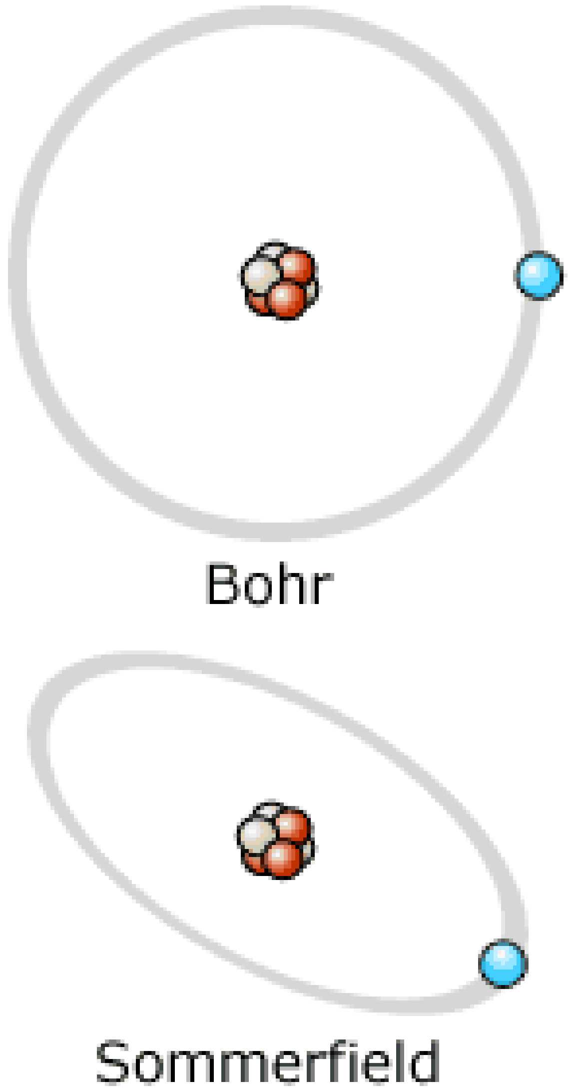
Some Quantum mechanics

Bohr-Sommerfeld I

- Bohr-Sommerfeld theory (classical quantum mechanics
- Assume a complete revolution of an electron around the atomic nucleus

$$\oint p_i dq_i = n_i h$$

$$n_i = 1,2,3...$$



Bohr-Sommerfeld II

$$\frac{Ze^2}{r^2} = \frac{m\upsilon^2}{r} = \frac{p\upsilon}{r}$$

Columb force = centrifugal force

$$\oint pdq = m\upsilon 2\pi r = 2\pi \cdot pr \equiv n\mathrm{h}$$

Bohr´s postulation

$$\upsilon = \frac{\mathrm{Ze}^2}{n\hbar} \text{ and } r = \frac{n\hbar}{m\upsilon} = \frac{n^2\hbar^2}{\mathrm{Ze}^2 m}$$

yields specific orbits

$$r = \frac{n^2\hbar^2}{Ze^2 m} = 0.5 \cdot 10^{-10} \frac{n^2}{Z} [\mathrm{cm}]$$

Bohr-Sommerfeld III

$$E = -\frac{Ze^2}{r} + \frac{mv^2}{2}$$

$$= -\frac{Ze^2 \cdot Ze^2 m}{n^2 \hbar^2} + \frac{Z^2 e^4 m}{2n^2 \hbar^2}$$

$$= -\frac{mZ^2 e^4}{2\hbar^2} \cdot \frac{1}{n^2}$$

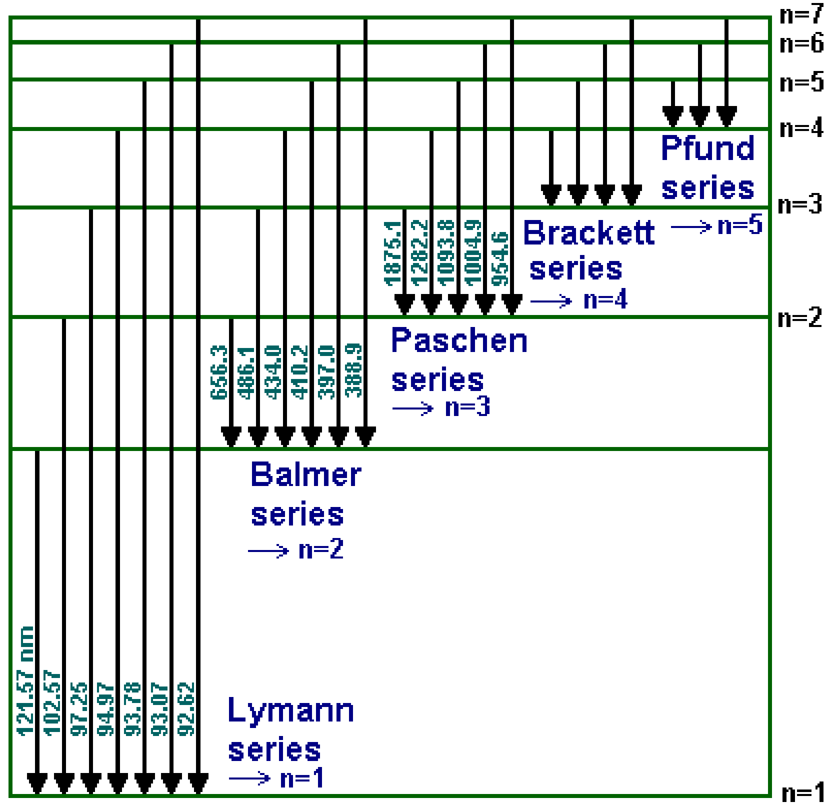
$$= const. \frac{Z^2}{n^2}$$

- The energy depends only on the **separation** between the nucleus and the electron

$$1Ry = \frac{m\ e^4}{2\hbar^2} \cdot Z^2 \cong 13.6\,\mathrm{eV} \cdot \mathrm{Z}^2$$

The hydrogen atom

$$\Delta E = const. \cdot Z^2 \left(\frac{1}{n_2^2} - \frac{1}{n_1^2} \right)$$



Note: the photon has spin 1

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Hydrogen atom (important transitions)

- Lyα 121.57 nm (UV)
- Hα 656.27 nm (visible)
- Hβ 486.13 nm (visible)
- Hγ 434.05 nm (visible)
- Paα 1.875 µm (ground base)
- Brα 4.051 µm (ground base)
- Brγ 2.166 µm (ground base)

Bohr-Sommerfeld IV

- Separating the equation in a radial and a spherical part yields

$$\oint p_r dr = n_r \mathrm{h}$$

$$\oint p_\varphi d\varphi = n_\varphi \mathrm{h} \text{ mit } n_\varphi = 1,2,3\ldots$$

$$n_\varphi \equiv l + 1 \text{ mit } l = 0,1,2\ldots$$

$$n = n_r + n_\varphi = n_r + l + 1$$

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Quantum mechanics I

$$i\hbar\frac{d\Psi}{dt} = H\Psi$$

$$H = -\frac{\hbar^2}{2m_e}\sum_i \nabla_i^2 - Ze^2\sum_i \frac{1}{r_i} + \sum_{i\neq j}\frac{e^2}{r_{ij}}$$

Separating space and time yields the ansatz

$$\Psi(\vec{r},t) = \Psi(\vec{r})e^{-\frac{iEt}{\hbar}} \text{ yields}$$

$$\mathrm{E}\Psi = \mathrm{H}\Psi \text{ (time independent)}$$

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Quantum mechanics II

- Central field

$$\Psi(r,\vartheta,\varphi) = R_{nl}(r)Y_{lm}(\vartheta,\varphi)$$

- Inserting this ansatz in the Schrödinger equation allows to separate the radial and the spherical term in two differential equations. This is only possible, when a constant is the result of each equation. The constant is called the separation constant.

  For simplicity, the separation constant is chosen to $l(l+1)$

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Quantum mechanics III

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}(E-V)=\ell(\ell+1)$$

$$-\frac{1}{Y}\left\{\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y}{\partial\vartheta}\right)+\frac{1}{\sin^2\vartheta}\frac{\partial^2 Y}{\partial\varphi^2}\right\}=\ell(\ell+1)$$

The spherical coordinates can be separated in two

$$Y(\vartheta,\varphi)=\Theta(\vartheta)\cdot\Phi(\varphi)$$

Quantum mechanics IV

$$\sin^2\vartheta\left\{\frac{1}{\Theta\sin\vartheta}\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right)+\ell(\ell+1)\right\}=-\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}=m^2$$

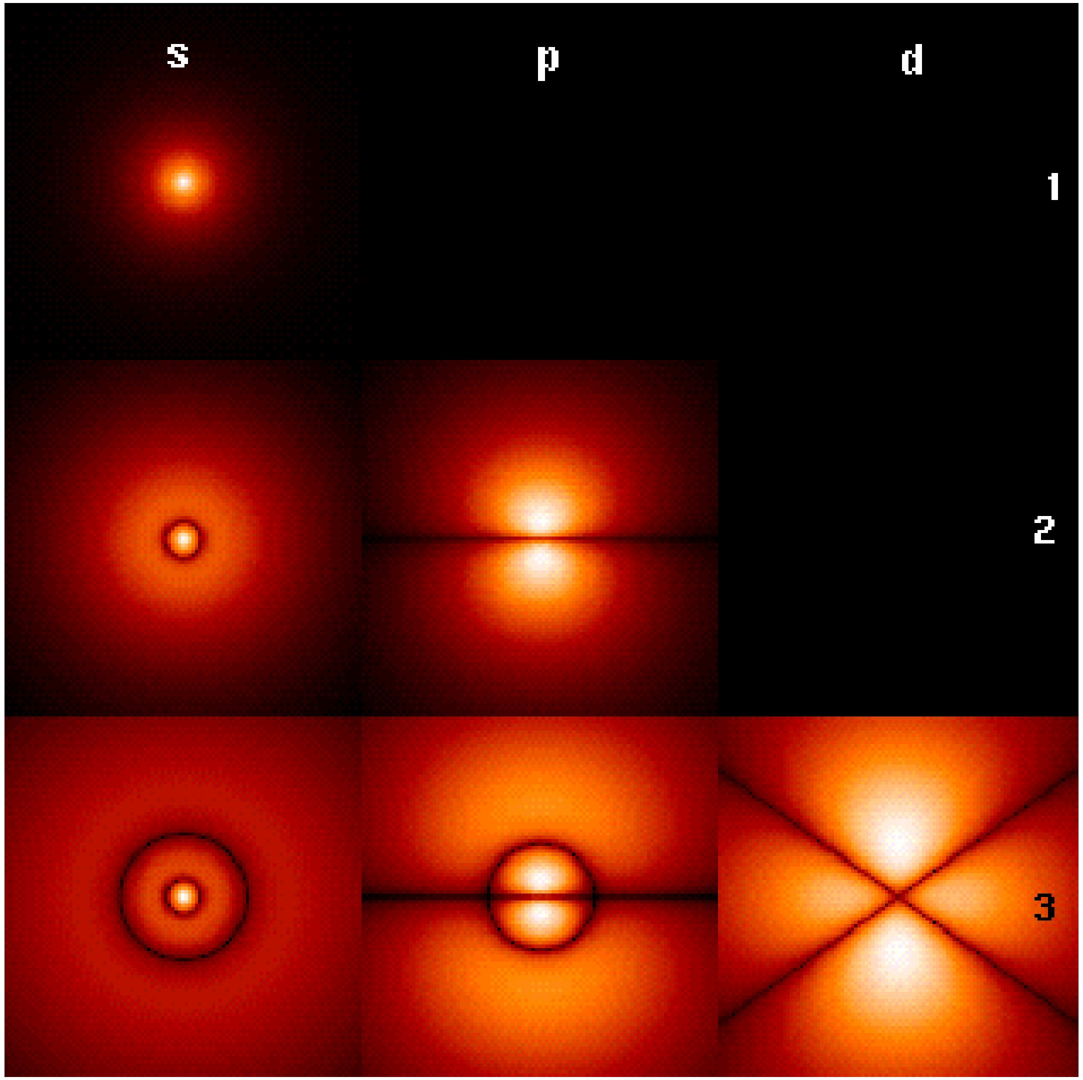
$$-\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}=m \text{ azimuthal term}$$

$$\frac{1}{\Theta\sin\vartheta}\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right)+\ell(\ell+1)-\frac{m^2}{\sin^2\vartheta}=0 \text{ polar term}$$

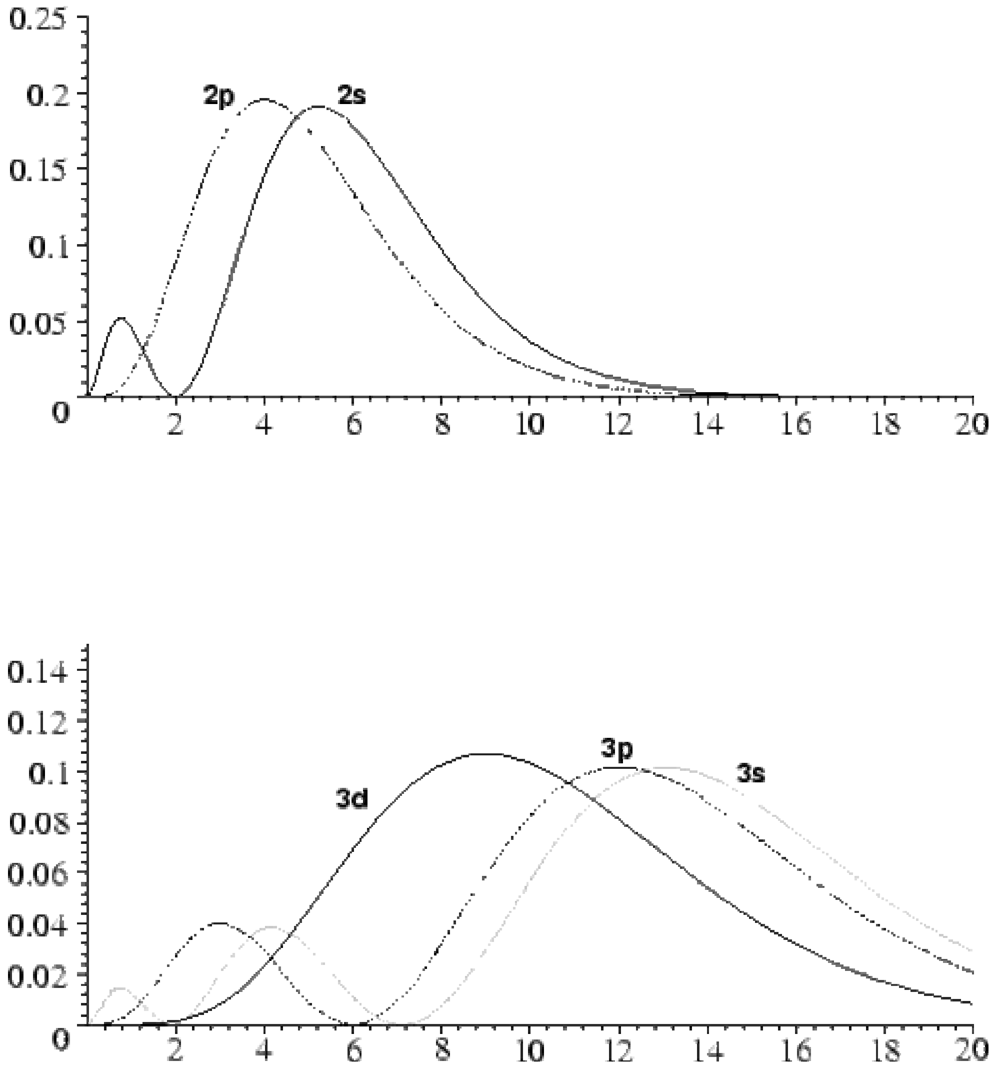
Quantum mechanics V

- The energy levels are $E_n = R \cdot 1/n^2$
- The quantum numbers are *n*, *l* and *m*
- $n = 1,2,3 \ldots$ (principal quantum number)
- $l = 0,1,2 \ldots n-1$ (orbital quantum number)
- $m = -l, -l+1 \ldots +l$ (magnetic quantum number)
- $m_s = \pm 1/2$ (Spin of the fermions)
- The magnetic quantum number resembles a "hidden" quantum number until the degeneracy is broken up

Visualisation of the wave function



Radial wave function



Hydrogen atom (example)

n	l	m	state	$n^{2S+1}L$
1	0	0	1s	1^2S
2	0 1	0 0,±1	2s $2p_0$, $2p_{\pm1}$	2^2S 2^2P
3	0 1 2	0 0,±1 0,±1,±2	3s $3p_0$,$3p_{\pm1}$ $3d_0$,$3d_{\pm1}$,$3d_{\pm2}$	3^2S 3^2P 3^2D

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Quantum mechanics VI

- Nucleus with many electrons, we can use the central field approximation

$$V(r) \approx \begin{cases} \dfrac{Z - N + 1}{r} \text{ for } r \to \infty \\ \dfrac{Z}{r} \text{ for } r \to 0 \end{cases}$$

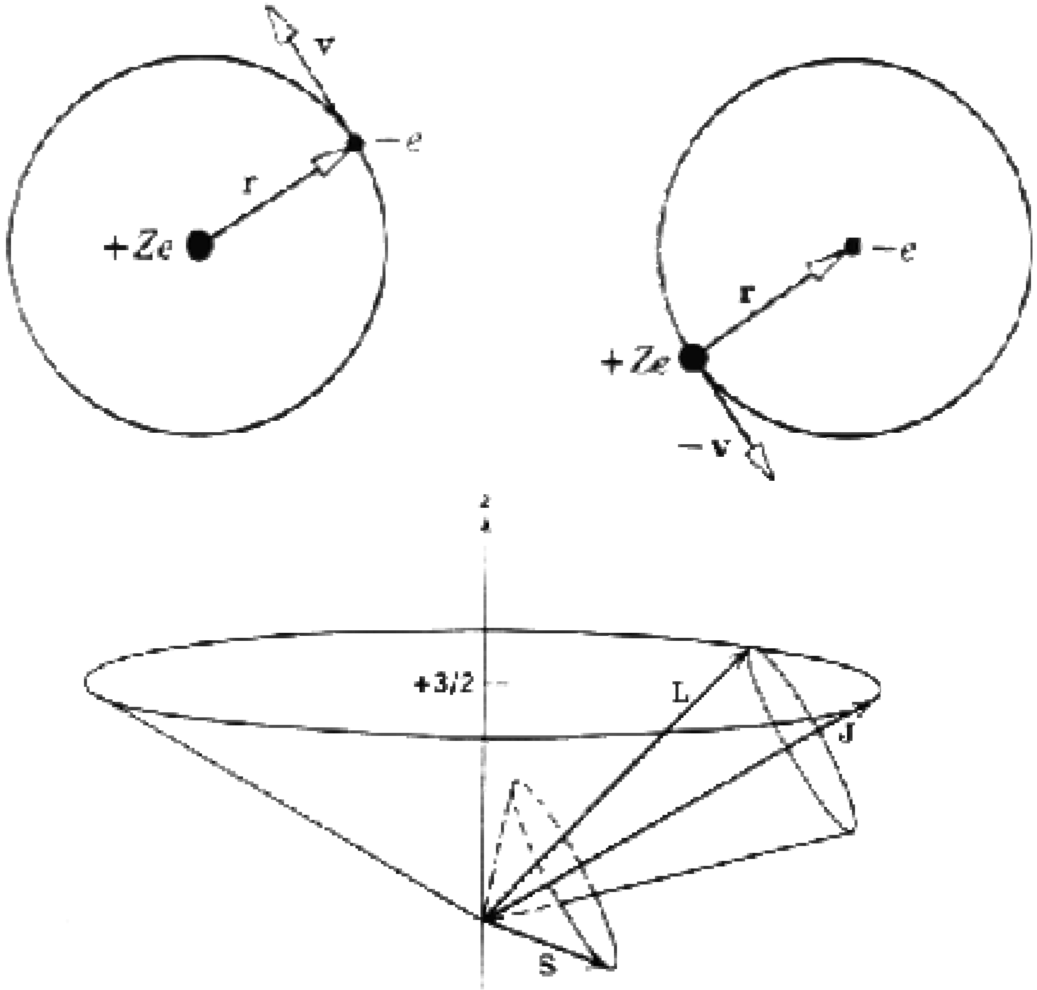
Quantum mechanics VII

- Wave function for atoms with many electrons

$$\Psi = u_a(1) \cdot u_b(2) \cdot \ldots \cdot u_k(N) \text{ with}$$

$$\mathrm{a} = (\mathrm{n}, \mathrm{l}, \mathrm{m}, \mathrm{m_s})$$

Spin-orbit coupling



Spin-orbit coupling

- The **magnetic moments** of the **electron** and the **orbital current** causes a small energetic shift leading to the **fine structure splitting**
- **Spin-orbit coupling is responsible for one of the most important cooling processes in the ISM due to fine structure emission lines**

$$\Phi_{ls} = \mu_B \vec{\sigma} \cdot \vec{B}_l = \frac{1}{2m^2c^2} \frac{1}{r} \frac{d\Phi(r)}{r} \left(\vec{\sigma} \cdot \vec{l} \right)$$

$$\cong \frac{Ze^2}{2m^2c^2} \frac{1}{r^3} \approx 10^{-4}\ \mathrm{eV\ for\ \ hydrogen}$$

Spin-spin coupling

- The **magnetic moment**s of the **nucleus** and the **electron spin** leads to a small shift of the energy levels and to overcome the degeneracy of the total angular momentum
- The **hyper-fine structure line splitting is m_e/m_H ~ 1/2000 smaller than the fine structure splitting**! Most important for hydrogen in space, 21-cm line emission.

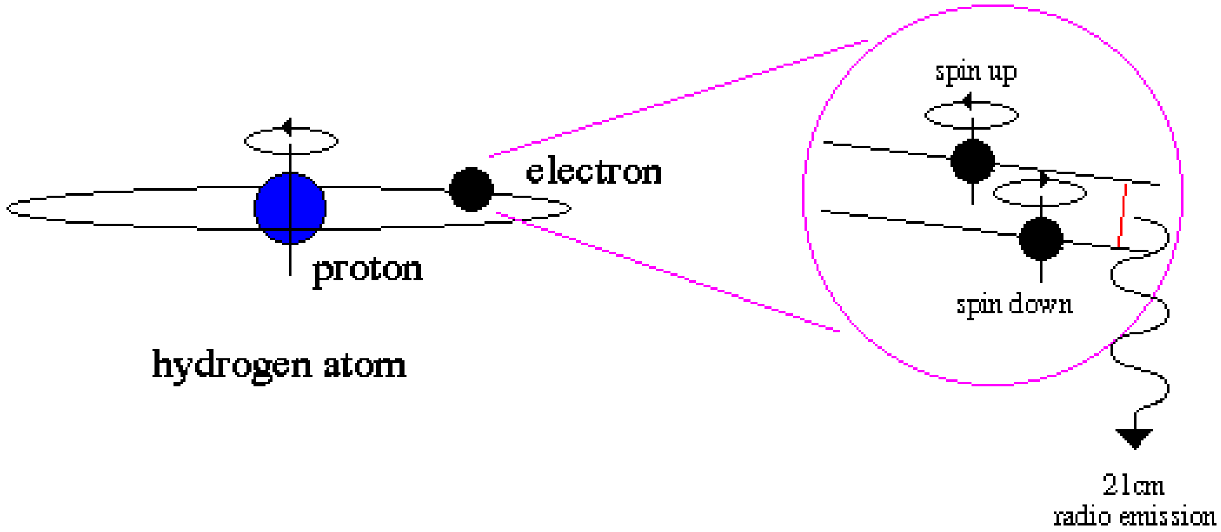
$$\Delta E_{HFS} = \frac{-\mu_p \mu_n \overline{B}_0}{2 s_p j} \left\{ F(F+1) - j(j+1) - s_p(s_p+1) \right\}$$

$$\approx 5 \cdot 10^{-6}\ \text{eV}$$

Spin-spin coupling

21 cm Radiation

The proton and electron in a hydrogen atom both have spin. They can be spinning in the same direction or in opposite directions. Spin in the same direction causes the electron to occupy a slightly higher energy state then spin in opposite directions.



About once ever 10 million years, the electron will flip its spin and emit a radio photon of wavelength 21 cm.

Quick summary

- The **atomic energy levels** are determined primarily by Z and are in the order of some eV
- The **spin-orbit coupling** leads to small shifts of the energy levels (α^2 ~ 1/137 times electronic energy 10 < E < 100 eV) yielding fine structure lines $\Delta E \sim 10^{-3}$ eV to 10^{-1} eV. These fine structure emissions lines lie in the wavelength region between 10 < λ < 300µm
- The **spin-spin coupling** shifts the location of the energy level in the order of $\Delta E \sim 10^{-6}$ eV yielding hyper-fine structure lines. Most important, easy to observe an THE diagnostic line of the Universe is the HI 21-cm line emission. The energetic separation between F=1 and F=0 is 5.9×10^{-6} eV which corresponds to a frequency of 1.421 GHz with an Einstein coefficient of 2.87×10^{-15} s^{-1}

Quick summary II

- some eV denotes temperatures of a few thousand Kelvin
- Fine structure lines $\Delta E \sim 10^{-4}$ eV are emitted by gas with a few hundred Kelvin
- Hyperfinestructure lines $\Delta E \sim 10^{-6}$ eV are emitted by gas with a few Kelvins

$$E = \mathrm{h}\nu = \frac{3}{2} n\mathrm{k}T \Rightarrow T \propto \frac{E}{\mathrm{k}}$$

$$\mathrm{k} \approx 1.16 \cdot 10^{4} \left[\frac{\mathrm{eV}}{\mathrm{K}} \right]$$

Einstein Coefficients

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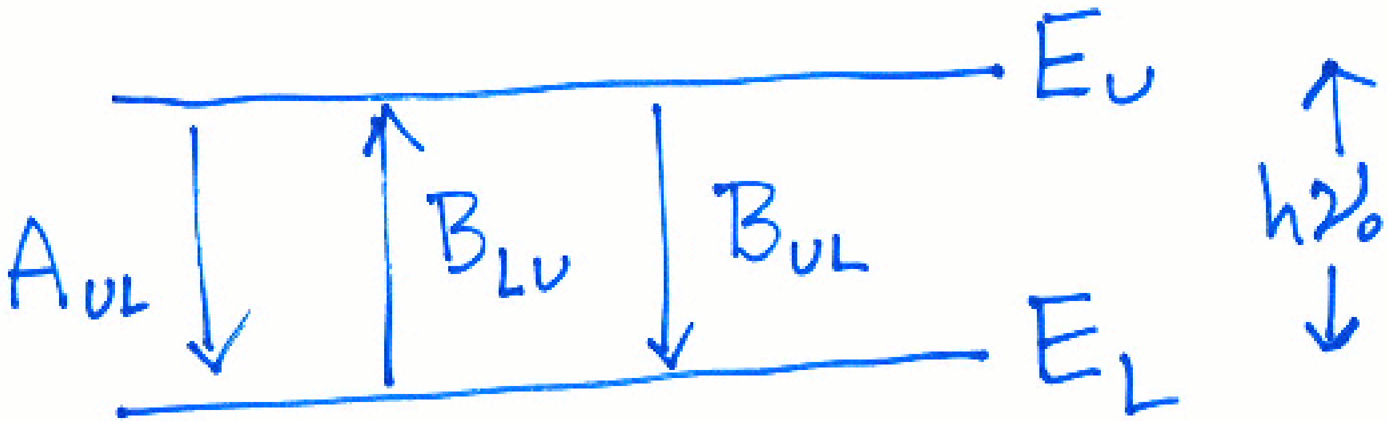
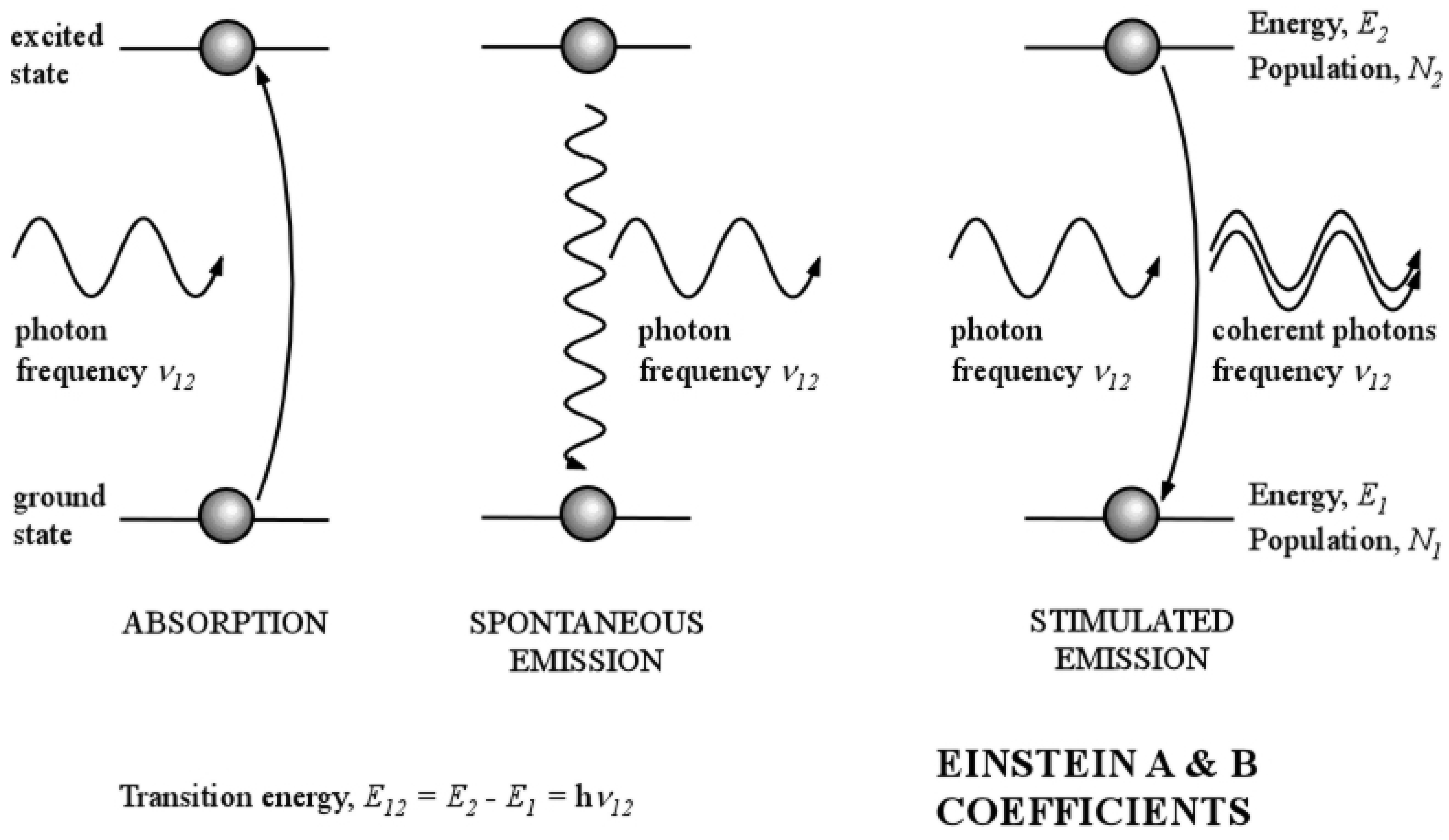
Einstein coefficients



Einstein coefficients



http://www.homepages.ucl.ac.uk/~ucapphj/EinsteinAandB.jpg

Einstein coefficients

We assume thermodynamic equilibrium

$$R_{mk} = R'_{km} = N_k \left(B_{km} I(\nu) + A_{km} \right)$$

Boltzmann Equation

$$N_k = N_m e^{-\frac{\hbar\nu}{\mathrm{k}T}} \text{ yields}$$

$$I(\nu) = \frac{1}{e^{\frac{\hbar\nu}{\mathrm{k}T}} - 1} \frac{A_{km}}{B_{mk}} \text{ using BB } I(\nu) = \frac{\hbar\nu^3}{\pi^2 \mathrm{c}^3} \frac{1}{e^{\frac{\hbar\nu}{\mathrm{k}T}} - 1}$$

gives

$$A_{km} = \frac{\hbar\nu^3}{\pi^2 \mathrm{c}^3} B_{mk}$$

Natural line width

The number of transitions N_k as a function of time from a level k is

$$\frac{dN_k}{dt} = -N_k P$$

solving this homogenous differential equation gives

$$N_K = N_0 e^{-Pt}$$

Using the quantum mechanical notation we find

$$P_k(t) = \left|\Psi_k(t)\right|^2 = \left|\Psi_{k0}\right|^2 e^{-\frac{\Gamma}{\hbar}t}$$

gives

$$\frac{\Gamma}{\hbar} = P = \frac{1}{\tau} \text{ and } \Gamma\tau = \hbar \text{ (energy - time uncertainty relation)}$$

Natural line width II

The line intensity is

$$I(\nu) \propto \frac{\hbar^2}{(E - E_k)^2 + \left(\frac{\Gamma}{2}\right)^2}$$

and the line shape

$$I(\nu) = I_0(\nu) \frac{\left(\frac{\Gamma}{2}\right)^2}{(E - E_k)^2 + \left(\frac{\Gamma}{2}\right)^2}$$ Lorentz distribution

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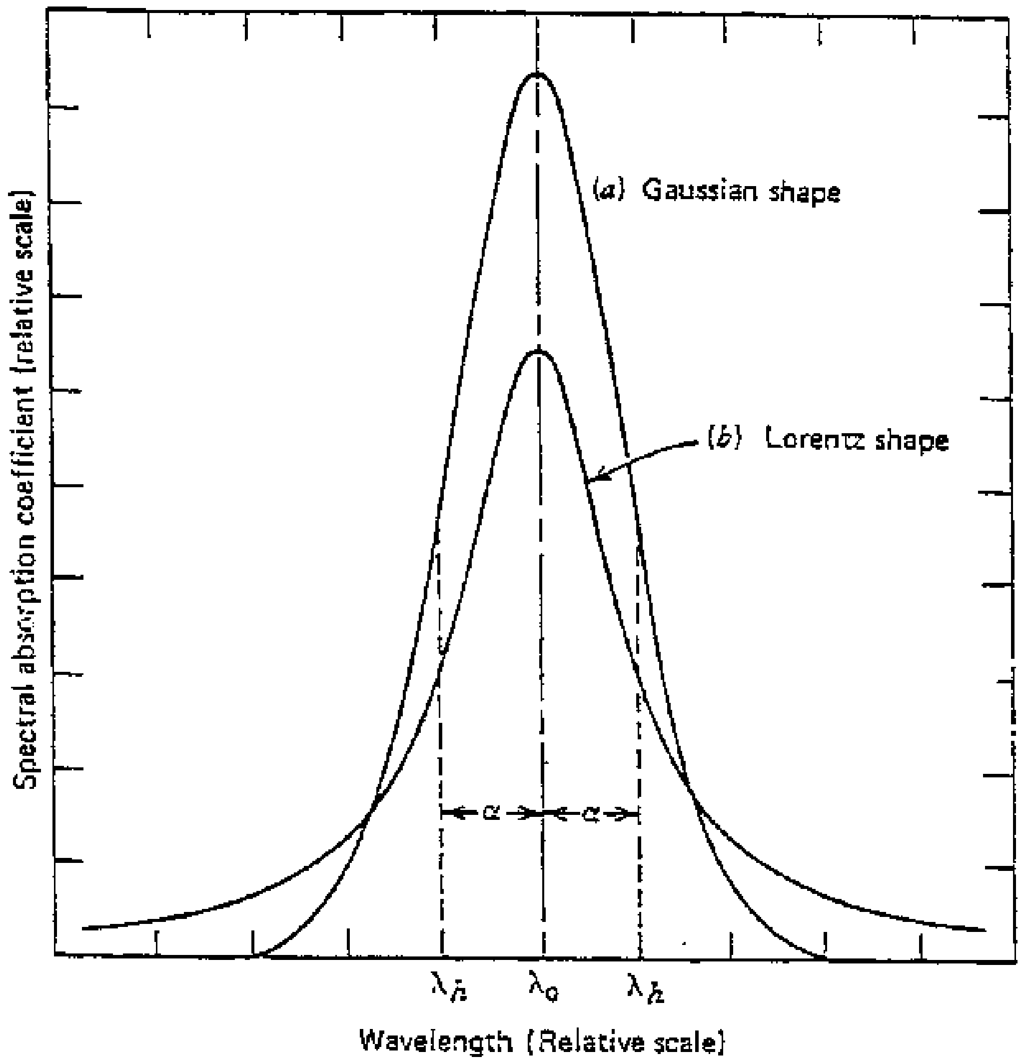
Transition propabilities

- The Einstein coefficients define the transition probabilities
- The "lifetime" of an excited is inverse proportional to the Einstein coefficient for spontaneous emission

Lorentz line shape



emission lines

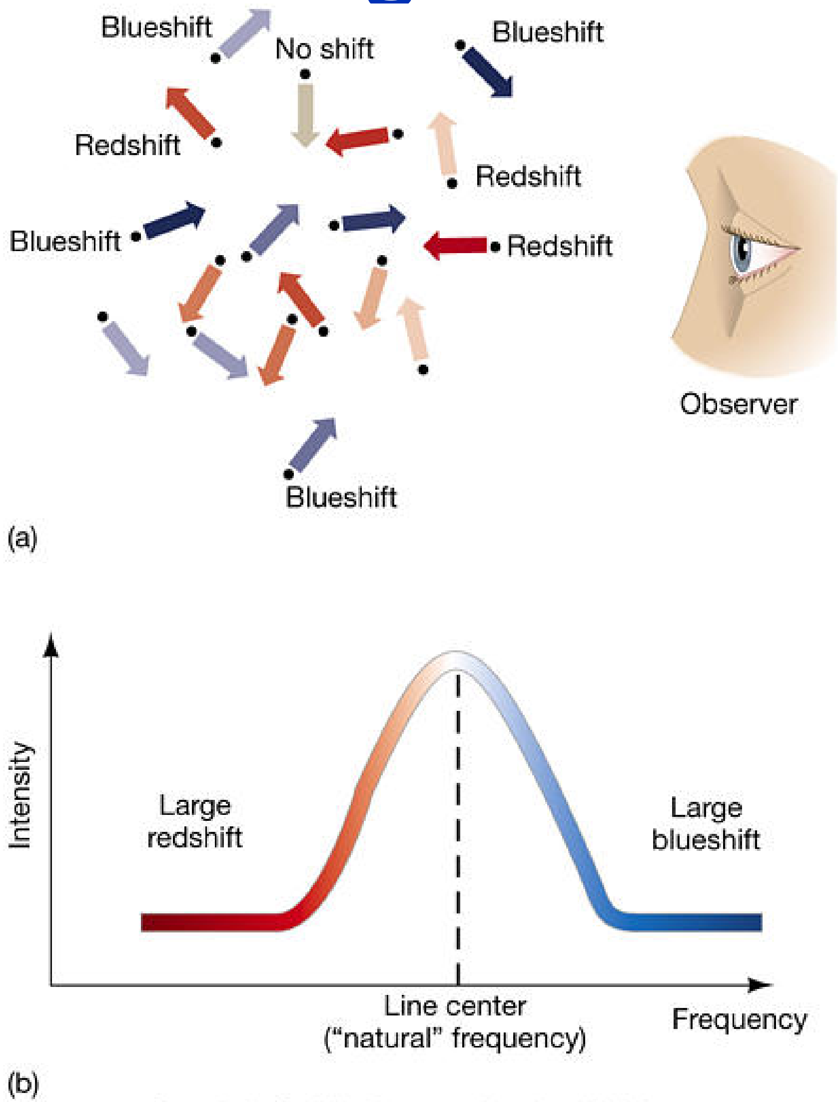
Dipole approximation

- $\Delta S=0$
- $\Delta L=0,\pm 1$
- $\Delta l= \pm 1$
- $\Delta J=0,\pm 1$(not $0 \rightarrow 0$)
- $\Delta M_J=0,\pm 1$(not $0 \rightarrow 0$ if $\Delta J=0$)

Line emission which do not follow these selection rules are denoted as forbidden lines.

Forbidden line emission does not imply that these emission lines are not observable in space but characterized by a much lower transition probability in comparison to allowed transitions.

Doppler broadening



Doppler broadening

- The gas temperature leads to thermal motions of the emitting and absorbing ions and atoms, these motions can be described by the Maxwell-Boltzmann distribution

$$n(v_r) = N\sqrt{\frac{m}{2\pi kT}}\, e^{\left(-\frac{mv_r^2}{2kT}\right)}$$

$$\upsilon - \upsilon_0 = \upsilon_0 \frac{v_r}{c} \Rightarrow v_r = c\left(\frac{\upsilon}{\upsilon_0} - 1\right)$$

and

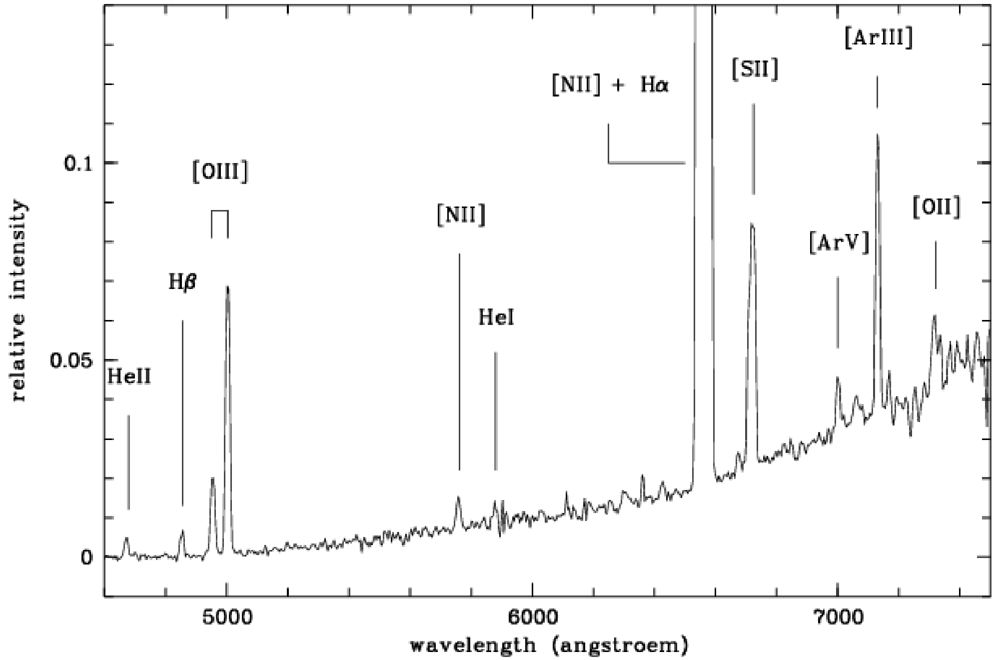
$$\Delta\nu_D = \frac{\nu_0}{c}\sqrt{\frac{2kT}{m}}$$

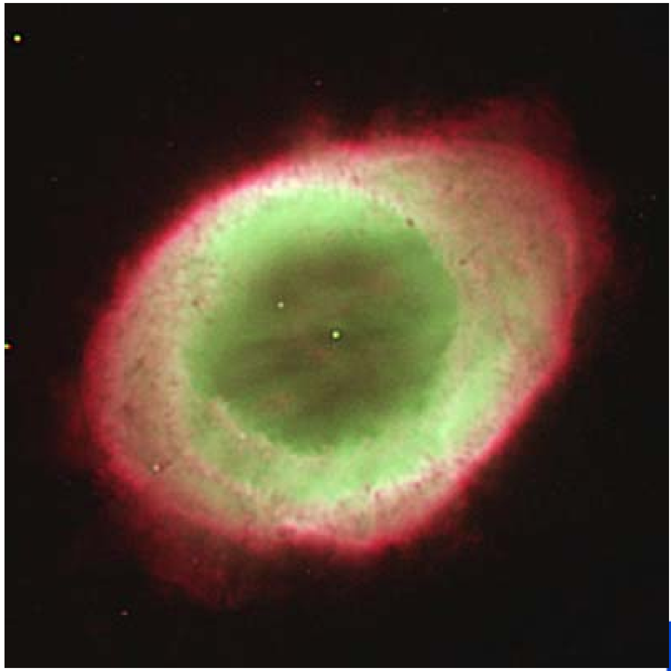
$$I(\nu) = \frac{1}{\Delta\nu_D\sqrt{\pi}}\, e^{\left(-\frac{(\nu-\nu_0)^2}{\Delta\nu_D^2}\right)}$$

Forbidden transitions

- Some transitions are metastable (lifetime ~ 0.1 sec) because they are "forbidden„ ($\Delta J=\pm1$, $\Delta L=0$, $\Delta S=0$), here 2-photon decay makes the work

2^2S -> 1^2S H(2S) -> $H(1s)+h\nu_1+h\nu_2$





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Infrared and radio recombination lines

- Important (forbidden) emission lines are in the radio range of hydrogen-like ions, namely H^+, He^+, He^{++}, C^+ ..., the wavelength of the emission line is

$$\lambda^{-1}_{n,n'} = R_A Z^2 \left(\frac{1}{n^2} - \frac{1}{n'^2} \right) \text{ with}$$

$$R_A = 1.097 \cdot 10^5 \left(1 - \frac{m_e}{m_A} \right) \left[\text{cm}^{-1} \right] \text{ for small n and}$$

$n \approx n'$ these lines are in the infared and radio regime

Infrared and radio recombination line

- Transitions between **fine structure** levels are **magnetic dipol transitions** ($\Delta J=\pm 1$, $\Delta L=0$, $\Delta S=0$)
- Their transition probability is about four orders of magnitude smaller than of the allowed electric dipole transition
- Accordingly, the emission lines are **usually optically thin** and are **excited by collisions** of the atoms
- Because the electronic masses of the different isotopes are pretty much comparable, the different isotopes can not be differentiated by their corresponding fine structure line emission, example[^{13}CII] and [^{12}CII] 158µm emission line

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Infrared and radio recombination line

- Fine structure lines of

  C^+, N^{++}, Ne^+, Ar^+, Si^+, O^{+++} and S^{+++} have 1p or 5p electrons in their valence shell, this yields fine structure doublets and a single fine structure line is the ground state

  C^0, O^0, Si^0, N^+, O^{++}, S^{++} and Ne^{++} with 2 p and 4 p electrons show up with triplets and doublets in the ground state

  Ne^0, Ar^0, He^0, O^+, S^+ with 3p electrons have ground fine structure line emission

Infrared and radio recombination line

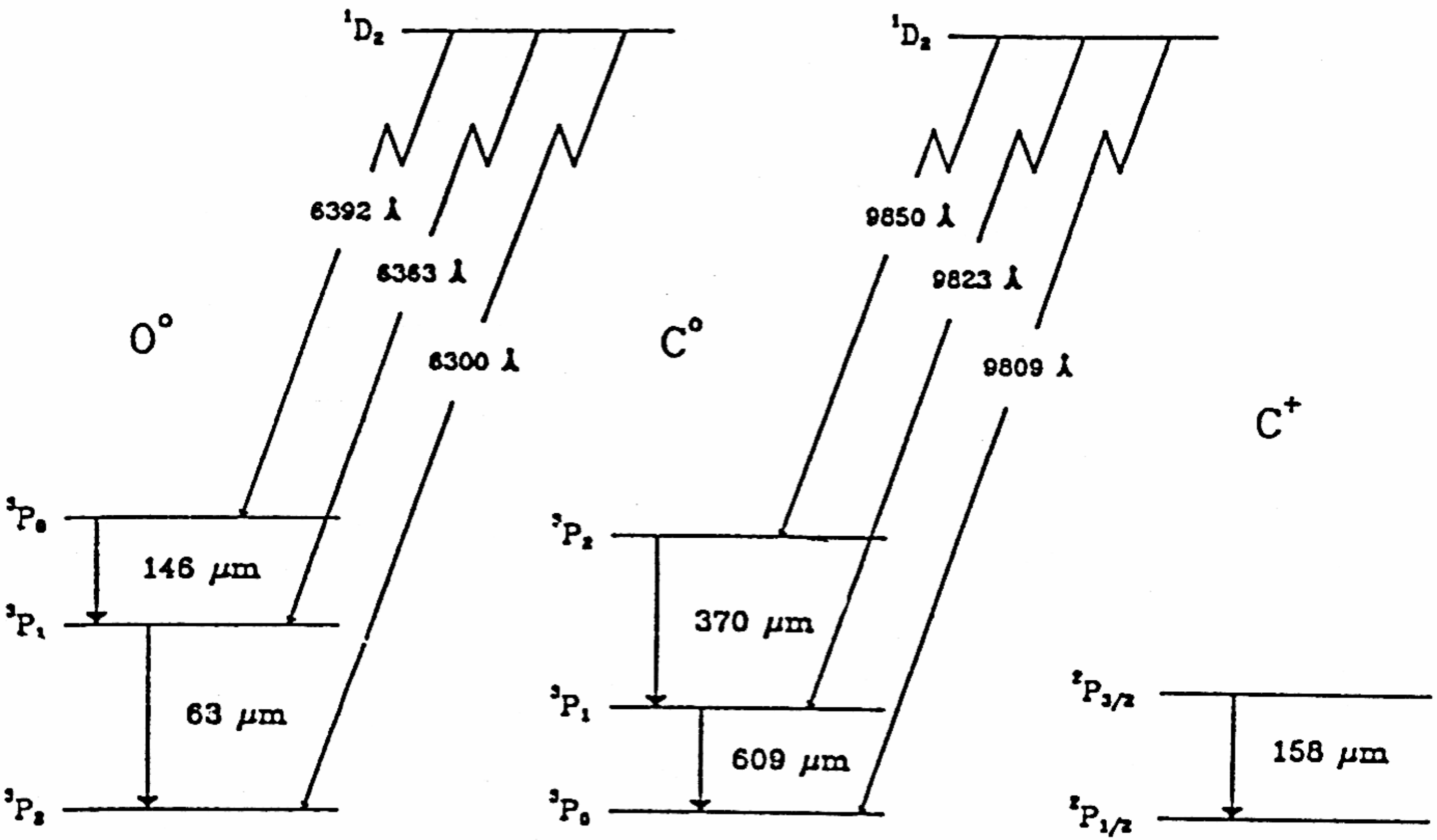

Fig. 2. Lowest energy levels and fine structure transitions of O^0, C^0 and C^+

Radiation transfer

Radiation transfer

- Emission

$$dE = j_\nu dV d\Omega dt = j_\nu ds dA d\Omega dt = dI_\nu dA d\Omega dt$$

$$dI_\nu = j_\nu ds \left[\mathrm{erg\ cm^{-3} s^{-1} sr^{-1} Hz^{-1} \cdot cm}\right]$$

- For an isotropic emitter

$$j_\nu = \frac{1}{4\pi} P_\nu$$

Radiative transfer

- Absorption
- Quantities: number of absorbing objects, cross section of the absorbing objects with photons

$$n \cdot dV = n \cdot dA \cdot ds \text{ total number of absorbers}$$

$$n \cdot \sigma_\nu \cdot dA \cdot ds \text{ total area of absorbers}$$

- The absorbed amount of energy

$$-dI_\nu \, dA d\Omega \, dt d\nu = I n \sigma_\nu \, dA ds d\Omega \, dt d\nu \text{ or}$$

$$dI_\nu = -I_\nu n \sigma_\nu ds = -\kappa_\nu I_\nu ds$$

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Radiative transfer

- The radiative transfer equation

$$\frac{dI_\nu}{ds} = j_\nu - \kappa_\nu I_\nu$$

- Only emission κ_ν =0

$$\frac{dI_\nu}{ds} = j_\nu$$

$$I_\nu = I_\nu(0) + \int_0^s j_\nu(s')ds'$$

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Radiative transfer

- Only absorption $j_\nu = 0$

$$\frac{dI_\nu}{ds} = -\kappa_\nu I_\nu$$

$$\Rightarrow I_\nu(s) = I_0 e^{-\int_0^s \kappa_\nu(s')ds'} = I_0 e^{-\tau_\nu}$$

- The optical depth is defined accordingly

$$\tau_\nu(s) = \int_0^s \kappa_\nu(s')ds' = \int_0^s n(s')\cdot\sigma_\nu\cdot ds' = n\cdot\sigma_\nu\cdot s$$

- $\tau<1$ optical thin
- $\tau>1$ optical thick

Radiative transfer

- Solution for mixed cases

$$\frac{dI_\nu}{ds} = \kappa_\nu \frac{dI_\nu}{d\tau_\nu} = j_\nu - \kappa_\nu I_\nu$$

$$\Rightarrow \frac{dI_\nu}{d\tau_\nu} = \frac{j_\nu}{\kappa_\nu} - I_\nu =: S_\nu - I_\nu$$

$$\Rightarrow I_\nu(\tau_\nu) = I_0 e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau'_\nu)} S(\tau'_\nu) d\tau'_\nu$$

Radiative transfer

- Thermodynamic equilibrium

$$\frac{dI_\nu}{ds} = S_\nu - I_\nu = 0$$

$$\Rightarrow S_\nu = I_\nu = B_\nu$$

- With

$$B_\nu = \frac{2h\nu^3}{c^2} \frac{1}{\exp\left(\frac{h\nu}{kT}\right) - 1}$$

which is the Planck-function

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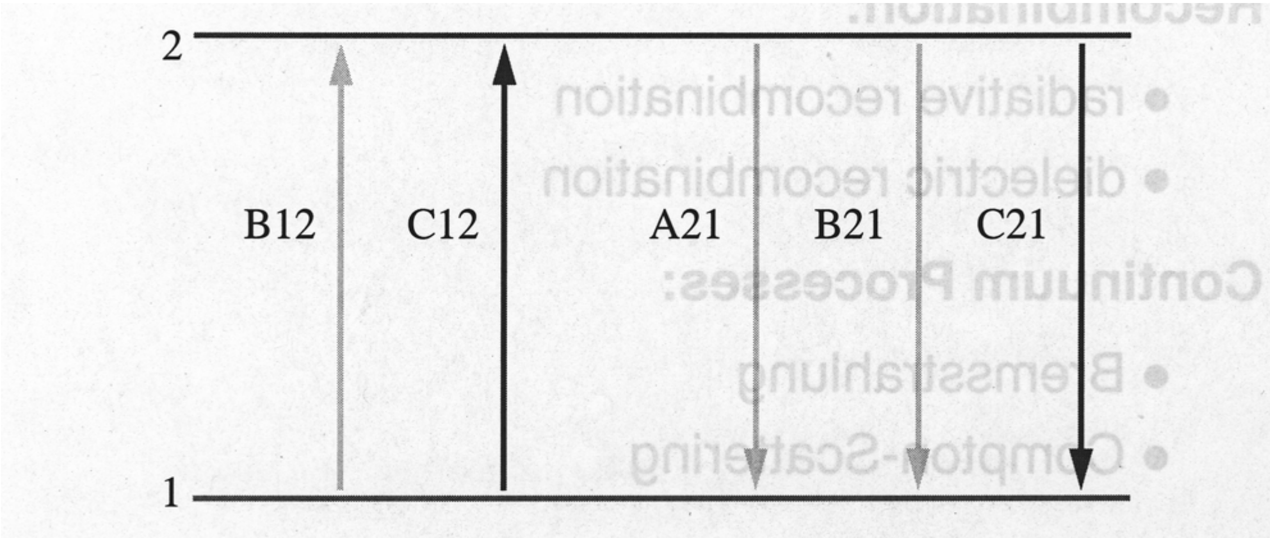
Excitation and de-excitation

Einstein coefficients and collisions



Photoionization

- $(Z,z) + \gamma \rightarrow (Z,z+1) + e^-$
- A photon with an energy in excess of 13.6 eV can ionize neutral hydrogen

  $H + h\nu \rightarrow H^+ + e$

  $E_{kin}(e) = h\nu - 13.6$ eV
- Cross section is roughly

$$\sigma(\nu) \approx 6.3 \cdot 10^{-18} \left(\frac{\nu_{ion}}{\nu} \right)^{-3} \mathrm{cm}^2$$

Collisional Ionization

- $(Z,z) + e^- \rightarrow (Z,z+1) + e^- + e^-$
- The collision cross section is a function of the gas temperature $\Leftrightarrow$ average velocity distribution and depends on the electron density

  $\gamma coll.(z,z+1)=n_e C_z(z,T_e) := \langle v\sigma_i \rangle$

Recombination

- Inverse process of ionization
- (Z,z+1) + e^- $\rightarrow$ (Z,z) + γ + γ ...
- Recombination rate depends on the electron and nucleon volume densities $n(H^+) \cdot n(e)$ and the average velocity distribution of the gas constituents
- The recombination cross section can be described by the Milne relation

$$\sigma_{rec}(\mathrm{v}) = \frac{g_{z,n}}{g_{z+1}} \cdot \left(\frac{\mathrm{h}\nu}{m c \mathrm{v}} \right)^2 \sigma_{ni}(\nu)$$

Dielectronic recombination

- $(Z,z+1) + e^- \rightarrow (Z,z+1)^* \rightarrow (Z,z) + \gamma + \gamma \ldots$
- The dielectric recombination describes a capture of an electron by an ion which binds the electron in an excited state followed by a relaxation of the system by the emission of photons.
- The transition probabilities depend on the same physical parameters as for the recombination plus the ionization structure of the gas.

Recombination

- The recombination rate can be approximated by the empirical formula

$$\alpha \approx 4 \cdot 10^{-13} \left(\frac{10^4 [\mathrm{K}]}{T} \right)^{\frac{3}{4}} \left[\mathrm{cm}^3\ \mathrm{s}^{-1}\right]$$

- The recombination time is

$$\tau \approx \frac{1}{n(e) \cdot \alpha} \approx \frac{3 \cdot 10^{12} [\mathrm{s}]}{\mathrm{n(e)}} \approx \frac{10^5}{n(e)} [\mathrm{a}]$$

Radiative transfer

- The amount of energy emitted spontaneously in a volume in a certain direction is
- The amount of energy absorbed by the same volume is
- The amount of energy emitted by stimulated emission is
- Using

$$dE_e(\nu) = \mathrm{h}\nu_0 N_2 A_{21} \varphi_e(\nu) dV \frac{d\Omega}{4\pi} d\nu dt$$

$$dE_a(\nu) = \mathrm{h}\nu_0 N_1 B_{12} \frac{4\pi}{\mathrm{c}} I_\nu \varphi_a(\nu) dV \frac{d\Omega}{4\pi} d\nu dt$$

$$dE_s(\nu) = \mathrm{h}\nu_0 N_2 B_{21} \frac{4\pi}{\mathrm{c}} I_\nu \varphi_e(\nu) dV \frac{d\Omega}{4\pi} d\nu dt$$

$$\varphi_e(\nu) = \varphi_a(\nu) = \varphi(\nu) \text{ and } dV = d\sigma \cdot ds$$

$$dE_e(\nu) + dE_s(\nu) - dE_a(\nu) = dI_\nu d\Omega d\sigma ds dt$$

$$= \frac{\mathrm{h}\nu}{4\pi}\left[N_2 A_{21} + N_2 B_{21} \frac{4\pi}{\mathrm{c}} I_\nu - N_1 B_{12} \frac{4\pi}{\mathrm{c}} I_\nu\right] \varphi_\nu d\Omega d\sigma ds dt$$

Radiative transfer

- This gives

$$\frac{dI_\nu}{ds} = -\frac{\mathrm{h}\nu}{\mathrm{c}}\left(N_1 B_{12} - N_2 B_{21}\right) I_\nu \varphi(\nu) + \frac{\mathrm{h}\nu_0}{4\pi} N_2 A_{21} \varphi(\nu)$$
$$= -\kappa_\nu I_\nu + \varepsilon_\nu$$

- Using the relation between spontaneous emission and absorption, we find for the absorption

$$\kappa_\nu = \frac{\mathrm{h}\nu}{\mathrm{c}} N_1 B_{12} \left(1 - \frac{g_1 N_2}{g_2 N_1}\right) \varphi(\nu)$$

- And for the emission

$$\varepsilon_\nu = \frac{\mathrm{h}\nu_0}{\mathrm{c}\pi} N_2 A_{21} \varphi(\nu)$$

- In case of LTE

$$\frac{N_2}{N_1} = \frac{g_2}{g_1} \exp\left\{-\frac{\mathrm{h}\nu_0}{\mathrm{k}T}\right\}$$

$$\kappa_\nu = \frac{\mathrm{c}^2}{8\pi} \frac{1}{\nu_0} \frac{g_2}{g_1} N_1 A_{21} \left(1 - \exp\left\{-\frac{\mathrm{h}\nu_0}{\mathrm{k}T}\right\}\right) \varphi(\nu)$$

Radiative transfer

- The exponential correction factor for stimulated emission becomes important in the ultraviolet wavelength regime only in very hot environments
- In the radio regime the correction term is important for mm-wavelength regime and extreme low temperature environments

Equilibrium considerations

ISM in equilibrium?

- Thermal equilibrium denotes, that each excitation process has the same likelihood as the corresponding de-excitation process.

  This is not realized in the ISM!

THE ISM IS NOT IN EQUILIBRIUM!

ISM in equilibrium?

- Maxwell velocity distribution
  - Collision thermalize the velocity distribution
  - $T_{\mathrm{kin}} = T_{\mathrm{e}} = T_{\mathrm{i}} = T_{\mathrm{n}}$
- Boltzmann population of energy levels
  - $T_{\mathrm{ex}} \neq T_{\mathrm{kin}}$
- Planck spectrum
  - ISM spectrum ≠ Black Body

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Radiation transfer in non-equilibrium situations

Radiative transfer: rate equation

- To quantify the emission and absorption coefficients it is necessary to know both, the Einstein coefficients and the number densities N_1 and N_2. As claimed above, this is not the case under „normal“ astronomical conditions within the ISM.
- In the special case of Local Thermal Equilibrium (LTE) the population of the energy levels is according to the Boltzmann distribution.
- In all other cases, one has to solve the rate equation

$$\frac{dN_j}{dt} = -N_j \sum_k \sum_y R^y_{jk} + \sum_k N_k \sum_y R^y_{kj}$$

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Rate equation I (absorption and emission)

- Assuming the simple case that only spontaneous emission and absorption changes the population of two different energy levels, the rate equation is

$$N_0 B_{01} \overline{U} = N_1 \left(A_{10} + B_{10} \overline{U} \right)$$

- With

$$\overline{U} = \frac{4\pi}{\mathrm{c}} \overline{I}\,,\ \mathrm{A}_{10} = \frac{g_0}{g_1} B_{01} \frac{8\pi \mathrm{h} \nu^3}{\mathrm{c}^3} \text{ and } \mathrm{g}_0 B_{01} = g_1 B_{10}$$

- We find

$$\frac{N_1}{N_2} = \frac{B_{01}}{B_{10}} \frac{\overline{I}}{\frac{2\mathrm{h}\nu^3}{\mathrm{c}^2} + \overline{I}} = \frac{g_1}{g_2} \exp\left(-\frac{\mathrm{h}\nu}{\mathrm{k}T} \right)$$

- Accordingly, in this simple case the level population is determined by the Boltzmann distribution. Note: the temperature is NOT the thermodynamic temperature of the considered system!

Rate equation II (+ collisions)

- Assuming that next to emission and absorption processes also collisions are involved:

$$N_1\left(C_{12}+B_{12}\overline{U}\right)=N_2\left(A_{21}+B_{21}\overline{U}+C_{21}\right)$$

- The collision rate is

$$C_{ik}=N\gamma_{ik}=N\int_0^\infty \sigma_{ik}(\mathrm{v})\mathrm{v}f(\mathrm{v})d\mathrm{v}$$

- Using

$$g_i\gamma_{ik}=g_k\gamma_{ki}\exp\left\{-\frac{h\nu}{kT_K}\right\}$$

- T_K is the temperature which determines the velocity distribution, the kinetic temperature

$$f(\upsilon)=\sqrt{\frac{2}{\pi}}\upsilon^2\left(\frac{m_r}{kT_K}\right)^{\frac{3}{2}}\exp\left\{-\frac{m_r\upsilon^2}{2kT_K}\right\}$$

$$\frac{N_2g_1}{N_1g_2}=\exp\left\{-\frac{h\nu}{kT_{ex}}\right\}$$

- It follows

$$=\exp\left\{-\frac{h\nu}{kT_b}\right\}\frac{A_{21}+C_{21}\exp\left(-\frac{h\nu}{kT_k}\right)\left\{\exp\left(\frac{h\nu}{kT_b}\right)-1\right\}}{A_{21}+C_{21}\left(1-\exp\left(\frac{h\nu}{kT_b}\right)\right)}$$

Line diagnostic

Diagnostics of the ISM

- Ionization
  - Photo ionization
  - Collisional ionization
  - Auger-Ionization
- Recombination
  - Radiative recombination
  - Dielectric recombination
- Continuum processes
  - Bremsstrahlung
  - Compton scattering

Line diagnostic (density)

- Choose element with two energy levels about the same excitation energy. Depending on the density the levels will be depopulated by radiation of collisional de-excitation

$$n_1 n_e C_{12} = n_2 A_{21} + n_2 n_e C_{21}$$

$$n_1 n_e C_{13} = n_3 A_{31} + n_3 n_e C_{31}$$

$$\Rightarrow \frac{n_2}{n_1} = \frac{n_e C_{12}}{A_{21} + n_e C_{21}} = (LTE) \frac{n_e}{A_{21} + n_e C_{21}} \frac{g_2}{g_1} C_{21} \exp\left(-\frac{E_{12}}{\mathrm{k}T} \right)$$

Line diagnostic (density)

- With

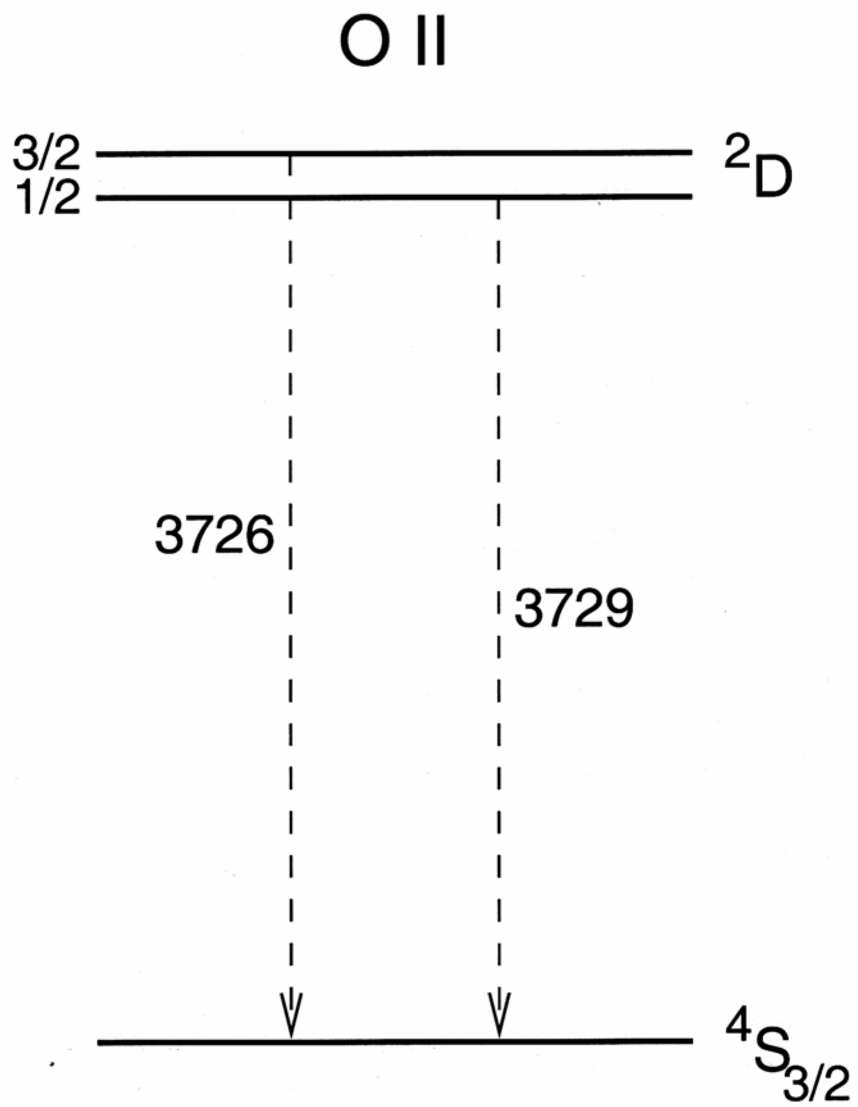
$$4\pi I_{21} = A_{21} n_2 \mathrm{h} \nu_{21}$$

- We find

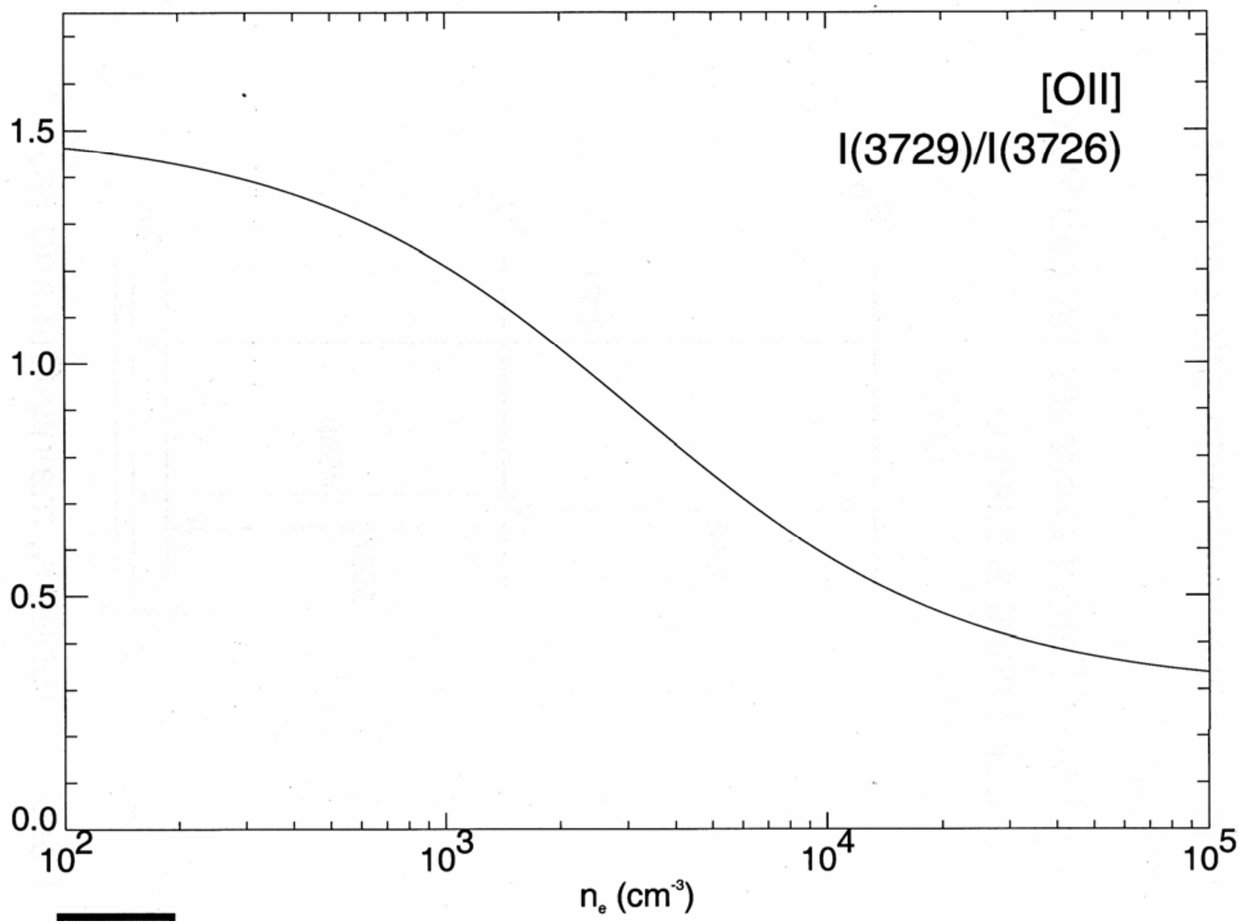
$$\frac{I_{21}}{I_{31}} = \frac{A_{21} n_2 \mathrm{h} \nu_{21}}{A_{31} n_3 \mathrm{h} \nu_{31}} \text{ using } \nu_{21} \approx \nu_{31}$$

$$\frac{I_{21}}{I_{31}} = \frac{A_{21} n_2}{A_{31} n_3}$$

Line diagnostic (density)



Line diagnostic (density)

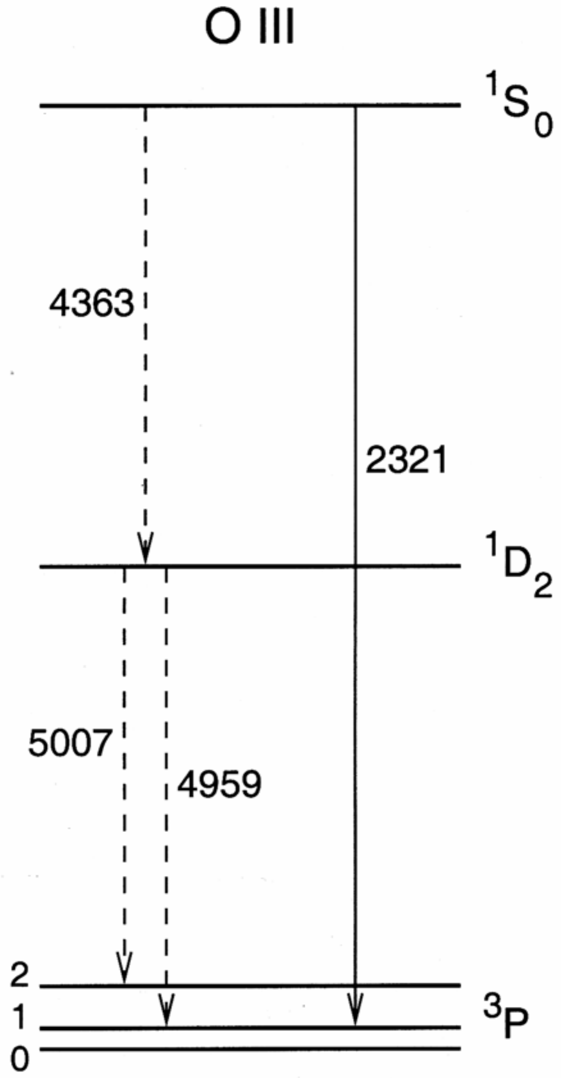


Line diagnostic (density)

Table 1. Infrared fine structure lines [d)]

Species	Excitational Potential [eV]	Ionization Potential [eV]	Transitions	λ [μm]	A [s^{-1}]	n_{crit} [cm^{-3}] [a)]
C	–	11.26	^{3}P, $J = 1 \rightarrow 0$	609.1354	7.9(-8)	4.7(2) 1. (4) for H_2 [a)]
			$2 \rightarrow 1$	370.415	2.7(-7)	1.2(3)
CII	11.26	24.38	^{2}P, $J = \frac{3}{2} \rightarrow \frac{1}{2}$	157.7409	2.4(-6)	2.8(3) 5. (3) for H_2 50 for electrons
O	–	13.62	^{3}P, $J = 1 \rightarrow 2$	63.18372	8.95(-5)	4.7(5) $T_{300}^{-1/2}$ [b)] 7. (5) $T_{300}^{-1/2}$ for H_2
			$0 \rightarrow 1$	145.52547	1.7(-5)	9.5(4) $T_{300}^{-1/2}$ $\geq$1. (5) $T_{300}^{-1/2}$ for H_2 [a)]
Si	–	8.15	^{3}P, $J = 1 \rightarrow 0$	129.68173	8.25(-6)	2.4(4)
			$2 \rightarrow 1$	68.473	4.2(-5)	8.4(4)
SiII	8.15	16.35	^{2}P, $J = \frac{3}{2} \rightarrow \frac{1}{2}$	34.814	2.1(-4)	3.4(5)
S	–	10.36	^{3}P, $J = 1 \rightarrow 2$	25.245	1.4(-3)	1.9(6)
			$0 \rightarrow 1$	56.309	3.0(-4)	7.2(5) but H_2 [a)]
Fe	–	7.87	^{5}D, $J = 3 \rightarrow 4$	24.0424	2.5(-3)	3.1(6)
			$3 \rightarrow 2$	34.7135	1.6(-3)	3. (6)
FeII	7.87	16.18	^{6}D, $J = \frac{7}{2} \rightarrow \frac{9}{2}$	25.9882	2.1(-3)	2.2(6)
			$\frac{5}{2} \rightarrow \frac{7}{2}$	35.491	1.6(-3)	3.3(6)

Line diagnostic (temperature)



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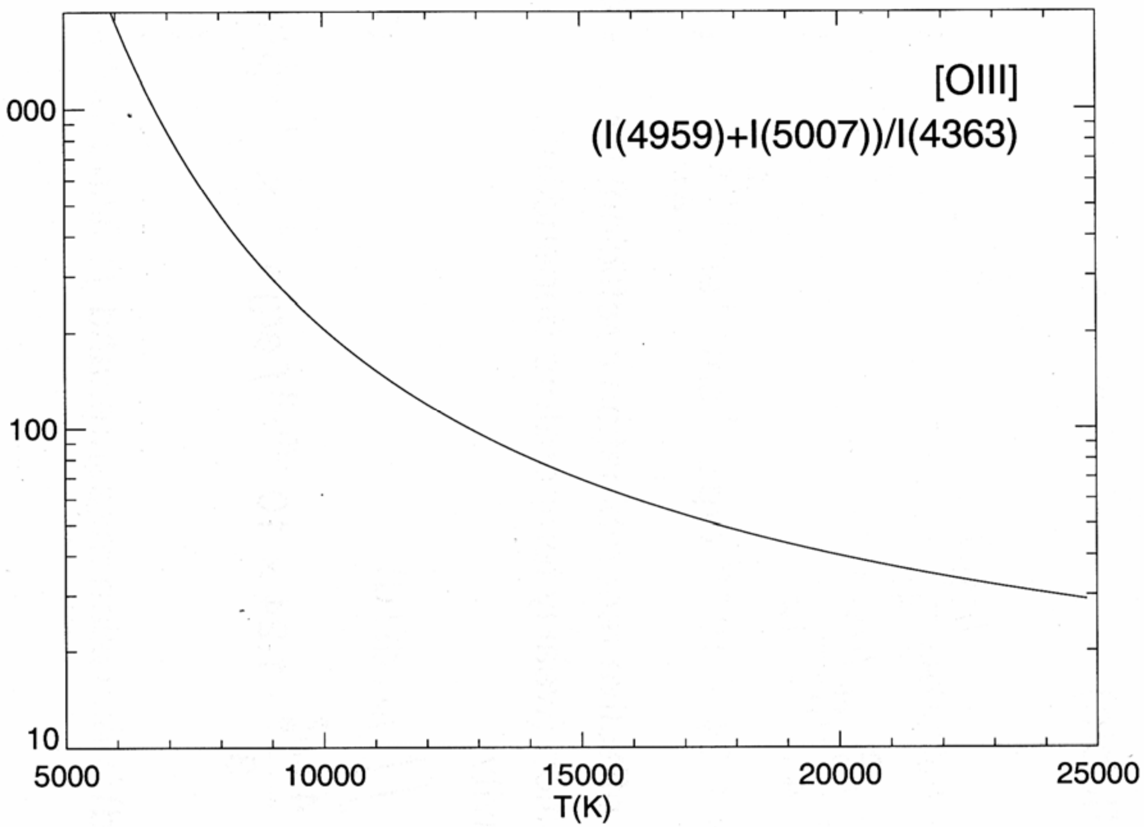
Line diagnostic (temperature)



$$\frac{I(4959+5007)}{4363}=\frac{7.7\exp(3.29\times 10^4/T)}{1+4.5\times 10^{-4}n_e T^{-1/2}}$$

Line diagnostic (temperature)

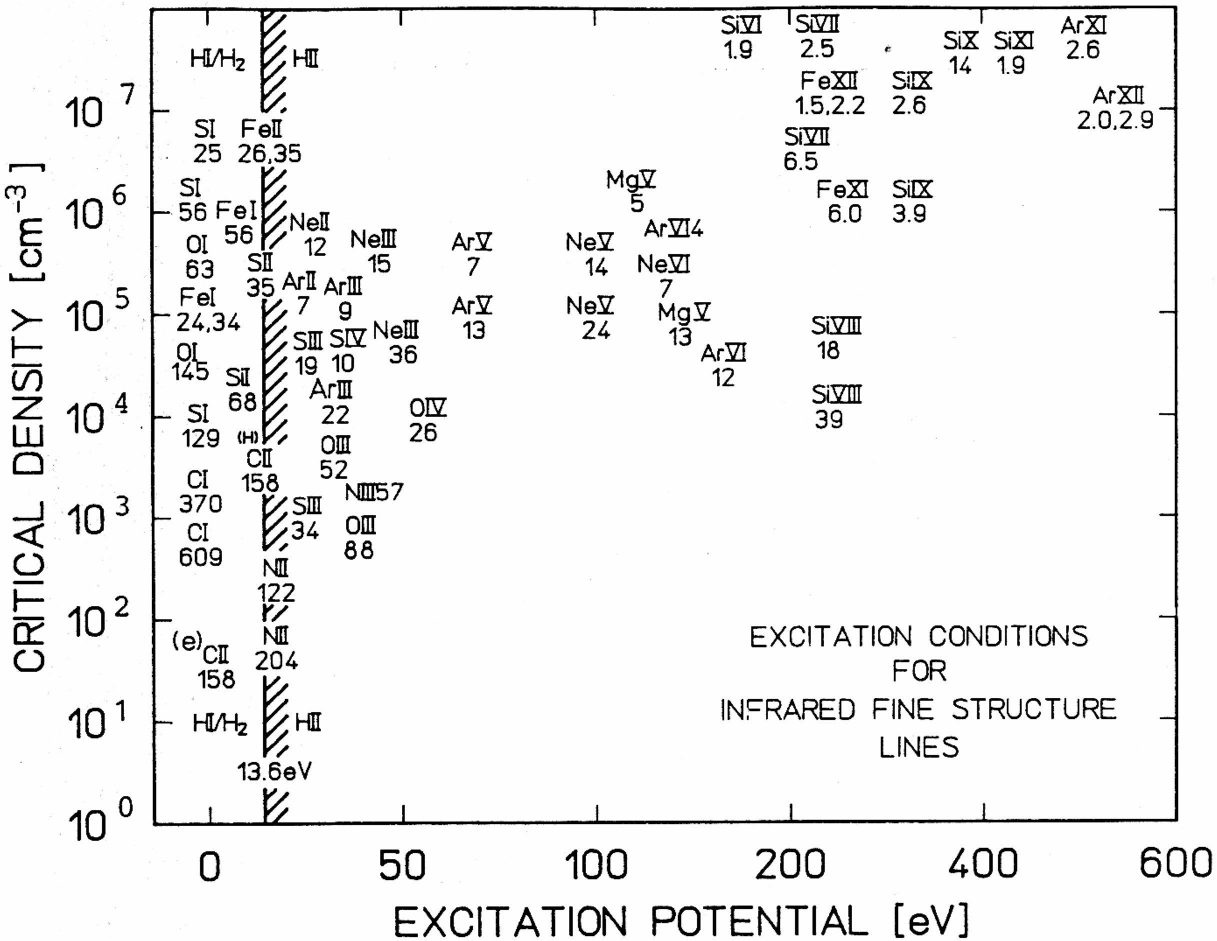


Fig. 7. Infrared fine structure lines as probes of physical conditions in interstellar clouds

Line diagnostic (temperature)

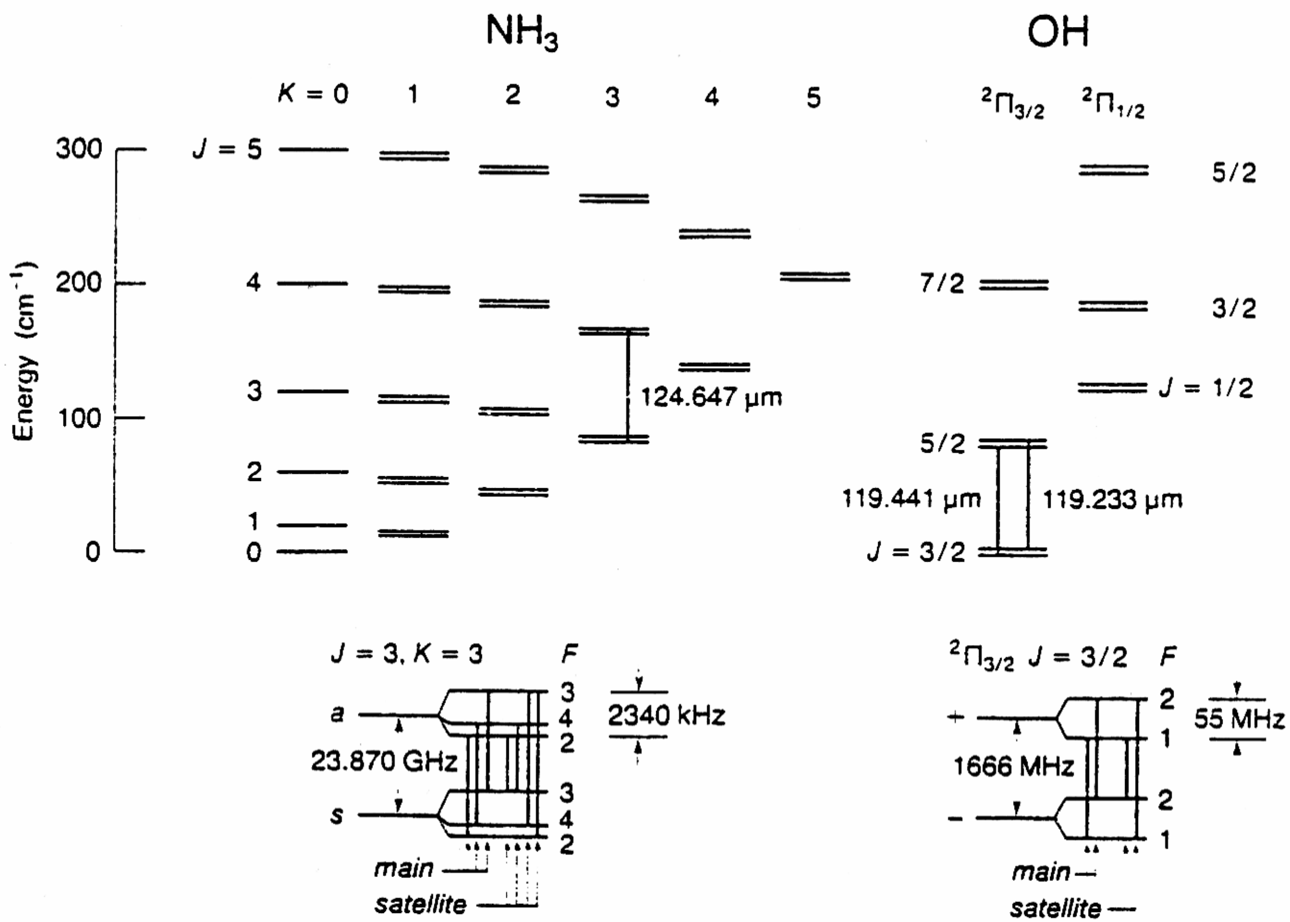


Fig. 5. Rotational levels of NH_3 (left) and OH (right) (adapted from Watson 1982)

Line diagnostic (temperature)

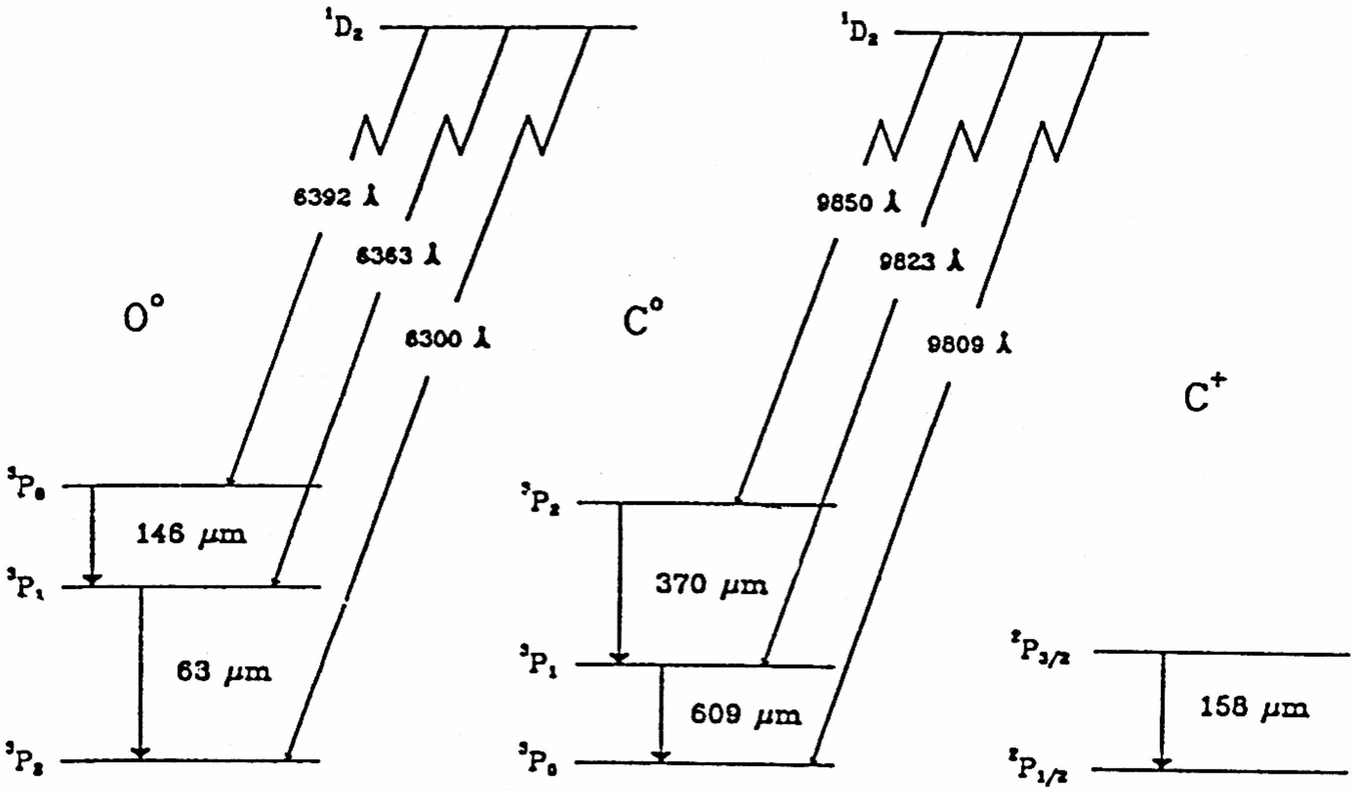


Fig. 2. Lowest energy levels and fine structure transitions of O^0, C^0 and C^+

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Line diagnostic (density and temperature)

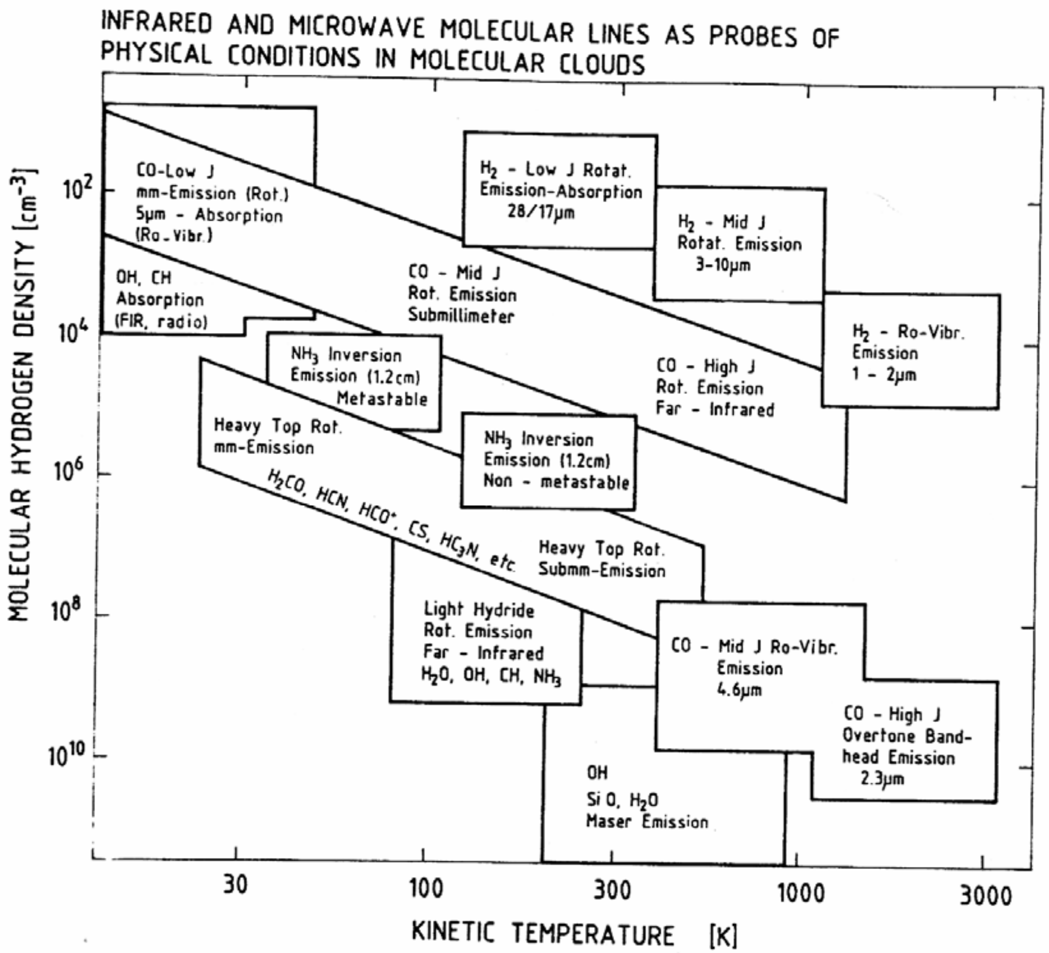


Fig. 8. Molecular lines as probes of physical conditions in interstellar clouds

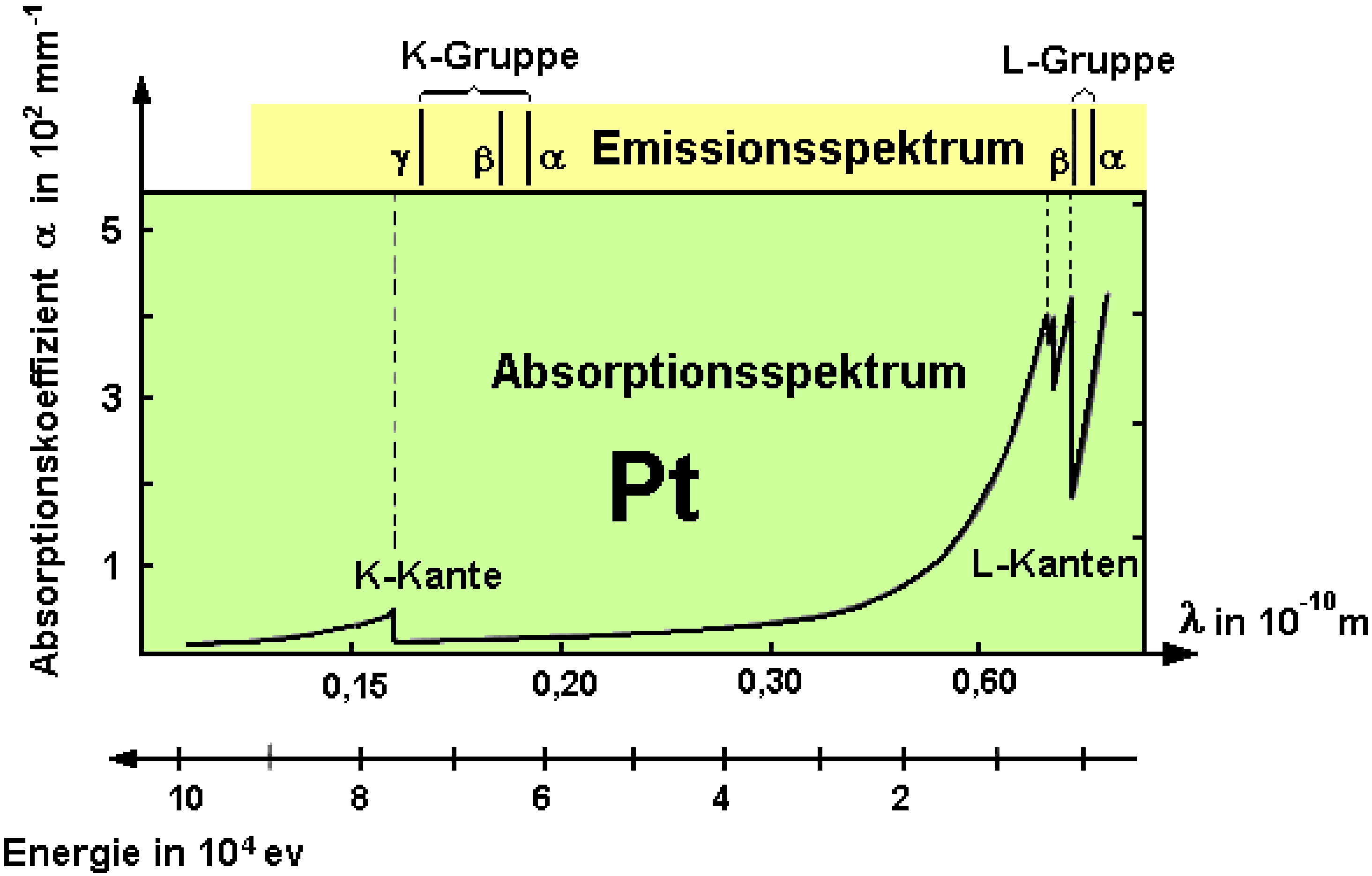
Practical example: soft X-ray radiation

Example: soft X-ray radiation

- The improvement in the diagnostic in medicine was immediately recognized after the the discovery of X-ray by Röntgen in 1895. The X-ray detector was the standard photographic plate.
- The human bones consist manly of Calcium (Z=20) while the muscles consists of Hydrogen (Z=1), Carbon (Z=6), Nitrogen (Z=7) and Oxigen (Z=8)
- Moseley-Gesetz:

$$\upsilon_{K\alpha} \propto (Z-1)^2$$

Example: soft X-ray radiation



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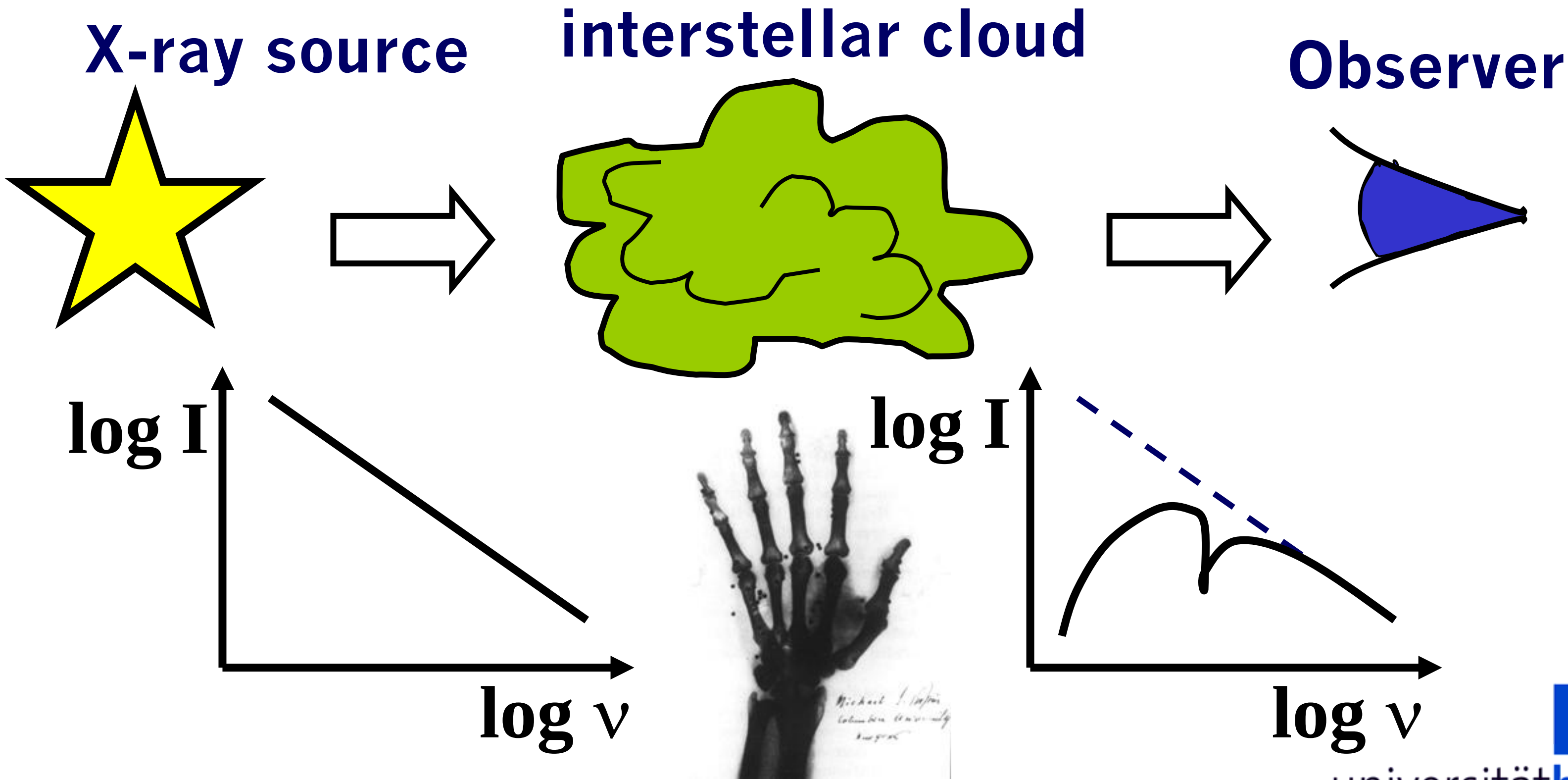
Example: Soft X-ray radiation



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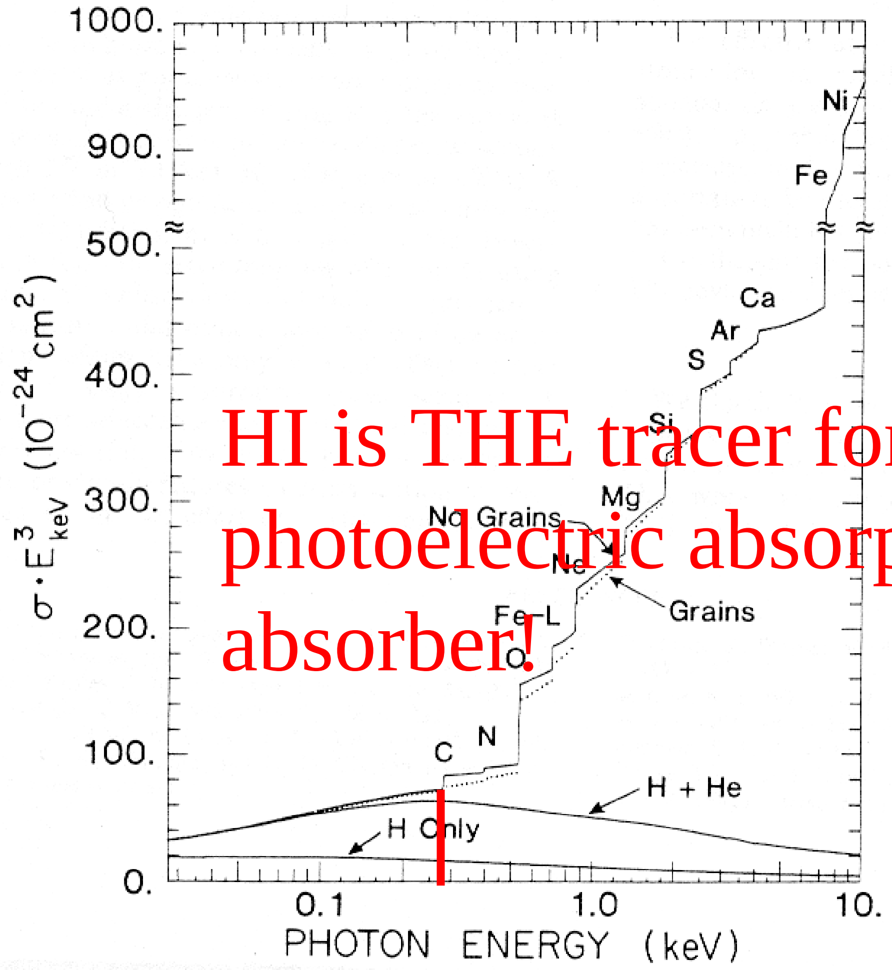
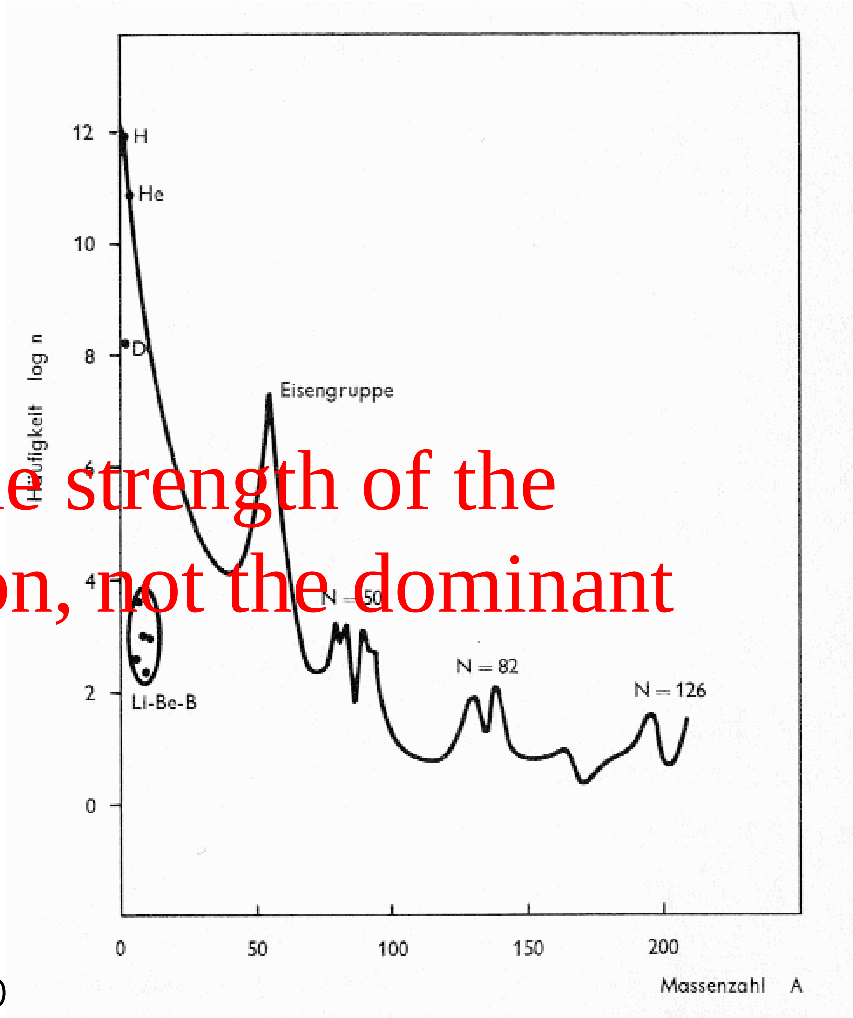
Example: Soft X-ray radiation





HI is THE tracer for the strength of the photoelectric absorption, not the dominant absorber!

Example: soft X-ray absorption

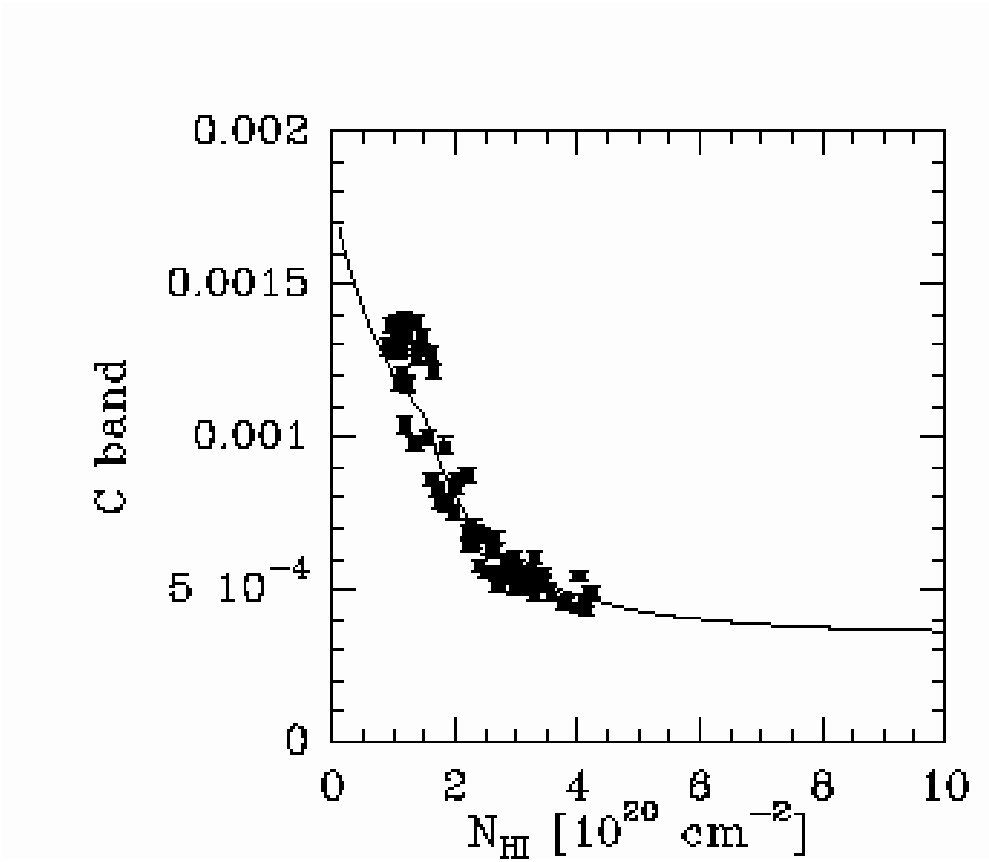
$$I = I_0 \exp(-\sigma_{eff}(E) \cdot N_H)$$

'τ' denotes the optical depth

$$\sigma_{eff} = \sum[-\sigma_Z(E) \cdot n_z/n_H]$$

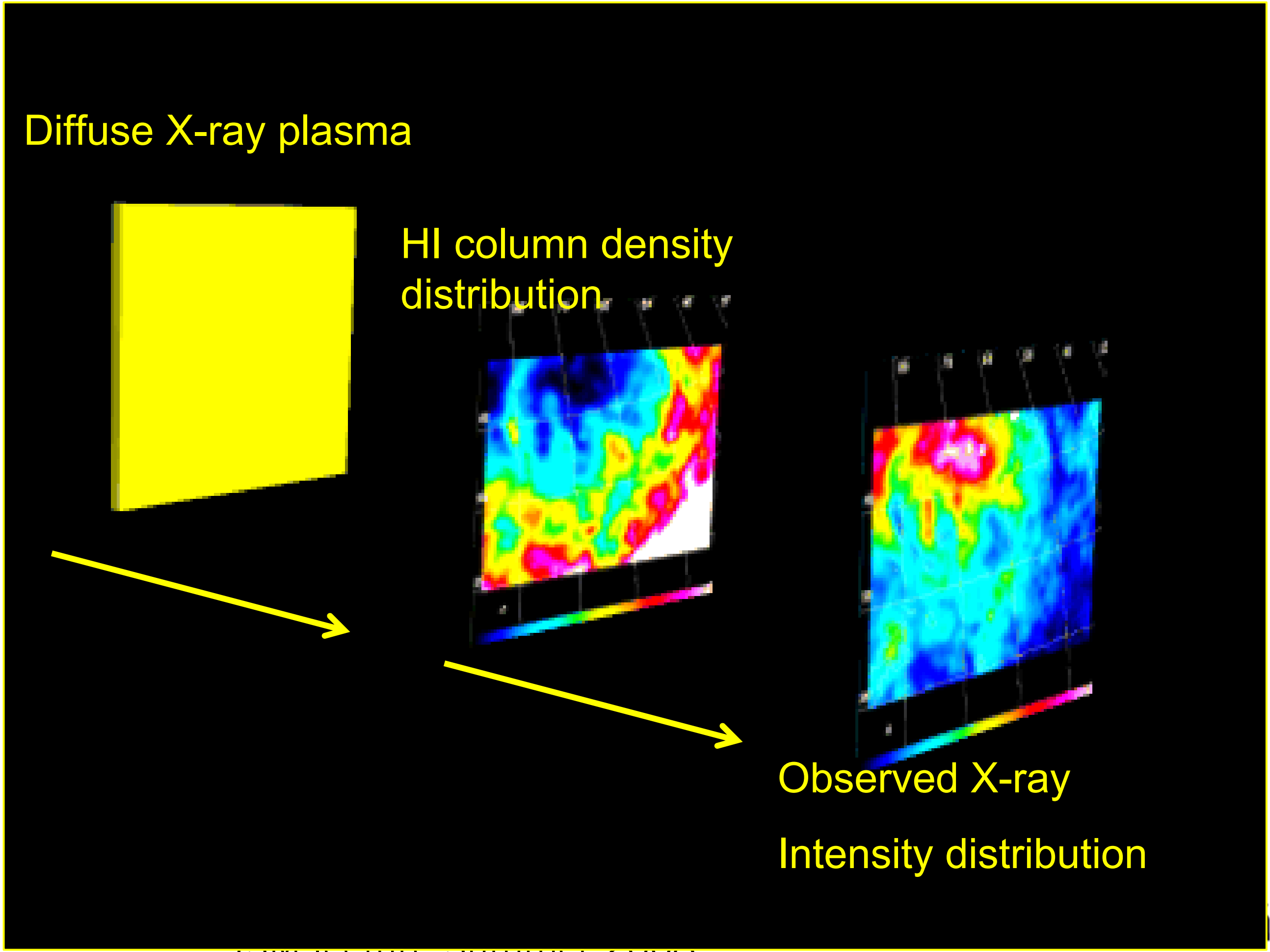
This is the so-called effective photo electric absorption cross section

Example: soft X-ray radiation

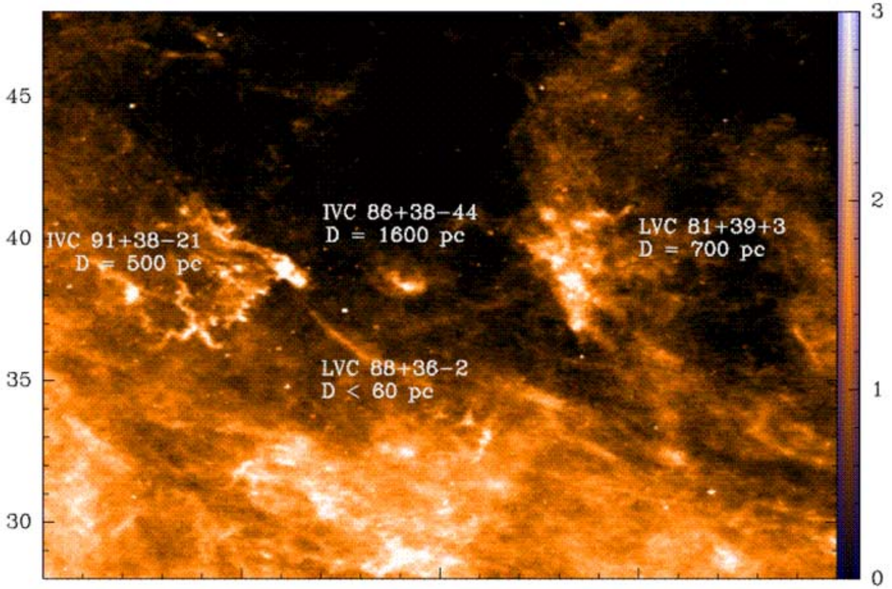


$$I = I_0 + I_1 \cdot \exp(-\sigma_{eff}(E) \cdot N_H)$$

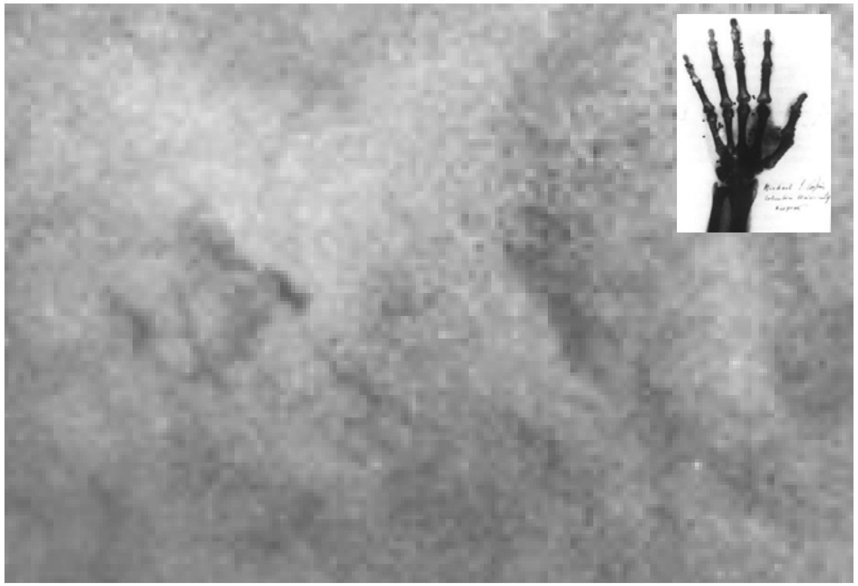
Kerp & Pietz (1998)


Diffuse X-ray plasma
HI column density distribution
Observed X-ray
Intensity distribution

Example: soft X-ray radiation

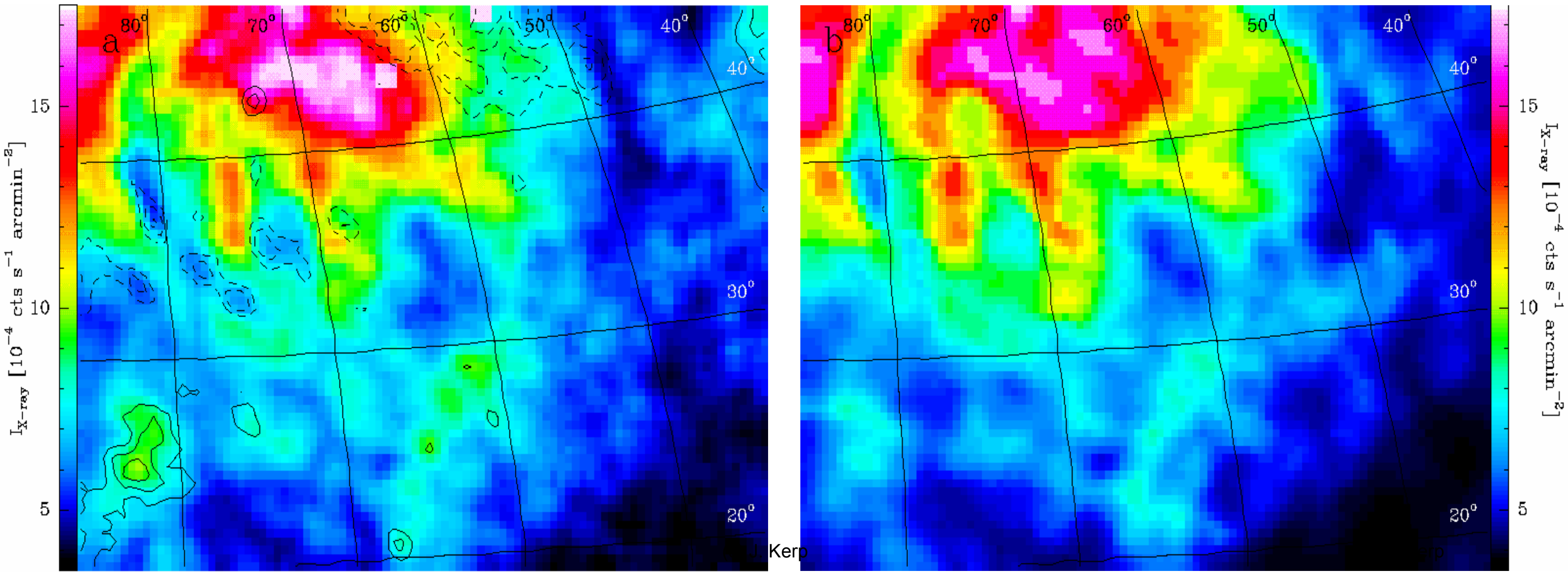


HI 21-cm



0.25 keV ROSAT

Example: soft X-ray radiation

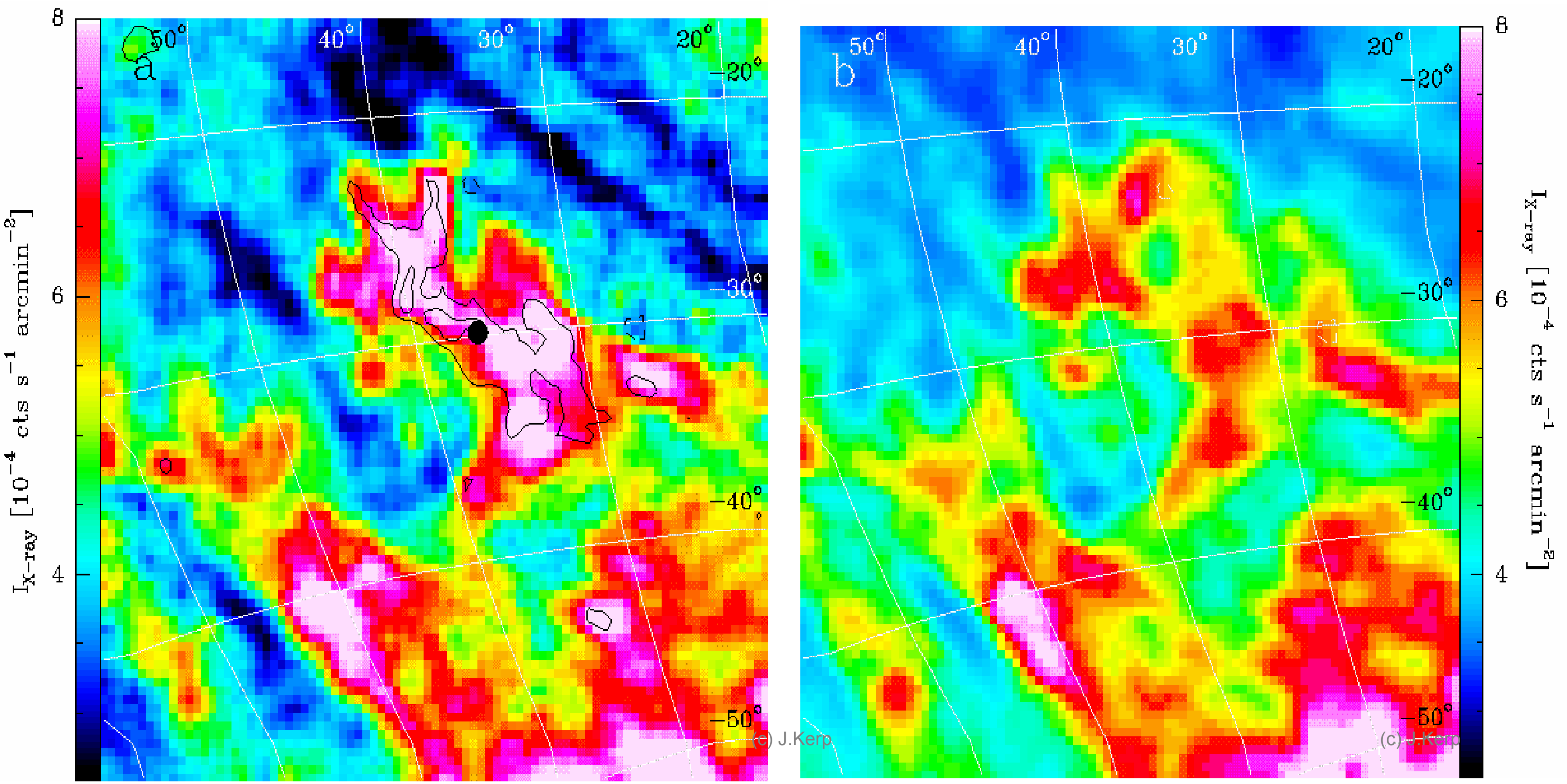


ROSAT 1/4 keV all-sky survey map

Modelled ROSAT map based on the Leiden/Dwingeloo HI 21-cm line data.

Kerp, Burton, Egger et al. 1999, A&A 342, 213

Example: soft X-ray radiation



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