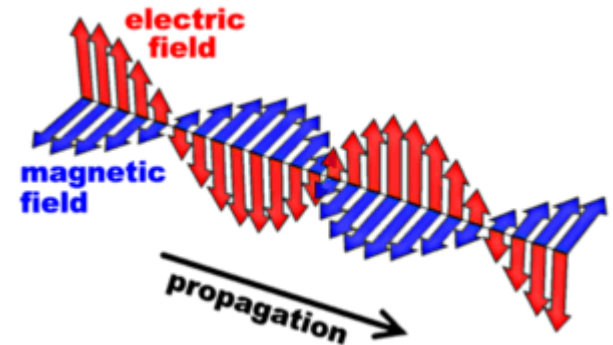
- **We may put further condition on *A***

$$\nabla\mathbf{A} = 0, \ \varphi = 0$$

- ***Coulomb gauge!***

In Coulomb gauge we show that *A* satisfies wave equation:

$$\nabla^2 A - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} = 0$$

Derive the wave equation for the vector potential **A**:

$$\nabla^2 \boldsymbol{A} - \frac{1}{c^2}\frac{\partial^2 \boldsymbol{A}}{\partial t^2} = 0$$

Monochromatic plane wave solutions

- **Let us solve wave equation as obtained in Coulomb gauge:**

$$\nabla^2 \boldsymbol{A} - \frac{1}{c^2}\frac{\partial^2 \boldsymbol{A}}{\partial t^2} = 0$$

- **For the monochromatic plane wave this solution reads as:**

$$\boldsymbol{A}(\omega;\boldsymbol{r},t) = A_0(\omega)\,\boldsymbol{\varepsilon}\left(\mathrm{e}^{i(\boldsymbol{kr}-\omega t+\delta_\omega)} + \mathrm{e}^{-i(\boldsymbol{kr}-\omega t+\delta_\omega)}\right)$$

- **It is rather easy to find general properties of *A*:**

  - **From gauge condition:** $\nabla \boldsymbol{A} = 0$ $\implies$ $\boldsymbol{k}\cdot\boldsymbol{\varepsilon} = 0$

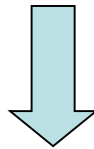 - **From wave equation:** $\implies$ $\omega = kc$

Monochromatic plane wave solutions

- **Let us solve wave equation as obtained in Coulomb gauge:**

$$\nabla^2 \boldsymbol{A} - \frac{1}{c^2}\frac{\partial^2 \boldsymbol{A}}{\partial t^2} = 0$$

- **For the monochromatic plane wave this solution reads as:**

$$\boldsymbol{A}(\omega; \boldsymbol{r}, t) = A_0(\omega)\, \boldsymbol{\varepsilon}\left(\mathrm{e}^{i(\boldsymbol{kr} - \omega t + \delta_\omega)} + \mathrm{e}^{-i(\boldsymbol{kr} - \omega t + \delta_\omega)}\right)$$
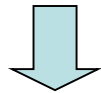
We can immediately get electric and magnetic fields:

$$\boldsymbol{E} = -2\,\omega\, A_0(\omega)\, \boldsymbol{\varepsilon}\, \sin(\boldsymbol{kr} - \omega t + \delta_\omega)$$

$$\boldsymbol{B} = -2\,\omega\, A_0(\omega)\, (\boldsymbol{k} \times \boldsymbol{\varepsilon})\, \sin(\boldsymbol{kr} - \omega t + \delta_\omega)$$

The direction of electric field is along the <u>polarization</u> vector ε!
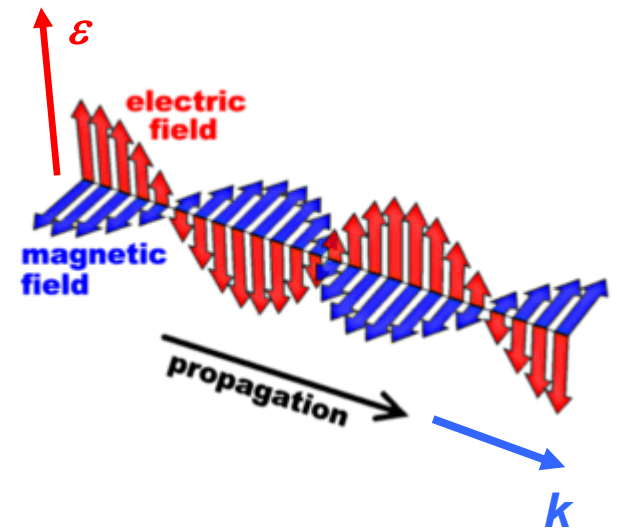
- **Finally, we may calculate the intensity of radiation:**

$$I(\omega) = 2\varepsilon_0 \omega^2 c A_0(\omega)$$

Monochromatic plane wave solutions

- **Let us solve wave equation as obtained in Coulomb gauge:**

- **For the mon**

We can immed

$$E = -2\,\omega\,A$$

$$B = -2\,\omega\,A$$

The direction of e

- **Finally, we may calculate the intensity of radiation:**

$$I(\omega) = 2\varepsilon_0\omega^2 c A_0(\omega)$$

✓ **Small comment**

In general case, a pulse of radiation can be considered as a superposition of monochromatic plane waves:

$$A(\boldsymbol{r},t) = \int_{\Delta_\omega} A_0(\omega)\,\boldsymbol{\varepsilon}\left(e^{i(\boldsymbol{k}\boldsymbol{r}-\omega t+\delta_\omega)} + c.c.\right)\mathrm{d}\omega$$

$$A_0(\omega)$$
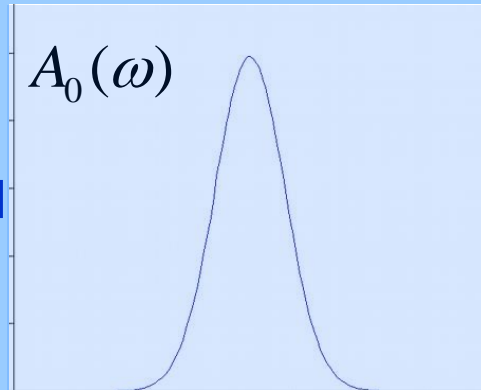
Pulse is nearly monochromatic

k

Plan of lecture

◆ **Spectral analysis: Basic ideas and a little bit history**

◆ **Transition rates for bound-bound transitions**

    ◈ **Electromagnetic field**

    ◈ **Interaction of EM field with hydrogen-like ions**

    ◈ **Transition matrix elements and their evaluation**

    ◈ **Selection rules**

Dirac particle for charged particle in EM field

- **Time-dependent Dirac equation for hydrogenic atom in electromagnetic field reads:**

$$i\hbar \frac{\partial}{\partial t} \Psi(\boldsymbol{r},t) = \left(-i\hbar c\,\boldsymbol{\alpha}\cdot\nabla + V(\boldsymbol{r}) + m_e c^2 \alpha_0 + ce\,\boldsymbol{\alpha}\cdot\boldsymbol{A}\right)\Psi(\boldsymbol{r},t)$$

Coulomb potential

Coupling to external field
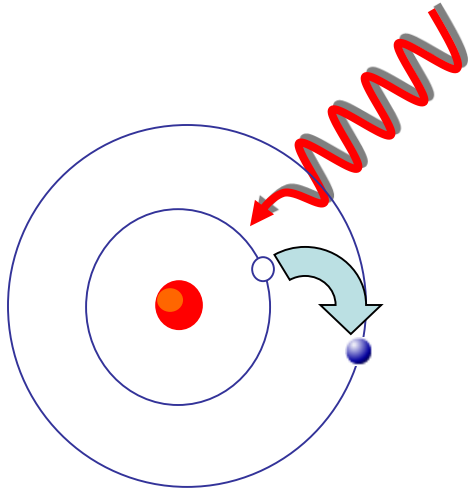
- **Of course, expression above is an approximation:**

  - ➤ **The influence of the ion on the external field is neglected.**

  - ➤ **The interaction between the radiation field and the nucleus is ignored.**

- **How to solve such a Dirac equation? One of the ways is to apply time-dependent perturbation theory!**

Time-dependent perturbation theory (1)

- **Time-dependent Dirac equation for hydrogenic atom in electromagnetic field reads:**

$$i\hbar \frac{\partial}{\partial t} \Psi(\boldsymbol{r},t) = \left(H_0 + \lambda H_{\text{int}}(t) \right) \Psi(\boldsymbol{r},t)$$

unperturbed time-independent Hamiltonian

$$\hat{H}_0 = -i\hbar c \boldsymbol{\alpha} \cdot \nabla + V(\boldsymbol{r}) + m_e c^2 \alpha_0$$

time-dependent perturbation

$$\hat{H}_{\text{int}} = ce\boldsymbol{\alpha} \cdot \boldsymbol{A}$$

- **We have discussed already eigenfunctions of the Hamiltonian H_0**

$$\hat{H}_0 \psi_k(\boldsymbol{r}) = E_k \psi_k(\boldsymbol{r})$$

For simplicity: $k \rightarrow (n, j, \text{parity})$

- **General solution of the time-dependent Dirac equation can be expanded:**

$$\Psi(\boldsymbol{r},t) = \sum_k c_k(t) \psi_k(\boldsymbol{r}) \; e^{-iE_k t / \hbar}$$

We need to find expansion coefficients $c_k(t)$!

Time-dependent perturbation theory (2)

- **To find expansion coefficients:**

$$\Psi(\boldsymbol{r},t) = \sum_k c_k(t)\psi_k(\boldsymbol{r})\; \mathrm{e}^{-iE_k t/\hbar}$$

$$i\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t) = \left(H_0 + \lambda H_{\mathrm{int}}(t)\right)\Psi(\boldsymbol{r},t)$$

- **... after some simple algebra we obtain:**

$$\frac{\partial c_b(t)}{\partial t} = \frac{1}{i\hbar}\sum_k \lambda\, c_k(t)\left\langle\psi_b\middle|H_{\mathrm{int}}\middle|\psi_k\right\rangle \mathrm{e}^{i(E_b - E_k)t/\hbar}$$

> **That is the system of coupled differential equations. To "decouple" it and, hence, to solve it we may use perturbation approach.**

- **If the perturbation λH_{int} is weak, we can expand c_k coefficients in powers of the parameter λ:**

$$c_k(t) = c_k^{(0)}(t) + \lambda\, c_k^{(1)}(t) + \lambda^2\, c_k^{(2)}(t) + \dots$$

Time-dependent perturbation theory

- **By substituting** $c_k(t) = c_k^{(0)}(t) + \lambda\, c_k^{(1)}(t) + \lambda^2\, c_k^{(2)}(t) + ...$ **into:**

$$\frac{\partial c_b(t)}{\partial t} = \frac{1}{i\hbar} \sum_k \lambda\, c_k(t) \left\langle \psi_b \left| H_{\text{int}} \right| \psi_k \right\rangle \mathrm{e}^{i(E_b - E_k)t/\hbar}$$

- **We easily find (with additional condition** $c_k^{(0)} = \delta_{ka}$ **):**

$$\lambda^0 : \quad \frac{\partial c_b^{(0)}}{\partial t} = 0$$

$$\lambda^1 : \quad c_b^{(1)}(t) = \frac{1}{i\hbar} \int_0^t dt' \left\langle \psi_b \left| H_{\text{int}}(t') \right| \psi_a \right\rangle \mathrm{e}^{i(E_b - E_a)t'/\hbar}$$

Time-dependent perturbation theory (3)

- **By using expansion of c_k coefficients and by assuming that the system was initially in the well-defined state a = (n_a, j_a, $parity_a$) we obtain:**

$$c_b^{(1)}(t) = \frac{ce}{i\hbar} \int\limits_0^t \left\langle \psi_b \left| \boldsymbol{\alpha}\, A \right| \psi_a \right\rangle e^{i(E_b - E_a)t'/\hbar}\, \mathrm{d}t'$$
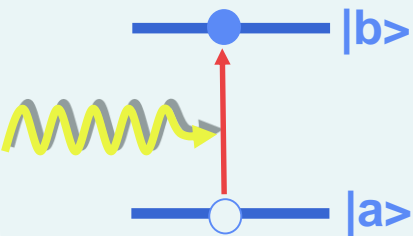
- **To proceed further we use the explicit form of the vector potential and finally obtain:**

$$c_b^{(1)}(t) = \frac{ce}{i\hbar} \int\limits_{\Delta_\omega} d\omega\, A_0(\omega) \left[e^{i\delta_\omega} \left\langle \psi_b \left| \boldsymbol{\alpha}\, \boldsymbol{\varepsilon}\, e^{i\boldsymbol{k}\boldsymbol{r}} \right| \psi_a \right\rangle \int\limits_0^t dt'\, e^{i(E_b - E_a - \hbar\omega)t'/\hbar} \right.$$

$$\left. + e^{-i\delta_\omega} \left\langle \psi_b \left| \boldsymbol{\alpha}\, \boldsymbol{\varepsilon}\, e^{-i\boldsymbol{k}\boldsymbol{r}} \right| \psi_a \right\rangle \int\limits_0^t dt'\, e^{i(E_b - E_a + \hbar\omega)t'/\hbar} \right]$$
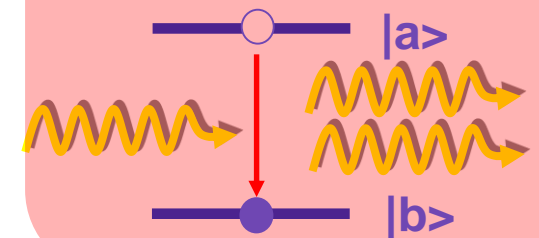
absorption

$$E_b = E_a + \hbar\omega$$

stimulated emission

$$E_b = E_a - \hbar\omega$$

Transition probability: Absorption

- **For the case of absorption:**

$$c_b^{(1)}(t) = \frac{ce}{i\hbar} \int_{\Delta_\omega} d\omega\, A_0(\omega)\, e^{i\delta_\omega} \langle \psi_b | \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\, e^{i\boldsymbol{kr}} | \psi_a \rangle \int_0^t dt'\, e^{i(E_b - E_a - \hbar\omega)t'/\hbar}$$

absorption

$$E_b = E_a + \hbar\omega$$

|b>

|a>

- **Probability that the system which was in t'=0 in state |a> is in t'=t in state |b> is:**

$$P_{ab}(t) = \left| c_b^{(1)}(t) \right|^2 = C\, \frac{I(\omega_{ba})}{\omega_{ba}^2} \left| \langle \psi_b | \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\, e^{i\boldsymbol{kr}} | \psi_a \rangle \right|^2 t$$

proportional to intensity

and to duration of pulse

laser pulse

t'=0   t'=t

- **It is more convenient to introduce the _transition rate_ (transition probability per unit time):**

$$\Gamma_{ab} = C\, \frac{I(\omega_{ba})}{\omega_{ba}^2} \left| \langle \psi_b | \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\, e^{i\boldsymbol{kr}} | \psi_a \rangle \right|^2$$

- **Sometimes it is useful to define also the rate of absorption of energy per atom related to intensity (cross section):**

$$\sigma_{ab} = C\, \frac{1}{\omega_{ba}} \left| \langle \psi_b | \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\, e^{i\boldsymbol{kr}} | \psi_a \rangle \right|^2$$
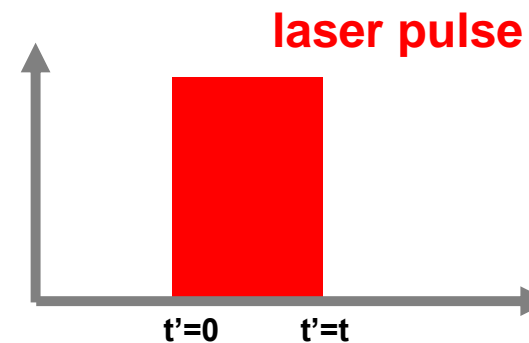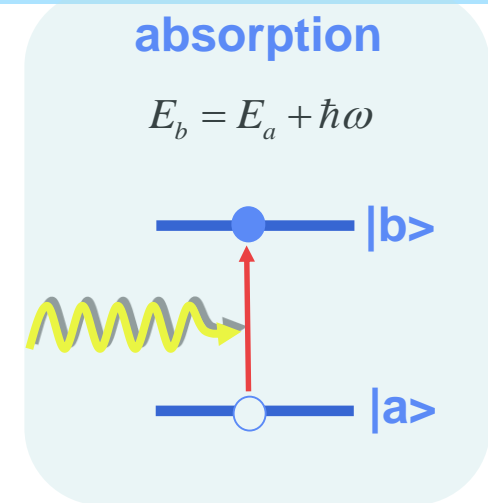
Transition probability: Emission

- **For the case of absorption:**

$$c_b^{(1)}(t) = \frac{ce}{i\hbar} \int_{\Delta_\omega} d\omega \, A_0(\omega) \, e^{-i\delta_\omega} \left\langle \psi_b \left| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\, e^{-i\boldsymbol{k}\boldsymbol{r}} \right| \psi_a \right\rangle \int_0^t dt' \, e^{i(E_b - E_a + \hbar\omega)t'/\hbar}$$

**stimulated emission**

$$E_b = E_a - \hbar\omega$$

|a>

|b>

- **Probability that the system which was in t'=0 in state |a> is in t'=t in state |b> is:**

$$P_{ab}(t) = \left| c_b^{(1)}(t) \right|^2 = C \, \frac{I(\omega_{ba})}{\omega_{ba}^2} \left| \left\langle \psi_b \left| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\, e^{-i\boldsymbol{k}\boldsymbol{r}} \right| \psi_a \right\rangle \right|^2 t$$

proportional to intensity

and to duration of pulse

laser pulse

t'=0   t'=t

- **It is more convenient to introduce the _transition rate_ (transition probability per unit time):**

$$\Gamma_{ab} = C \, \frac{I(\omega_{ba})}{\omega_{ba}^2} \left| \left\langle \psi_b \left| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\, e^{-i\boldsymbol{k}\boldsymbol{r}} \right| \psi_a \right\rangle \right|^2 = C \, \frac{I(\omega_{ba})}{\omega_{ba}^2} \left| \left\langle \psi_a \left| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\, e^{i\boldsymbol{k}\boldsymbol{r}} \right| \psi_b \right\rangle \right|^2$$

Transition probability: Emission

- **For the case of absorption:**

$$c_b^{(1)}(t) = \frac{ce}{i\hbar} \int_{\Delta_\omega} d\omega \, A_0(\omega) \, \mathrm{e}^{-i\delta_\omega} \left\langle \psi_b \middle| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\,e^{-ikr} \middle| \psi_a \right\rangle \int_0^t dt' \, \mathrm{e}^{i(E_b - E_a + \hbar\omega)t'/\hbar}$$

- P...................in t'=0 in state |a>
  i...........

$$\left| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\,e^{-ikr} \middle| \psi_a \right\rangle \right|^2 t$$

and to duration of pulse

- **It is more convenient to intro........ the *transition rate* (transition probability per unit time).**
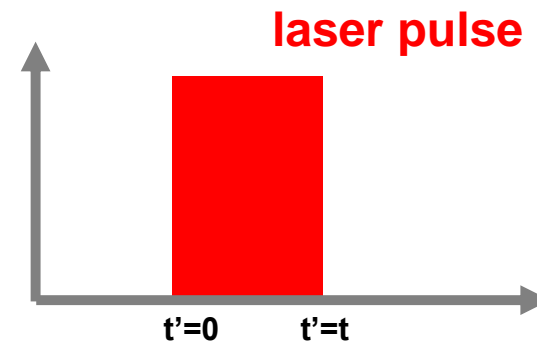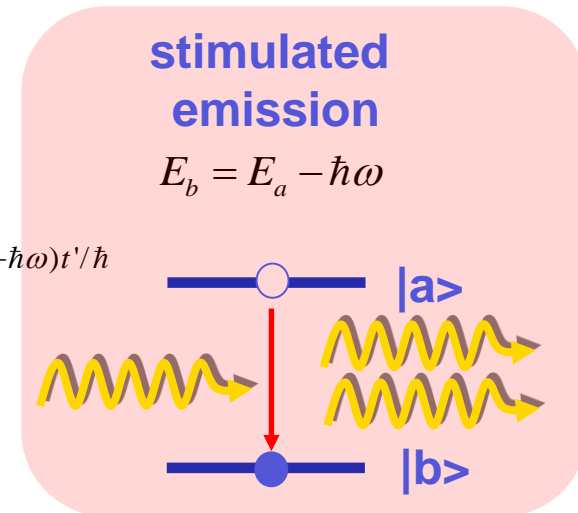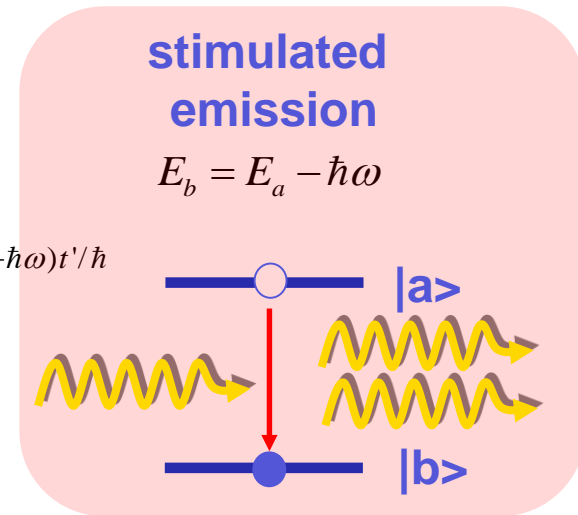
Note that rates for absorption and emission are the same!!!

It is consistent with the principle of detailed balance.

stimulated emission

$$E_b = E_a - \hbar\omega$$

|a>

|b>

laser pulse

t'=0   t'=t
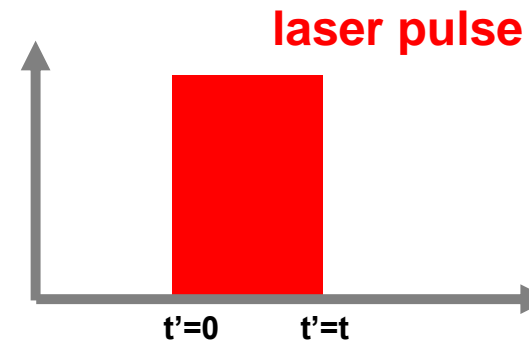
$$\Gamma_{ab} = C \frac{I(\omega_{ba})}{\omega_{ba}^2} \left| \left\langle \psi_b \middle| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\,e^{-ikr} \middle| \psi_a \right\rangle \right|^2 = C \frac{I(\omega_{ba})}{\omega_{ba}^2} \left| \left\langle \psi_a \middle| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\,e^{ikr} \middle| \psi_b \right\rangle \right|^2$$

# Light amplification by stimulated emission of radiation

- Under certain conditions, stimulated emission can provide a physical mechanism for <u>optical amplification</u>.

- Usually, stimulated emission is much weaker than absorption because the initial population of the upper level is smaller that that of the lower level.

- However, if a population inversion is achieved between the upper and lower levels, stimulated emission becomes a dominant process.

- We need at least three-level system to achieve a population inversion.
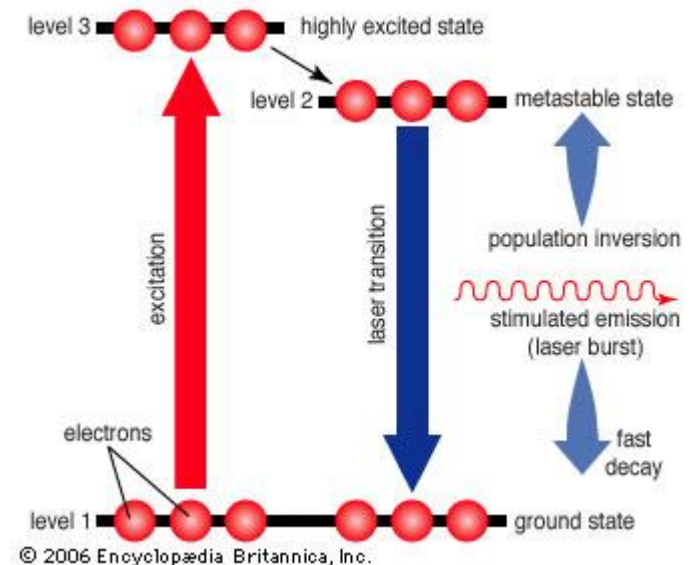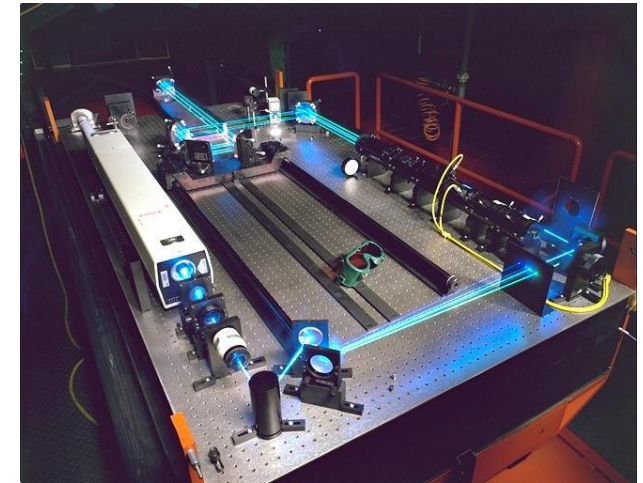
Photos from www.wikipedia.org

Spontaneous emission

- **Quantum mechanics explicitly prohibits spontaneous transitions.**

- **Rigorous treatment of the spontaneous decay can be done within the framework of QED.**

- **Spontaneous emission in free space depends upon vacuum fluctuations to get started.**

spontaneous emission

$$E_b = E_a - \hbar\omega$$

$|a>$

$|b>$
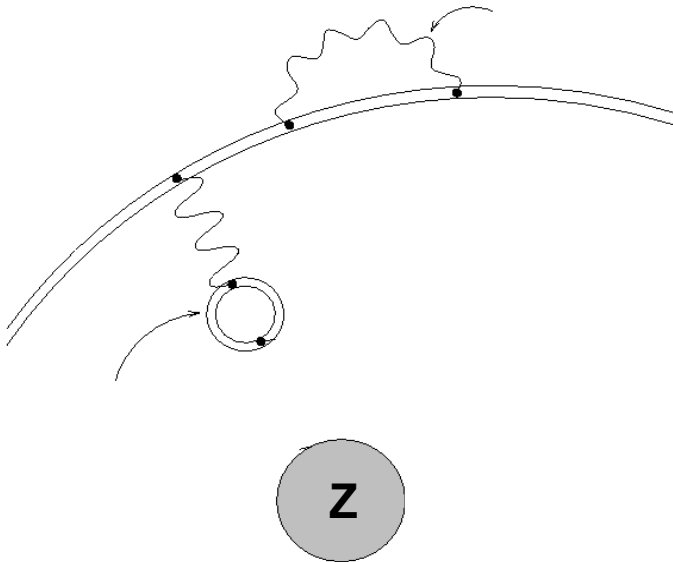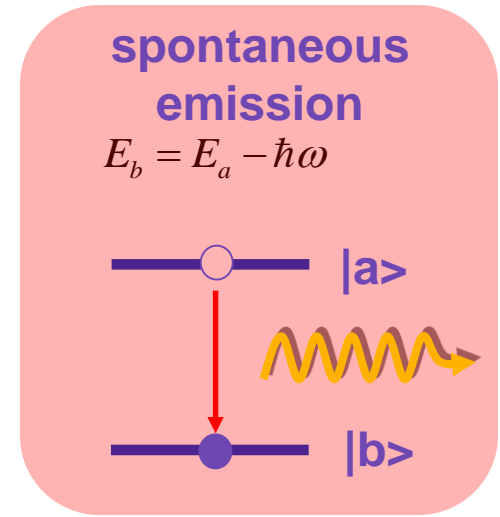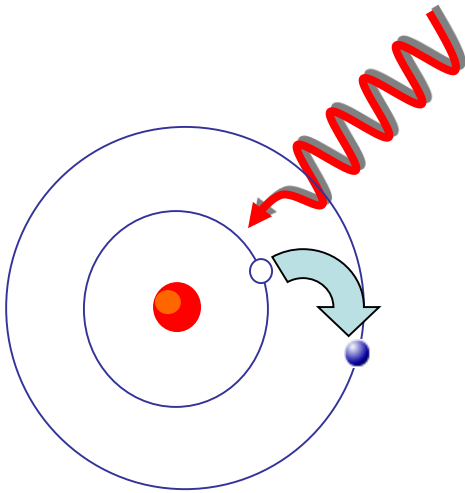
- **Transition rate is given by (Fermi's golden rule):**

$$\Gamma_{ab} = \frac{2\pi}{\hbar}\left|\left\langle\psi_b\left|\boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\,e^{-i\boldsymbol{kr}}\right|\psi_a\right\rangle\right|^2 \rho_b(\omega)$$

density of final photon states

Z

Emission/absorption rates

$$P_{ab}(t) \approx \left| \left\langle \psi_b \left| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\,e^{ikr} \right| \psi_a \right\rangle \right|^2 t$$
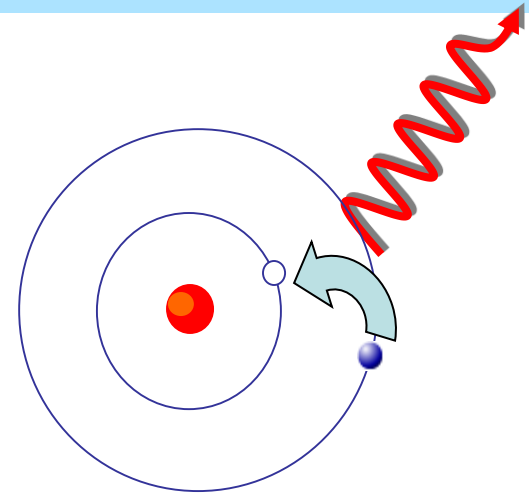
- **We have found that transition probabilities for the interaction of atom (ion) with electromagnetic filed can be traced back to evaluation of the transition matrix element:**

$$M_{ab} = \left\langle \psi_a \left| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\,e^{ikr} \right| \psi_b \right\rangle \equiv \int \psi_a^{+}(\boldsymbol{r})\,\boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\,e^{ikr}\,\psi_b(\boldsymbol{r})d\boldsymbol{r}$$

- **Now we shall learn how to calculate this matrix element!**

Plan of lecture

◆ **Spectral analysis: Basic ideas and a little bit history**

◆ **Transition rates for bound-bound transitions**

    ✦ **Electromagnetic field**

    ✦ **Interaction of EM field with hydrogen-like ions**

    ✦ **Transition matrix elements and their evaluation**

    ✦ **Selection rules**

Evaluation of matrix element

- **We wish to find a way for calculation of the transition matrix element:**

$$M_{ab} = \left\langle \psi_a \middle| \boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\,e^{ikr} \middle| \psi_b \right\rangle \equiv \int \psi_a^+(\boldsymbol{r})\,\boldsymbol{\alpha}\,\boldsymbol{\varepsilon}\,e^{ikr}\,\psi_b(\boldsymbol{r})\,d\boldsymbol{r}$$

final state

photon plane wave

initial state

- **We learned already in the previous lecture the possibility of <u>multipole expansion</u> of plane wave solution. (Remind yourself: we did it for free electron wavefunction).**

- **There are few routes to perform such an expansion but we will for the moment take the simplest one (standard Taylor series):**

$$e^{ikr} = 1 + i\boldsymbol{kr} + \frac{1}{2}(i\boldsymbol{kr})^2 + \ldots$$
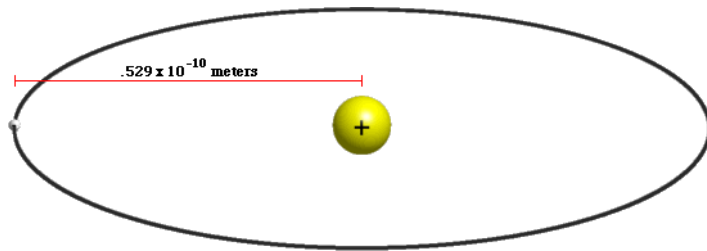
⇒ Very important question: how many terms in this expansion we shall take into account?

Nonrelativistic dipole approximation

- **Let us start from the strongly *non-relativistic* case:**

neutral hydrogen

$$r \approx 10^{-8} \ cm$$

visible light

$$k \approx 10^5 \ cm^{-1}$$

$$kr << 1$$
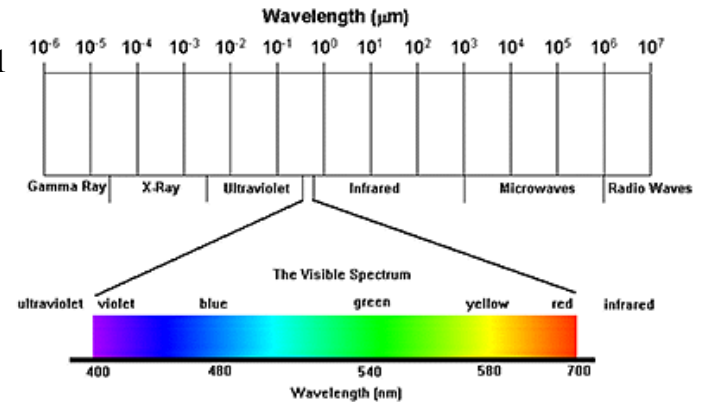
- **We can keep only the first term in multipole expansion:**

$$e^{ikr} = 1 + ikr + \frac{1}{2}(ikr)^2 + ... \approx 1$$

- **In such approximation matrix element reads:**

$$M_{ab} = \int \psi_a^+(r) \, \boldsymbol{\alpha} \, \boldsymbol{\varepsilon} \, \psi_b(r) dr$$

✅ Task 2

Does the non-relativistic dipole approximation holds for the radiative transitions in high-*Z* (say, Z~92) hydrogen-like ions? Why?

Nonrelativistic dipole approximation
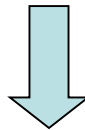
- **Since we are considering strongly *non-relativistic* case, we may (for the moment) take non-relativistic Schrödinger wavefunctions in our matrix element:**

$$M_{ab} = \int \psi_a^*(\boldsymbol{r}) \, \boldsymbol{\alpha} \, \boldsymbol{\varepsilon} \, \psi_b(\boldsymbol{r}) d\boldsymbol{r}$$

$$M_{ab} = \int \psi_a^*(\boldsymbol{r}) \, \boldsymbol{p} \, \boldsymbol{\varepsilon} \, \psi_b(\boldsymbol{r}) d\boldsymbol{r} = m\boldsymbol{\varepsilon} \int \psi_a^*(\boldsymbol{r}) \, \dot{\boldsymbol{r}} \, \boldsymbol{\varepsilon} \, \psi_b(\boldsymbol{r}) d\boldsymbol{r}$$

- **For the further evaluation of this matrix element we shall recall Heisenberg equation:**

$$\frac{d\hat{Q}}{dt} = \frac{i}{\hbar}\left[\hat{H}_0, \hat{Q}\right] \quad\Longrightarrow\quad \dot{\boldsymbol{r}} = \frac{i}{\hbar}\left[\hat{H}_0, \boldsymbol{r}\right]$$

- **By using this equation, we finally may find:**

$$M_{ab} = \frac{\boldsymbol{\varepsilon}}{i\hbar}(E_a - E_b)\int \psi_a^*(\boldsymbol{r}) \, \boldsymbol{r} \, \psi_b(\boldsymbol{r}) d\boldsymbol{r} = -\frac{\boldsymbol{\varepsilon}}{i\hbar e}(E_a - E_b)\int \psi_a^*(\boldsymbol{r}) \underbrace{(-e\boldsymbol{r})}_{} \psi_b(\boldsymbol{r}) d\boldsymbol{r}$$

electric dipole moment

E1 selection rules

- **From our discussion above it is clear that in order to understand whether some particular transition from level n_b, l_b, m_b to level n_a, l_a, m_a is allowed we have to find whether transition matrix element is zero or not:**

$$M_{ab} = -\frac{1}{i\hbar e}(E_a - E_b)\int \psi^*_{n_a l_a m_a}(\boldsymbol{r})(-e\boldsymbol{r})\psi_{n_b l_b m_b}(\boldsymbol{r})d\boldsymbol{r} =$$

$$\propto \int_0^\infty R_{n_a l_a}(r)R_{n_b l_b}(r)r^3\,dr \int Y^*_{l_a m_a}(\theta,\varphi)\left(\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{r}}\right)Y_{l_b m_b}(\theta,\varphi)\,d\Omega$$

- **For the further evaluation of this matrix element let us write vector product $\boldsymbol{\varepsilon r}$ in terms of spherical components:**

$$\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{r}} = \sum_q \varepsilon^*_q\, r_q$$

Few words about spherical components

Plan of lectures

- 1   15.04.2015   Preliminary Discussion / Introduction

- 2   22.04.2015   Experiments (discovery of the positron, formation of antihydrogen, ...)
- 3   29.04.2015   Experiments (Lamb shift, hyperfine structure, quasimolecules and MO spectra)
- 4   06.05.2015   Theory (from Schrödinger to Dirac equation, solutions with negative energy)
- 5   13.05.2015   Theory (bound-state solutions of Dirac equation, quantum numbers)
- 6   20.05.2015   Theory (bound-state Dirac wavefunctions, QED corrections)

- 7   27.05.2015   Experiment (photoionization, radiative recombination, ATI, HHG...)
- 8   03.06.2015   Theory (description of the light-matter interaction)
- 9   10.06.2015   Experiment (Kamiokande, cancer therapy, ….)

- 10   17.06.2015   Experiment (Auger decay, dielectronic recombination, double ionization)
- 11   24.06.2015   Theory (interelectronic interactions, extension of Dirac (and Schrödinger) theory for the description of many-electron systems, approximate methods)

- 12   01.07.2015   Theory (atomic-physics tests of the Standard Model, search for a new physics)
- 13   08.07.2015   Experiment (Atomic physics PNC experiments (Cs,...), heavy ion PV research)