Radiative Processes in Astrophysics

Lecture 13

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Kwang-Il Seon
UST / KASI

Terms for *ns* and *np* subshells

- Draine, Chap. 4

Table 4.1 Terms for ns and np Subshells

Ground configuration	Terms (in order of increasing energy)	Examples
$...ns^1$	$^2S_{1/2}$	H I, He II, C IV, N V, O VI
$...ns^2$	$^1S_0$	He I, C III, N IV, O V
$...np^1$	$^2P^o_{1/2,3/2}$	C II, N III, O IV
$...np^2$	$^3P_{0,1,2}$, $^1D_2$, $^1S_0$	C I, N II, O III, Ne V, S III
$...np^3$	$^4S^o_{3/2}$, $^2D^o_{3/2,5/2}$, $^2P^o_{1/2,3/2}$	N I, O II, Ne IV, S II, Ar IV
$...np^4$	$^3P_{2,1,0}$, $^1D_2$, $^1S_0$	O I, Ne III, Mg V, Ar III
$...np^5$	$^2P^o_{3/2,1/2}$	Ne II, Na III, Mg IV, Ar IV
$...np^6$	$^1S_0$	Ne I, Na II, Mg III, Ar III

- Configurations

  Terms

  Fine Structure (Spin-Orbit Interaction)

  Hyperfine Structure (Interaction with Nuclear Spin)

- Zeeman Effect: When a static magnetic field $\mathbf{B}_0$ is applied, each of the fine-structure levels $\mathcal{L}_J$ splits into $2J{+}1$ energy levels, with energies depending on the value of $\mathbf{J} \cdot \mathbf{B}_0$. The energy splittings are small, of order $\mu_{\rm B} B_0 \approx 5.78 \times 10^{-15} (B_0 / \,\mu{\rm G})\,{\rm eV}$, where $\mu_{\rm B} \equiv e\hbar/2m_e c$ is the **Bohr magneton**. Interstellar magnetic field strengths are of order $1 - 100\,\mu$G, and therefore the Zeeman shifts are too small to be measured for transitions in the sub-mm or shortward ($h\nu \gtrsim 10^{-4}\,{\rm eV}$).

  However, in the case of atomic hydrogen, the hyperfine splitting gives rise to the 21-cm transition, with an energy $h\nu = 5.9 \times 10^{-6}\,{\rm eV}$, and, therefore, an applied field of order $10\,\mu$G shifts the frequency by about one part in 10^8. This shift is much smaller than the frequency shift $v/c \sim 10^{-5}$ due to a radial velocity of a few ${\rm km\,s^{-1}}$, and it would be nearly impossible to detect, except that it leads to a shift in frequency between the two circular polarization modes. The Zeeman effect in H I 21-cm can therefore be detected by taking the *difference* of the two circular polarization signals. This technique has been used to measure the magnetic field strength in a number of H I regions.

2.9 Collisional Excitation

1. Under the conditions of very low density and weak radiation fields,

   (a) The vast majority of the atoms reside in the ground state.

   collisional excitation timescale $\gg$ radiative decay time scale

   This condition will remain true even if the excited state has a radiative lifetime of several second. This is frequently the case for the forbidden transitions observed in ionized astrophysical plasmas.

   (b) flux of an emission line $\propto$ flux number of collisions

   $\propto$ product of the number densities of the two colliding species by the probability that a collision will produce a collisional excitation

   (c) If the energy gap between the ground state and the excited state, E_{12}, is much larger than the mean energy of the colliding species $\sim T$, then, because there are few very energetic collisions, relatively few collisional excitations can occur. Therefore, the resulting emission line will be very much weaker than when $E_{12} \leq kT$.

   $\Longrightarrow$ This gives us the possibility of measuring temperature from the relative strengths of lines coming from excited levels at different energies above the ground state.

2. At high enough densities,
    (a) The collisional timescales are short.
    (b) The population in any upper level is set by the balance between collisional excitation, and the collisional deexcitation out of these levels, and are governed by the Boltzmann equlibrium.
3. At intermediate densities,
    (a) The collisional rates and the radiative decay rates are compatible.
    (b) The intensity of an emission line is determined by both the temperature and the density.
    (c) If the temperature is known, the density can be determined from the intensity ratio of two such lines.

4. Collisional Rate (Two Level Atom)

(a) The collisional cross section is in general varying approximately inversely as the impact energy (because of the focusing effect of the Coulomb force).

$$\begin{aligned}
\sigma_{12}(v) &= \left(\pi a_0^2\right)\left(\frac{hR}{\frac{1}{2}m_e^2 v^2}\right)\frac{\Omega_{12}}{g_1}\ \text{cm}^2 \text{ for } \frac{1}{2}m_e^2 v^2 > E_{12} \\
&= \frac{\pi \hbar^2}{m_e^2 v^2}\frac{\Omega_{12}}{g_1} \\
\text{or } \sigma_{12}(E) &= \frac{h}{8\pi m_e E}\frac{\Omega_{12}}{g_1} \\
\text{where, } a_0 &= \frac{\hbar^2}{m_e e^2} = 5.12 \times 10^{13} \text{ cm, Bohr radius} \\
R &= \frac{m_e e^4}{4\pi \hbar^3} = 109,737 \text{ cm}^{-1}\text{, Rydberg constant}
\end{aligned}$$

(b) The collision strength Ω_{12} is a function of electron velocity (or energy) but is often approximately constant near the threshold, g_1 is the statistical weight of the lower level.

(c) Advantage of using the collision strength

i. It removes the primary energy dependence for most atomic transitions.

ii. The symmetry between the upper and the lower states.

Using the principle of detailed balance, which states that in thermodynamic equilibrium each microscopic process is balanced by its inverse,

$$n_e n_1 v_1 \sigma_{12}\left(v_1\right) f\left(v_1\right) dv_1 = n_e n_2 v_2 \sigma_{21}\left(v_2\right) f\left(v_2\right) dv_2,$$

where v_1 and v_2 are related by $\frac{1}{2}m_e v_1^2 = \frac{1}{2}m_e v_2^2 + E_{12}$, and using the Boltzman equation of thermodynamic equilibrium,

$$\frac{n_2}{n_1} = \frac{g_2}{g_1}\exp\left(-\frac{E_{12}}{kT}\right)$$

we derive the following relation

$$g_1 v_1^2 \sigma_{12}\left(v_1\right) = g_2 v_2^2 \sigma_{21}\left(v_2\right),$$

and the symmetry of the collision strength between levels

$$\Omega_{12} = \Omega_{21}.$$

(d) Collisional excitation and de-excitation rates

If Ω_{21} is a constant, the total collisional de-excitation rate per unit volume per unit time is

$$\begin{aligned} R_{21} &= n_e n_2 q_{21} \\ &= n_e n_2 \int_0^\infty v \sigma_{21}(v) f(v)\, dv \\ &= n_e n_2 \left(\frac{2\pi \hbar^4}{k m_e^2} \right)^{1/2} T^{-1/2} \frac{\Omega_{21}}{g_2}. \\ &= n_e n_2 \frac{8.62942 \times 10^{-6}}{T^{1/2}} \frac{\Omega_{21}}{g_2} \text{ cm}^{-3}\text{s}^{-1}, \end{aligned}$$

and the collisional excitation rate per unit volume per unit time is $R_{12} = n_e n_1 q_{12}$, where

$$\begin{aligned} q_{12} &= \int_{v_{\min}}^\infty v \sigma_{12}(v) f(v)\, dv \\ &= \left(\frac{2\pi \hbar^4}{k m_e^2} \right)^{1/2} T^{-1/2} \frac{\Omega_{12}}{g_1} \exp\left(-\frac{E_{12}}{kT} \right) \\ &= \frac{g_2}{g_1} q_{21} \exp\left(-\frac{E_{12}}{kT} \right). \end{aligned}$$

(e) Quantum mechanical sum rule for collision strengths for the case where one term consists of a single level and the second consists of a multiplet, if either $S = 0$ or $L = 0$,

$$\Omega_{(SLJ,S'L'J')} = \frac{(2J'+1)}{(2S'+1)(2L'+1)}\Omega_{(SL,S'L')}$$

Here, $(2J'+1)$ is the statistical weight of an individual level (or term) in the multiplet, and $(2S'+1)(2L'+1)$ is the statistical weight of the multiplet. We can regard the collision strength as “shared” amongst these levels in proportion to the statistical weights of the individual levels ($g_J = 2J+1$).

i. C-like ions $\left(1s^2 2s^2 2p^2 \rightarrow 1s^2 2s^2 2p^2,\right.$ same electron configurations$\left.\right)$ → forbidden or intercombination transitions.

ground states (triplet) – ${}^3P_0 :{}^3P_1 :{}^3P_2 = 1/9 : 3/9 : 5/9$

excited states (singlets) – ${}^1D_2, {}^1S_1$

ii. Li-like ions $\left(1s^2 2s^1 \rightarrow 1s^2 2p^1\right)$ → resonance transitions

ground state (single) – ${}^2S_{1/2}$

excited states (doublet) – ${}^2P_{3/2} :{}^2P_{1/2} = 2/3 : 1/3$

(f) Limiting Cases

i. In the low density limit, the collisional rate between atoms and electrons is much slower than the radiative deexcitation rate of the excited level. Thus, we can balance the collisional feeding into level 2 by the rate of radiative transitions back down to level 1. The collision rate is

$$\begin{aligned} R_{12} &= A_{21} n_2, \\ n_2 &= \frac{n_e n_1 q_{12}}{A_{21}}, \end{aligned}$$

where A_{21} is the Einstein coefficient for spontaneous emission. Emission line flux is

$$\begin{aligned} F_{21} &= E_{12} A_{21} n_2 = E_{12} R_{12} \\ &= n_e n_1 E_{12} \frac{8.62942 \times 10^{-6}}{T^{1/2}} \left(\frac{\Omega_{12}}{g_1}\right) \mathrm{exp}\left(-\frac{E_{12}}{kT}\right) \ \mathrm{erg\ cm^{-3}\ s^{-1}} \\ &\simeq \chi n_e^2 \beta E_{12} T^{-1/2} \left(\frac{\Omega_{12}}{g_1}\right) \mathrm{exp}\left(-\frac{E_{12}}{kT}\right) \end{aligned}$$

For low temperatures, the exponential term dominates. At high temperature, the $T^{-1/2}$ term controls the cooling rate.

ii. In high-density limt, the level populations are set by the Boltzman equilibrium,

$$\begin{aligned} F_{21} &= E_{12} A_{21} n_2 \\ &= n_1 E_{12} A_{21} \frac{g_2}{g_1} \exp\left(-\frac{E_{12}}{kT}\right) \\ &\simeq \chi n_e E_{12} A_{21} \frac{g_2}{g_1} \exp\left(-\frac{E_{12}}{kT}\right) \end{aligned}$$

iii. Critical density defined as the density where the radiative depopulation rate matches the collisional deexcitation for the excited state,

$$\begin{aligned} A_{21} n_2 &= R_{21} \\ A_{21} n_2 &= n_e n_2 \frac{\beta}{T^{1/2}} \frac{\Omega_{21}}{g_2} \\ n_{\mathrm{crit}} &= \frac{A_{21} g_2 T^{1/2}}{\beta \Omega_{12}} \ \mathrm{cm}^{-3}. \end{aligned}$$

At around this density, the line emissivity plotted in log-scale changes slope from $+2$ to $+1$.

5. The Three-Level Atom (Line diagnostics)

   (a) Let C_{ij} be the collision rate ($C_{ij} = n_e q_{ij}$ s^{-1}) between any two levels. The equations of statistical equilibrium for a three level atom are

$$
\begin{aligned}
N_1 C_{13} + N_2 C_{23} &= N_3 \left(C_{31} + C_{32} + A_{32} + A_{31}\right), \\
N_1 C_{12} + N_3 \left(C_{32} + A_{32}\right) &= N_2 \left(C_{23} + C_{21} + A_{21}\right), \\
N_1 + N_2 + N_3 &= 1.
\end{aligned}
$$

   (b) Electron temperature

      i. Low-Density Limit; $E_{12} \sim E_{23}$

      ii. In this limit, $C_{31} \sim C_{32} \sim 0$. Also, because of the increasing threshold energies to excite each level, $N_3 \ll N_2 \ll N_1$ so that the equations are reduced to

$$
\begin{aligned}
N_3 &= \frac{N_1 C_{13}}{(A_{32} + A_{31})} \\
N_2 &= \frac{N_1 C_{12}}{A_{21}}.
\end{aligned}
$$

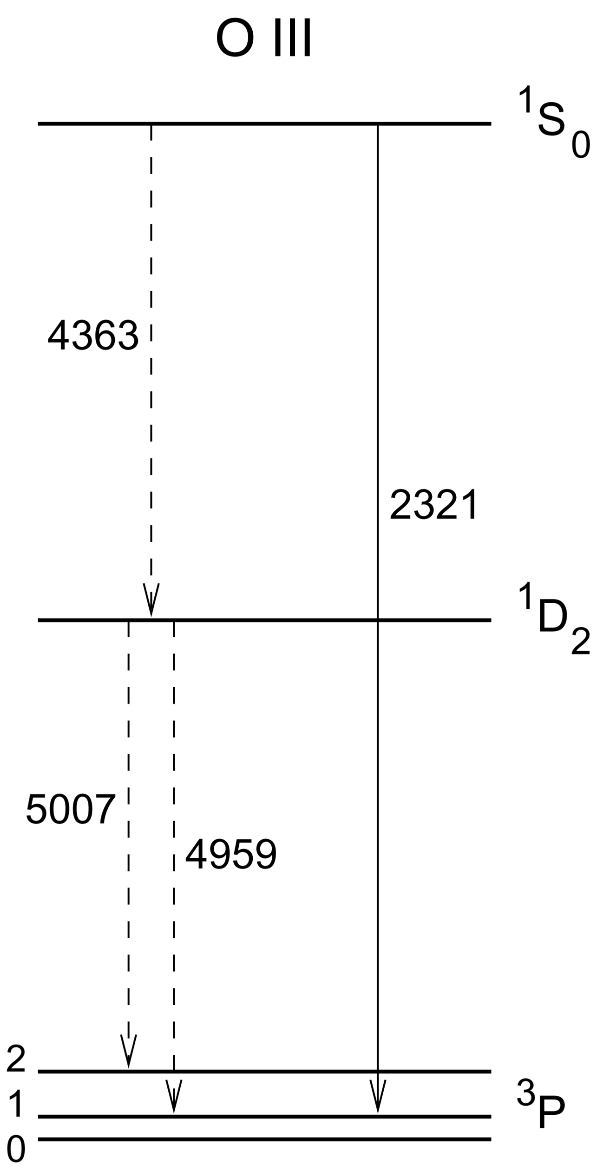
If we now form the line intensity ratio for the 3 → 2 and 2 → 1 transitions, we have

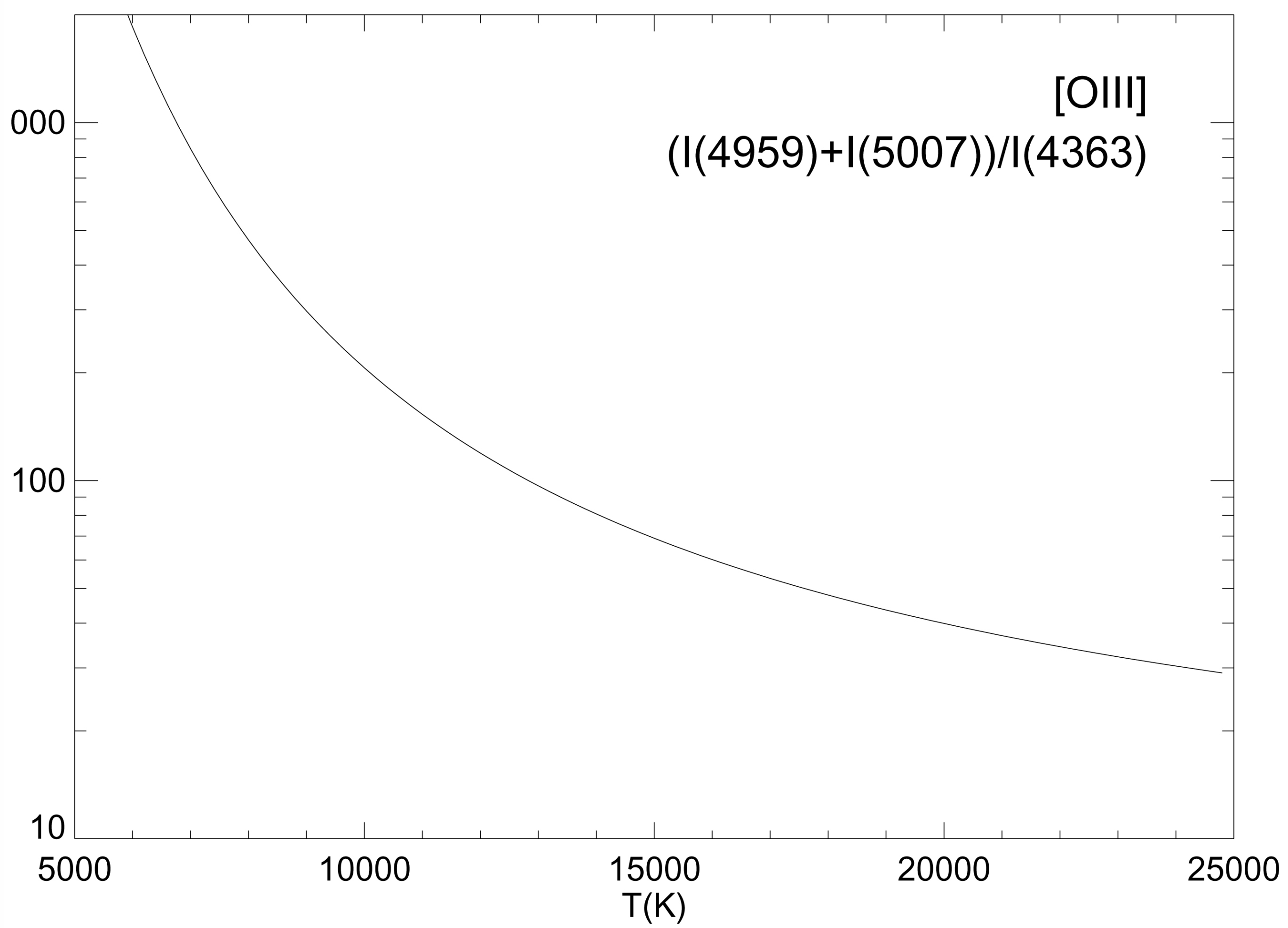
$$\begin{aligned}\frac{F_{32}}{F_{21}} &= \frac{E_{23}N_3A_{32}}{E_{12}N_2A_{21}} \\ &= \frac{E_{23}A_{32}C_{13}}{E_{12}(A_{32}+A_{31})C_{12}} \\ &= \frac{E_{23}A_{32}q_{13}}{E_{12}A_{31}q_{12}} \\ &= \frac{E_{23}A_{32}\Omega_{13}}{E_{12}A_{31}\Omega_{12}}\,\mathsf{exp}\left(-\frac{E_{23}}{kT}\right).\end{aligned}$$

provided that A_{32} is very much less than A_{31}.

Temperature

Use two levels with different excitation energy.





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

(c) Ions in which $E_{23} \ll E_{12}$

i. In low density limit

$$N_1 C_{13} = N_3 A_{31},$$
$$N_1 C_{12} = N_2 A_{21},$$

$$\frac{F_{31}}{F_{21}} = \frac{E_{31} A_{31} N_3}{E_{21} A_{21} N_2} = \frac{E_{31} C_{13}}{E_{21} C_{12}} \sim \frac{\Omega_{31}}{\Omega_{21}} \exp\left(-\frac{E_{23}}{kT}\right) \sim \frac{\Omega_{31}}{\Omega_{21}} = \frac{g_3}{g_2}.$$

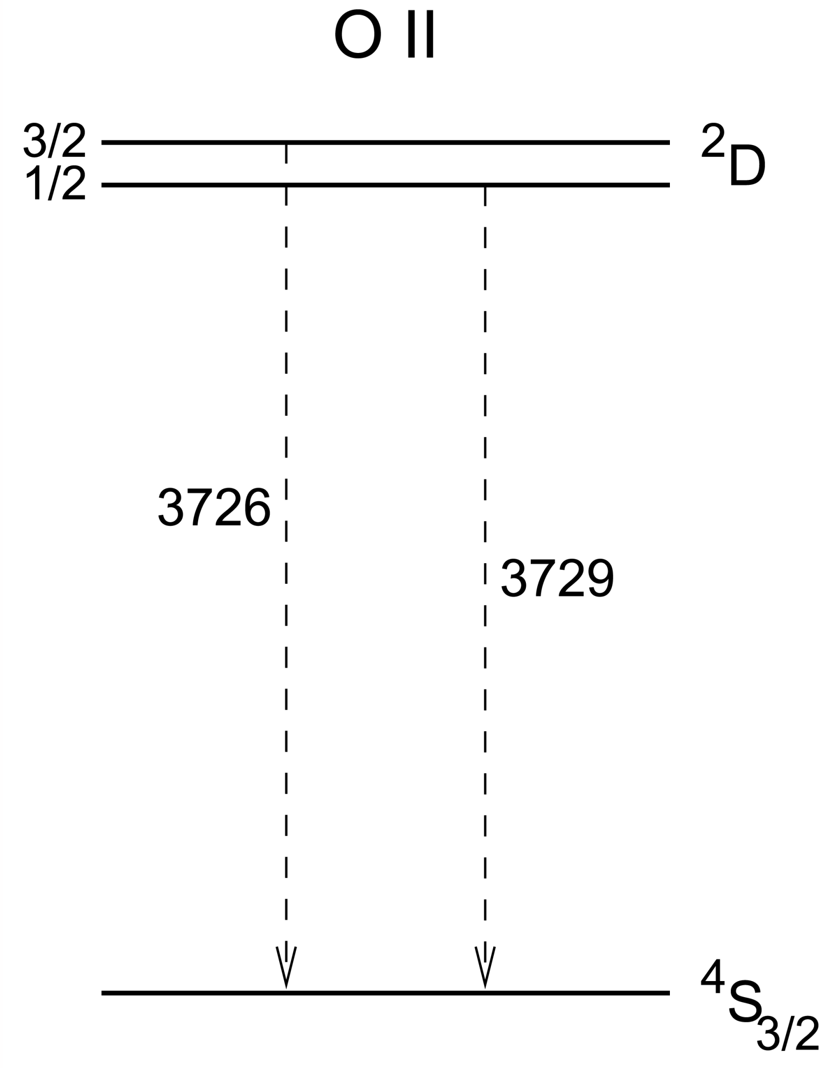
using the quantum-mechanical sum rule for collision strengths.

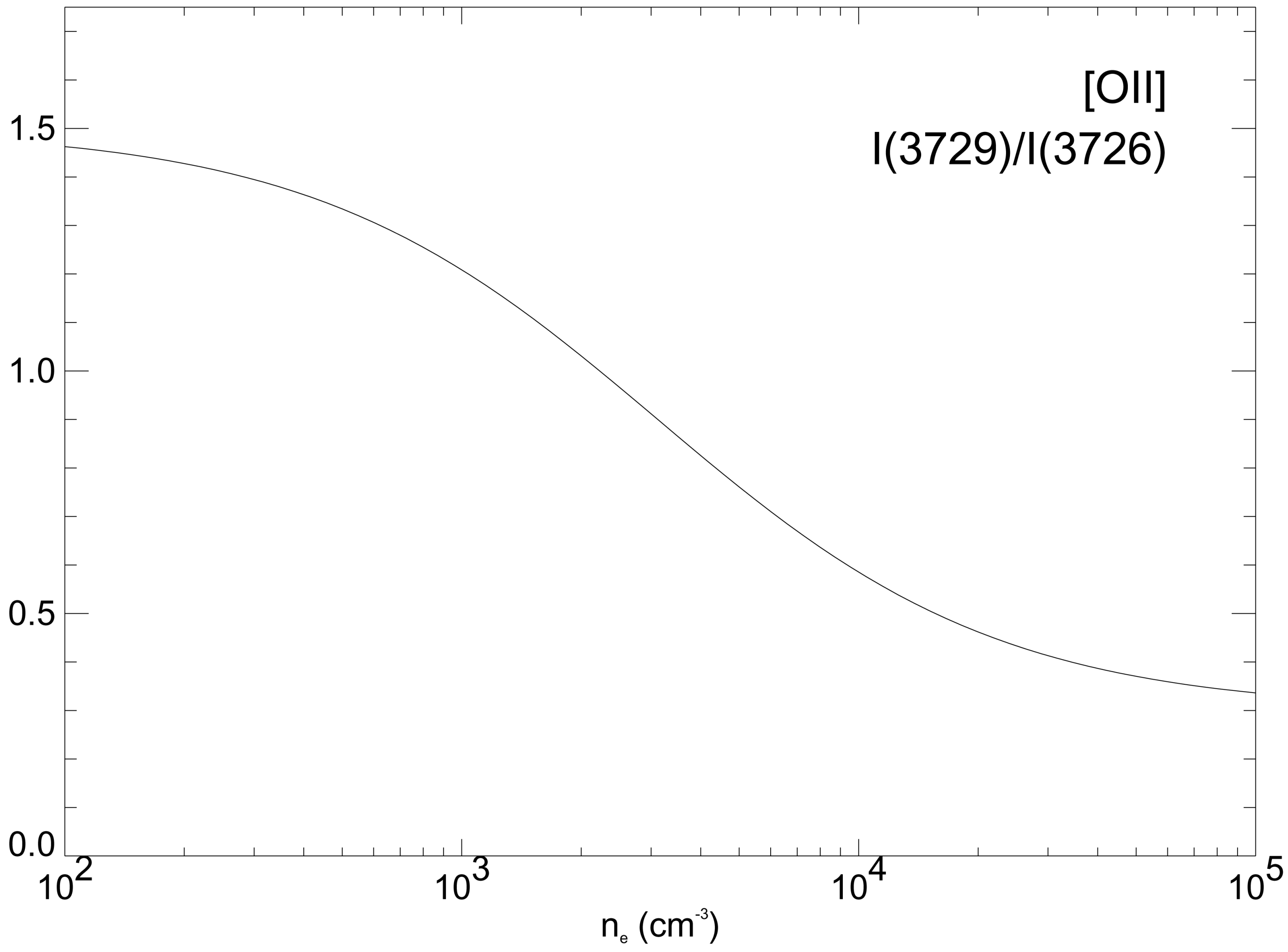
ii. In high density limit, the upper levels are populated according to their Bolzmann ratios,

$$\frac{F_{31}}{F_{21}} = \frac{E_{31} A_{31} N_3}{E_{21} A_{21} N_2} \sim \frac{A_{31} g_3}{A_{21} g_2}$$

Density

Choose atom with two levels with almost same excitation energy.





[Einstein Coefficients and Oscillator Strengths]

- Recall resonance scattering cross-section and the Einstein relations:

$$\sigma_{lu}(\nu) = \frac{\pi e^2}{mc} \frac{\gamma / 4\pi^2}{(\nu - \nu_0)^2 + (\gamma / 4\pi)^2} \qquad \begin{aligned} g_l B_{lu} &= g_u B_{ul} \\ A_{ul} &= \frac{2h\nu_{lu}^3}{c^2} B_{ul} \end{aligned} \qquad \text{where } \nu_{lu} \equiv \frac{E_u - E_l}{h} \; (= \nu_0)$$

- The Einstein (absorption) *B* coefficient associated with a classical oscillator can be defined in terms of the total energy extracted from a beam of radiation.

$$\int_0^\infty \sigma_{lu}(\nu) d\nu = \frac{\pi e^2}{mc} \equiv B_{lu}^{\text{classical}} \frac{h\nu_{lu}}{4\pi} \quad \rightarrow \quad B_{lu}^{\text{classical}} = \frac{4\pi^2 e^2}{h\nu_{lu} mc}$$

It is convenient to define the **absorption and emission oscillator strengths** (f_{lu} and f_{ul}) by the formulae:

$$B_{lu} = B_{lu}^{\text{classical}} f_{lu} = \frac{4\pi^2 e^2}{h\nu_{lu} mc} f_{lu} \qquad B_{ul} = \frac{4\pi^2 e^2}{h\nu_{ul} mc} f_{ul} \quad (\text{note that } \nu_{ul} = -\nu_{lu} < 0 \text{ and } f_{\text{ul}} < 0)$$

The oscillator strength (or *f* value) is the factor which corrects the classical result. The quantum mechanical process can be interpreted as being due to a (fractional) number *f* of equivalent classical electron oscillators of the same frequency.

- In quantum mechanics, the absorption oscillator strength is given by

$$f_{lu} = \frac{2m}{3\hbar^2 g_l e^2}\left(E_u - E_l\right)\sum\left|d_{lu}\right|^2 \qquad d_{lu} \equiv \left\langle \phi_u \middle| e\mathbf{r} \middle| \phi_l \right\rangle$$

where the sum is over all substates of the upper and lower levels.

We also have the following relations.

$$g_l f_{lu} = -g_u f_{ul} \qquad \sigma(\nu) = \frac{\pi e^2}{mc} f_{lu}$$

$$g_u A_{ul} \equiv -\frac{8\pi^2 e^2 \nu_{ul}^2}{mc^3} g_u f_{ul} = \frac{8\pi^2 e^2 \nu_{lu}^2}{mc^3} g_l f_{lu} \qquad = \frac{\pi e^2}{mc} f_{lu}\phi(\nu)$$

- *Thomas-Reiche-Kuhn sum rule*

$$\sum_{n'} f_{nn'} = N = \text{total number of electrons in the atom}$$

Here, the summation is over all states of the atom. Where there is a close shell and a smaller number q of electrons outside the closed shells that are involved in a more limited set of transitions, we also have

$$\sum_{n'} f_{nn'} = q$$

where the sum is now only over those states involve transitions of these outer electrons.

We note that $f \sim 1$ for strong allowed transitions.

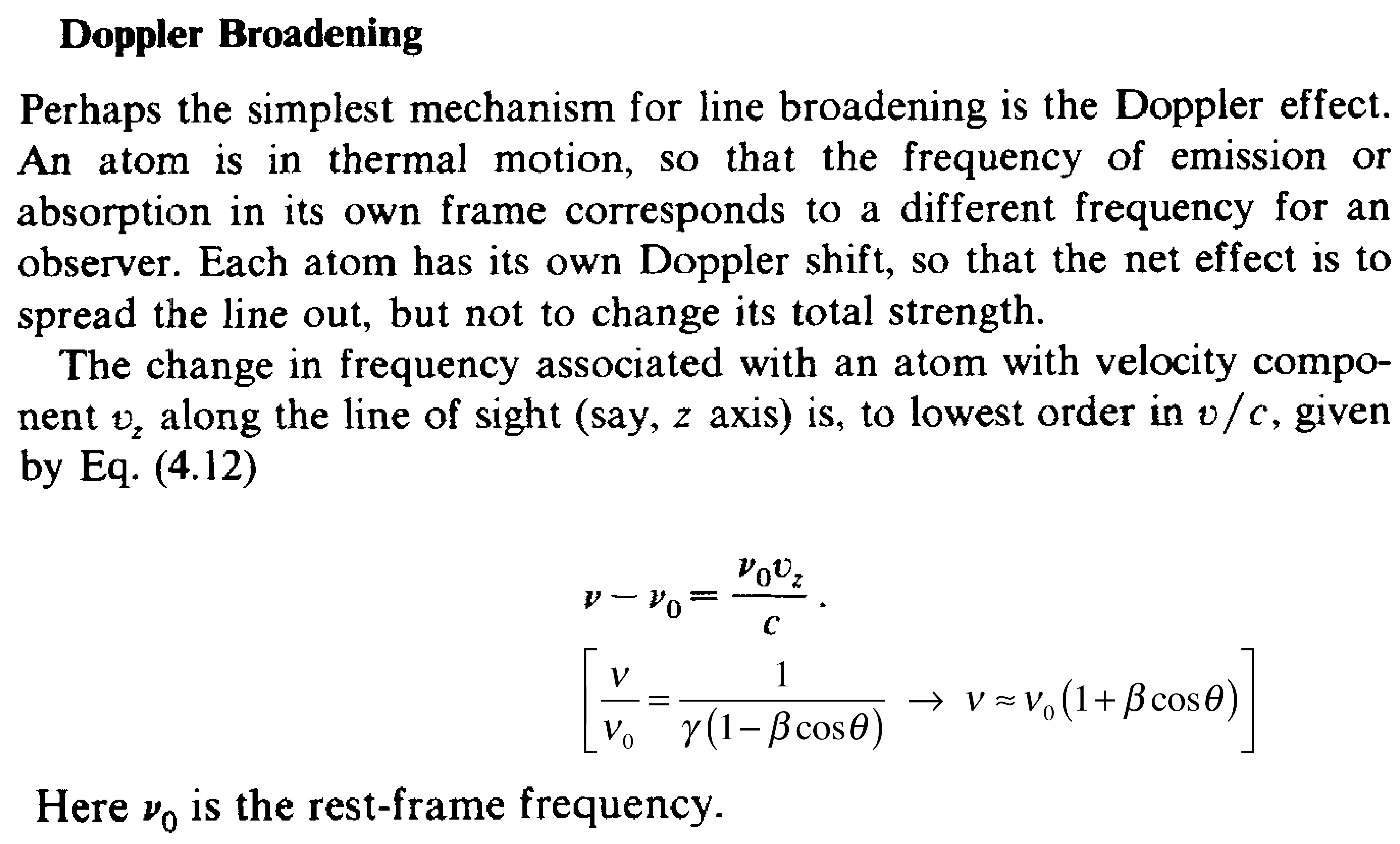
[Line Broadening Mechanisms]

- Atomic levels are not infinitely sharp, nor are the lines connecting them.

(1) Doppler Broadening

(2) Natural Broadening

(3) Collisional Broadening



Doppler Broadening

Perhaps the simplest mechanism for line broadening is the Doppler effect. An atom is in thermal motion, so that the frequency of emission or absorption in its own frame corresponds to a different frequency for an observer. Each atom has its own Doppler shift, so that the net effect is to spread the line out, but not to change its total strength.

The change in frequency associated with an atom with velocity component v_z along the line of sight (say, z axis) is, to lowest order in v/c, given by Eq. (4.12)

$$\nu-\nu_0=\frac{\nu_0 v_z}{c}.$$

$$\left[\frac{\nu}{\nu_0}=\frac{1}{\gamma(1-\beta\cos\theta)}\rightarrow\nu\approx\nu_0(1+\beta\cos\theta)\right]$$

Here ν_0 is the rest-frame frequency.

The number of atoms having velocities

in the range v_z to $v_z + dv_z$ is proportional to the Maxwellian distribution

$$\exp\left(-\frac{m_a v_z^2}{2kT}\right) dv_z$$

where m_a is the mass of an atom. From the above we have the relations

$$v_z = \frac{c(\nu - \nu_0)}{\nu_0},$$

$$dv_z = \frac{c\,d\nu}{\nu_0}.$$

Therefore, the strength of the emission in the frequency range ν to $\nu + d\nu$ is proportional to

$$\exp\left[-\frac{m_a c^2 (\nu - \nu_0)^2}{2\nu_0^2 kT}\right] d\nu,$$

Then, the profile function is

$$\phi(\nu) = \frac{1}{\Delta\nu_D\sqrt{\pi}} e^{-(\nu-\nu_0)^2/(\Delta\nu_D)^2}.$$

Here the *Doppler width* $\Delta\nu_D$ is defined by

$$\Delta\nu_D = \frac{\nu_0}{c}\sqrt{\frac{2kT}{m_a}} \quad .$$

The constant $(\Delta\nu_D\sqrt{\pi})^{-1}$ in the formula for $\phi(\nu)$ is determined by the normalization condition $\int\phi(\nu)\,\mathrm{d}\nu = 1$ under the (reasonable) assumption that $\Delta\nu_D \ll \nu_0$. The *line-center* cross section for each atom, neglecting stimulated emission, is therefore

$$\sigma_{\nu_0} = B_{12}\frac{h\nu_0}{4\pi}\phi(\nu_0) = \frac{1}{\Delta\nu_D\sqrt{\pi}}\frac{h\nu_0}{4\pi}B_{12}$$

$$= \frac{\pi e^2}{mc}f_{12}\frac{1}{\Delta\nu_D\sqrt{\pi}}$$

for the case of Doppler broadening. Numerically this is

$$\sigma_{\nu_0} = 1.16 \times 10^{-14} \lambda_0 \sqrt{A/T}\, f_{12}\ \mathrm{cm}^2,$$

where λ_0 is in $\mathring{A}$, T in K, and A is the atomic weight for the atom.

In addition to thermal motions there can also be turbulent velocities associated with macroscopic velocity fields. When the scale of the turbulence is small in comparison with a mean free path (called *microturbulence*) these motions are often accounted for by an effective Doppler width

$$\Delta\nu_D = \frac{\nu_0}{c}\left(\frac{2kT}{m_a} + \xi^2\right)^{1/2},$$

where ξ is a root mean-square measure of the turbulent velocities. This assumes that the turbulent velocities also have a Gaussian distribution.

Natural Broadening

A certain width to the atomic level is implied by the uncertainty principle, namely, that the spread in energy ΔE and the duration Δt in the state must satisfy $\Delta E\,\Delta t \sim \hbar$. We note that the spontaneous decay of an atomic state n proceeds at a rate

$$\gamma = \sum_{n'} A_{nn'},$$

where the sum is over all states n' of lower energy. If radiation is present, we should add the induced rates to this. The coefficient of the wave function of state n, therefore, is of the form $e^{-\gamma t/2}$ and leads to a decay of the electric field by the same factor. (The energy then decays proportional to $e^{-\gamma t}$.) Therefore, we have an emitted spectrum determined by the decaying sinusoid type of electric field, as given in §2.3 and Fig. 2.3. Thus the profile is of the form

$$\phi(\nu) = \frac{\gamma/4\pi^2}{(\nu-\nu_0)^2 + (\gamma/4\pi)^2}.$$

This is called a *Lorentz* (or *natural*) *profile*.

Actually, the above result applies to cases in which only the upper state is broadened (e.g., transitions to the ground state). If both the upper and lower state are broadened, then the appropriate definition for γ is

$$\gamma = \gamma_u + \gamma_l,$$

where γ_u and γ_l are the widths of the upper and lower states involved in the transition. Thus, for example, we can have a weak but broad line if the lower state is broadened substantially.

Collisional Broadening

The Lorentz profile applies even more generally to certain types of collisional broadening mechanisms. For example, if the atom suffers collisions with other particles while it is emitting, the phase of the emitted radiation can be altered suddenly (see Fig. 10.3). If the phase changes completely randomly at the collision times, then information about the emitting frequencies is lost. If the collisions occur with frequency $\nu_{\rm col}$, that is, each atom experiences $\nu_{\rm col}$ collisions per unit time on the average, then the profile is (see Problem 10.7).

$$\phi(\nu)=\frac{\Gamma/4\pi^2}{(\nu-\nu_0)^2+(\Gamma/4\pi)^2},$$

Lorentz or Cauchy distribution

where

$$\Gamma=\gamma+2\nu_{\rm col}.$$

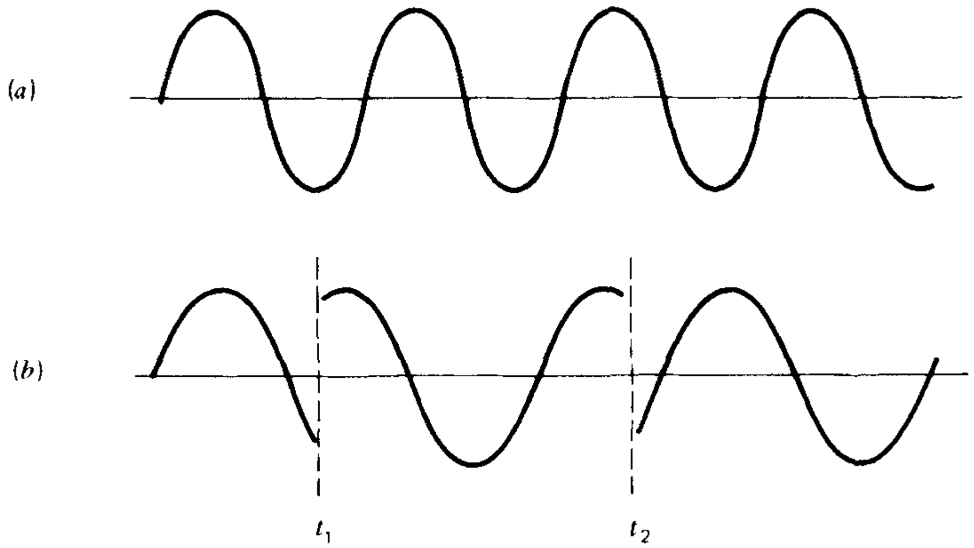


***Figure 10.3** Time-dependence of the electric field of emitted radiation which is (a) purely sinusoidal and (b) subject to random phase interruptions by atomic collisions.*

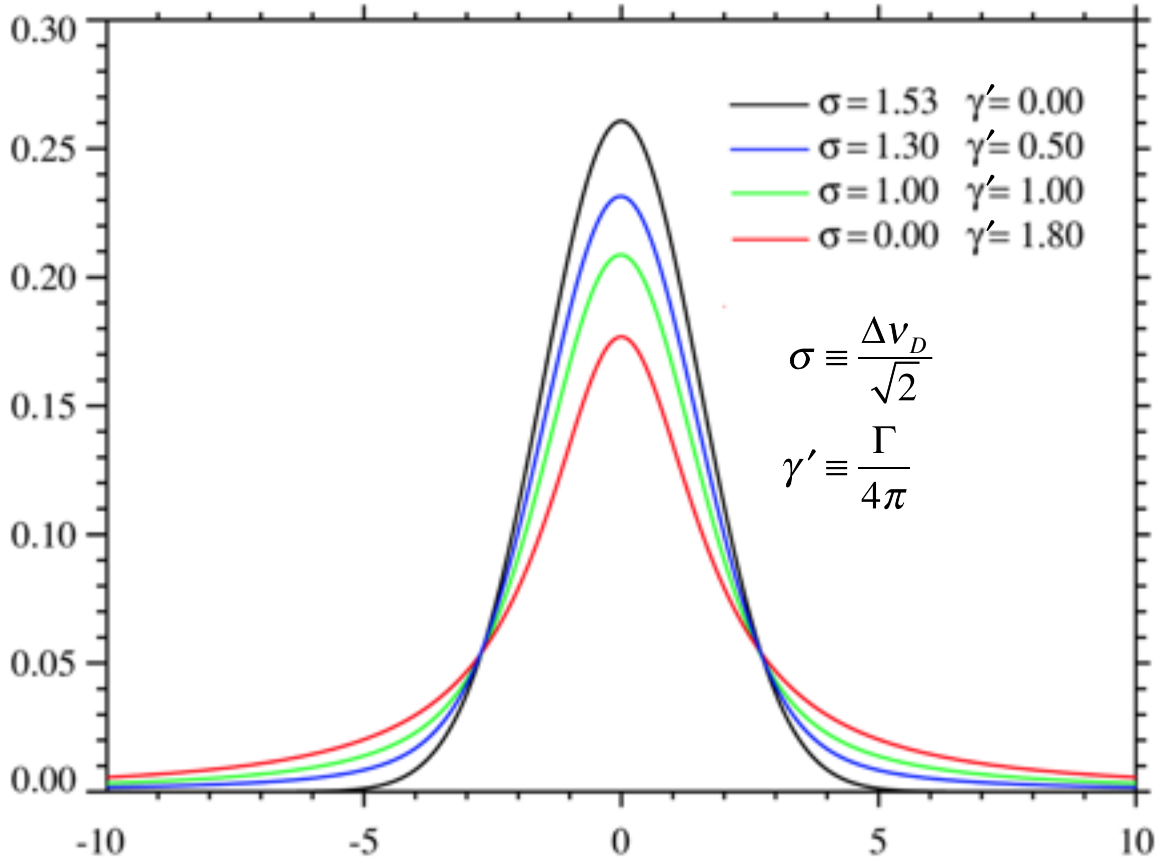
Combined Doppler and Lorentz Profiles

Quite often an atom shows both a Lorentz profile plus the Doppler effect. In these cases we can write the profile as an average of the Lorentz profile over the various velocity states of the atom:

$$\phi(\nu)=\frac{\Gamma}{4\pi^2}\int_{-\infty}^{\infty}\frac{(m/2\pi kT)^{1/2}\exp(-mv_z^2/2kT)}{(\nu-\nu_0-\nu_0 v_z/c)^2+(\Gamma/4\pi)^2}\,dv_z. \qquad (10.76)$$

We can write this more compactly using the definition of the *Voigt function*

$$H(a,u)\equiv\frac{a}{\pi}\int_{-\infty}^{\infty}\frac{e^{-y^2}\,dy}{a^2+(u-y)^2}.$$



Then Eq. (10.76) can be written as

$$\phi(\nu)=(\Delta\nu_D)^{-1}\pi^{-1/2}H(a,u),$$

where

$$a\equiv\frac{\Gamma}{4\pi\,\Delta\nu_D},$$

$$u\equiv\frac{\nu-\nu_0}{\Delta\nu_D}.$$

For small values of a, the center of the line is dominated by the Doppler profile, whereas the "wings" are dominated by the Lorentz profile.

[Energy Levels of Molecules] - Draine Chap. 5

5.1 Diatomic Molecules

It is helpful to consider first the hypothetical case where the nuclei are fixed, and only the electrons are free to move – this is known as the **Born-Oppenheimer approximation**. In atoms and atomic ions, the electrons move in a spherically symmetric potential, and the total electronic orbital angular momentum L_e is a good quantum number. In molecules, the electrons move in a Coulomb potential due to two or more nuclei, and spherical symmetry does not apply. However, in the case of diatomic molecules (or, more generally, linear molecules), the Coulomb potential due to the nuclei is symmetric under rotation around the nuclear axis (the line passing through the two nuclei), and L_{ez} =(the projection of the electronic angular momentum onto the internuclear axis)$/\hbar$ is a good quantum number. It is conventional to define $\Lambda \equiv |L_{ez}|$. Because the potential is axially symmetric, the two states $L_{ez} = \pm\Lambda$ have the same energy.

5.1.1 Fine-Structure Splitting

In addition, S_{ez} =(projection of the total electron spin onto the internuclear axis)$/\hbar$ is also a good quantum number; define $\Sigma \equiv |S_{ez}|$.

J_{ez} =(projection of the total electronic angular momentum on the internuclear axis)$/\hbar$ is also a good quantum number. If Λ and Σ are both nonzero, then there are two possible values: $J_{ez} = |\Lambda - \Sigma|$ and $J_{ez} = \Lambda + \Sigma$.

States with different $|J_{ez}|$ will differ in energy due to fine-structure splitting.

5.1.2 Hyperfine Splitting

If one or more nuclei have nonzero nuclear spin *and* $J_{ez} \neq 0$, then there will be an interaction between the nuclear magnetic moment and the magnetic field generated by the electrons, resulting in “hyperfine splitting”: the energy will depend on the orientation of the nuclear angular momentum (or angular momenta) relative to the axis. As in atoms, this splitting is small, of order $\sim 10^{-6}\,\mathrm{eV}$.

5.1.3 Designation of Energy Levels: Term Symbols

Diatomic molecules with identical nuclei (e.g., H_2, N_2, O_2) are referred to as **homonuclear**. Note that the nuclei must be truly *identical* – HD and $^{16}O^{17}O$ are not homonuclear molecules. The energy levels of homonuclear diatomic molecules are designated by **term symbols**

$$^{(2\Sigma+1)}\mathcal{L}_{u,g} \quad ,$$

$\Lambda =$	0	1	2	3	4 …
Orbitals	σ	π	δ	ϕ	γ …
States	Σ	Π	Δ	Φ	Γ …
Degeneracy	1	2	2	2	2 …

where

$\mathcal{L} = \Sigma$, Π, Δ, ... for $\Lambda = 0, 1, 2, \ldots$, where $\Lambda\hbar$ = projection of the electron orbital angular momentum onto the internuclear axis,

$\Sigma\hbar$ = projection of the electron spin angular momentum onto the internuclear axis.

$$u, g = \begin{cases} g & (\text{“gerade”}) \text{ if symmetric under reflection through the center of mass,} \\ u & (\text{“ungerade”}) \text{ if antisymmetric under reflection through the center of mass.} \end{cases}$$

For the special case of Σ states, a superscript + or – is added to the term symbol:

$$^{(2\Sigma+1)}\Sigma^{\pm}_{u,g} \; ,$$

where the superscript

$$\pm \; = \begin{cases} + & \text{if symmetric under reflection through (all) planes} \\ & \text{containing the nuclei,} \\ - & \text{if antisymmetric under reflection through a plane} \\ & \text{containing the nuclei.} \end{cases}$$

In the case of a **heteronuclear** diatomic molecule (e.g., HD, OH, or CO), the energy levels are designated

$$^{(2\Sigma+1)}\mathcal{L}_{J_{e,z}}$$

where $\mathcal{L}$ and Σ have the same meaning as for homonuclear diatomic molecules, but now $J_{e,z}$ is indicated as a subscript. As for homonuclear molecules, if the term symbol is Σ, then an additional superscript $\pm$ is applied, specifying the symmetry of the wave function under reflection through planes containing the nuclei.

Because a given molecule may have more than one electronic state with the same term symbol, the electronic states are distinguished by a letter X, A, B, ..., a, b, ... appearing in front of the term symbol. The letter X is customarily used to designate the electronic ground state. The ground terms for a number of diatomic molecules of astrophysical interest are given in Table 5.1

X labels the ground electronic state;
A, B, C, . . . label states of same spin multiplicity as the ground state;
a, b, c, . . . label states of different spin multiplicity to the ground state.

	Ground term
H_2	$^1\Sigma_g^+$
CH	$^2\Pi_{1/2,3/2}$
CH^+	$^1\Sigma_0^+$
OH	$^2\Pi_{3/2,1/2}$
CN	$^2\Sigma_{1/2}^+$
CO	$^1\Sigma_0^+$
SiO	$^1\Sigma_0^+$
CS	$^1\Sigma_0^+$

The electronic ground state of H_2 (two electrons) has zero electronic orbital angular momentum ($L_e = 0$), has zero electron spin ($S_e = 0$), is symmetric under reflection through the center of mass (g), and is symmetric under reflection through planes containing the nuclei ($+$). The ground state is X $^1\Sigma_g^+$.

CO has 2 p electrons contributed by C and 4 p electrons contributed by O; together, these 6 p electrons fill the $2p$ subshell, and as a result, the ground electronic state of CO has zero electronic angular momentum and zero electronic spin: $^1\Sigma_0^+$, just like H_2. The reduced mass of CO is $(12 \times 16/28)$ amu ≈ 6.9 amu. The C=O

OH is an example of a molecule with the ground electronic state having nonzero electronic orbital angular momentum: with seven electrons, the OH ground state has $L_{ez} = 1$ and $S_{ez} = 1/2$, and is therefore designated by $^2\Pi_{1/2,3/2}$. The electron spin and orbital angular momenta can couple to give $J_e = 1/2$ or $3/2$, with energies that are separated due to spin-orbit coupling (i.e., fine-structure splitting in atoms or ions); the $J_e = 3/2$ state has the lower energy.

Molecular Hydrogen

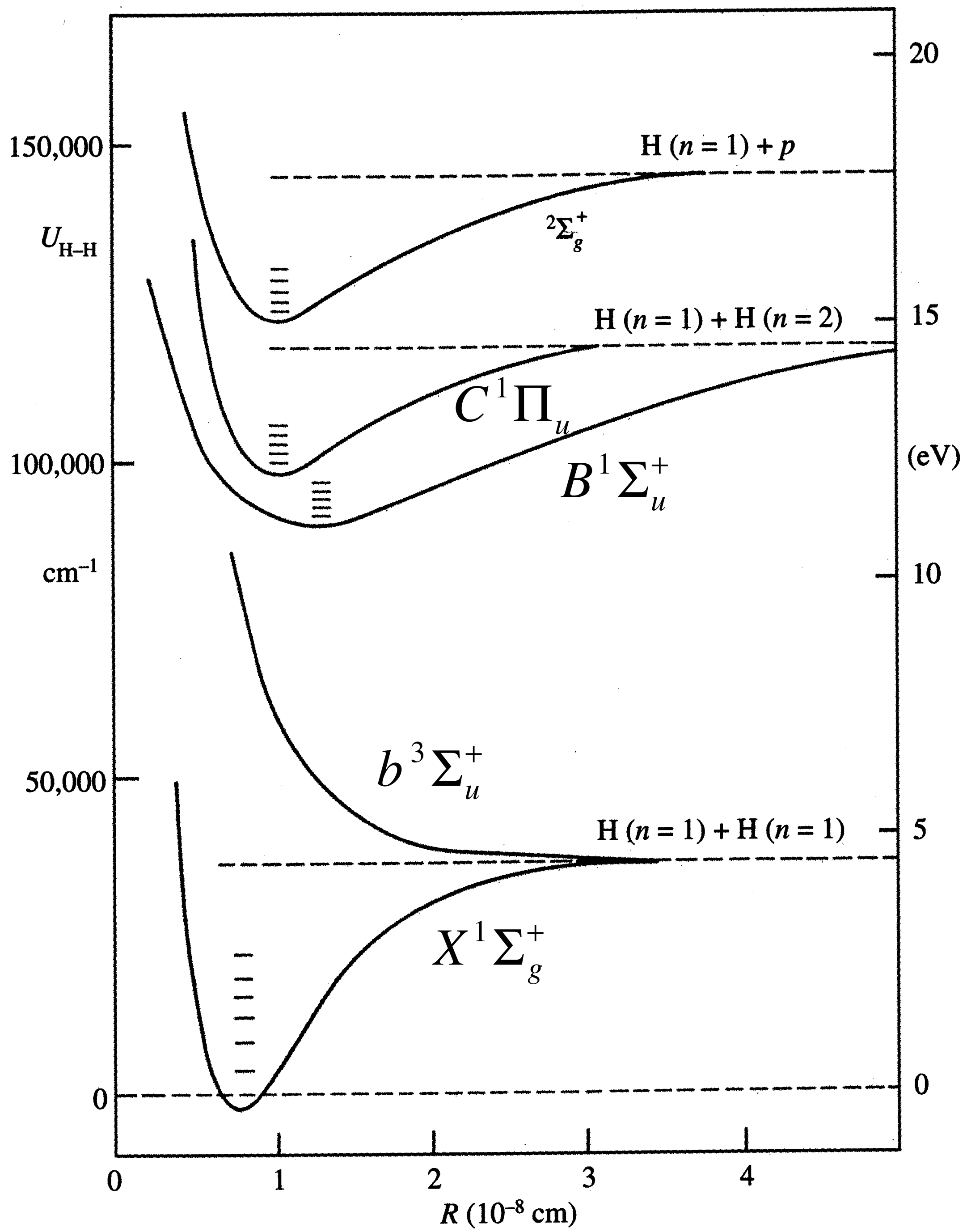


Figure 7.1

Energy diagram of the lower electronic states of H_2. The short horizontal lines in each of the bound states indicate the vibrational levels. The transitions from the ground state $^1\Sigma_g^+$ to the excited states $^1\Sigma_u^+$ and $^1\Pi_u$ are called Lyman and Werner bands, respectively. (Figure adapted from Watson, 1975, in *Atomic and Molecular Physics and the Interstellar Matter*, Les Houches, p. 177.)

- Energy Levels

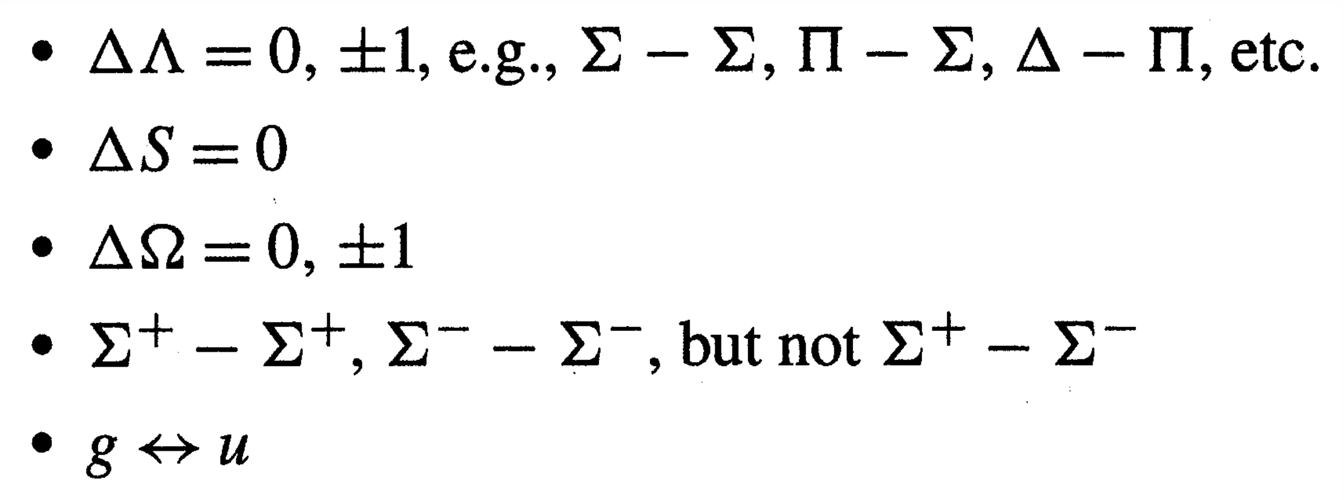
  An electronic transition consists of vibrational bands, which in turn are made up of rotational transitions.

$$E_q(v, J) = V_q(r_0) + h\nu_0 \left(v + \frac{1}{2} \right) + B_v J(J+1)$$

$$\nu_0 \equiv \frac{\omega_0}{2\pi} \qquad B_v = \frac{\hbar^2}{2m_r r_0^2} \quad .$$

  Here, q denotes an electronic state.

- Electric-dipole selection rules for electronic transitions in a diatomic molecule



  - $\Delta\Lambda = 0, \pm 1$, e.g., $\Sigma - \Sigma$, $\Pi - \Sigma$, $\Delta - \Pi$, etc.
  - $\Delta S = 0$
  - $\Delta\Omega = 0, \pm 1$
  - $\Sigma^+ - \Sigma^+$, $\Sigma^- - \Sigma^-$, but not $\Sigma^+ - \Sigma^-$
  - $g \leftrightarrow u$

5.1.4 O, P, Q, R, and S Transitions

A diatomic molecule can vibrate (stretch) along the internuclear axis, and it can rotate around an axis perpendicular to the internuclear axis. The rotational angular momentum adds (vectorially) to the electronic angular momentum.

The rotational levels of diatomic molecules are specified by a single vibrational quantum number v and rotational quantum number J. Transitions will change J by either 0, ±1, or ±2. It is customary to identify transitions by specifying the upper and lower electronic states, upper and lower vibrational states, and one of the following: $O(J_\ell)$, $P(J_\ell)$, $Q(J_\ell)$, $R(J_\ell)$, $S(J_\ell)$, where the usage is given in Table 5.2. Thus, for example, a transition from the $v_\ell = 0$, $J_\ell = 1$ level of the ground electronic state to the $v_u = 5$, $J_u = 2$ level of the first electronic excited state would be written B–X 5–0 $R(1)$.

Table 5.2 Usage of O, P, Q, R, and S

Designation	$(J_u - J_\ell)$	Note
$O(J_\ell)$	-2	Electric quadrupole transition
$P(J_\ell)$	-1	Electric dipole transition
$Q(J_\ell)$	0	Electric dipole or electric quadrupole; $Q(0)$ is forbidden
$R(J_\ell)$	$+1$	Electric dipole transition
$S(J_\ell)$	$+2$	Electric quadrupole transition

5.1.6 Ortho-H_2 and Para-H_2

In the case of H_2, the electronic wave function is required to be antisymmetric under exchange of the two electrons. The two protons, just like the electrons, are identical fermions, and therefore the Pauli exclusion principle antisymmetry requirement also applies to exchange of the two protons. The protons are spin 1/2 particles – the two protons together can have total spin 1 (spins parallel) or total spin 0 (spins antiparallel). Without going into the quantum mechanics, the consequence of the antisymmetry requirement is that if the protons have spin 0, the rotational quantum number J must be even; this is referred to as **para-H_2**, with $J = 0$, 2, 4, ... If the two protons are parallel, with total spin 1, the rotational quantum number J must be odd: this is referred to as **ortho-H_2**, with $J = 1$, 3, 5, ... Because the nuclear spins are only weakly coupled to the electromagnetic field, ortho-H_2 and para-H_2 behave as almost distinct species, with conversion of ortho to para, or para to ortho, happening only very slowly.

Because H_2 has no permanent electric dipole moment, the vibrational states and the rotational states radiate very weakly, via the time-variation of the electric quadrupole moment as the molecule vibrates or rotates. Because the nuclear spin state does not change, the rovibrational radiative transitions of H_2 must have $\Delta J = 0$ or $\Delta J = \pm 2$ – i.e., ortho→ortho or para→para.

The vibration–rotation emission spectrum of H_2 therefore consists of electric quadrupole transitions. The downward transitions are identified by

$$\begin{aligned} v_u - v_\ell \;\; \mathrm{S}(J_\ell) & \quad \text{if } J_\ell = J_u - 2 \quad , \\ v_u - v_\ell \;\; \mathrm{Q}(J_\ell) & \quad \text{if } J_\ell = J_u \quad , \\ v_u - v_\ell \;\; \mathrm{O}(J_\ell) & \quad \text{if } J_\ell = J_u + 2 \quad . \end{aligned}$$

For example, 1–0 S(1) refers to the transition $(v=1, J=3) \rightarrow (v=0, J=1)$. This transition is indicated in Fig. 5.2.

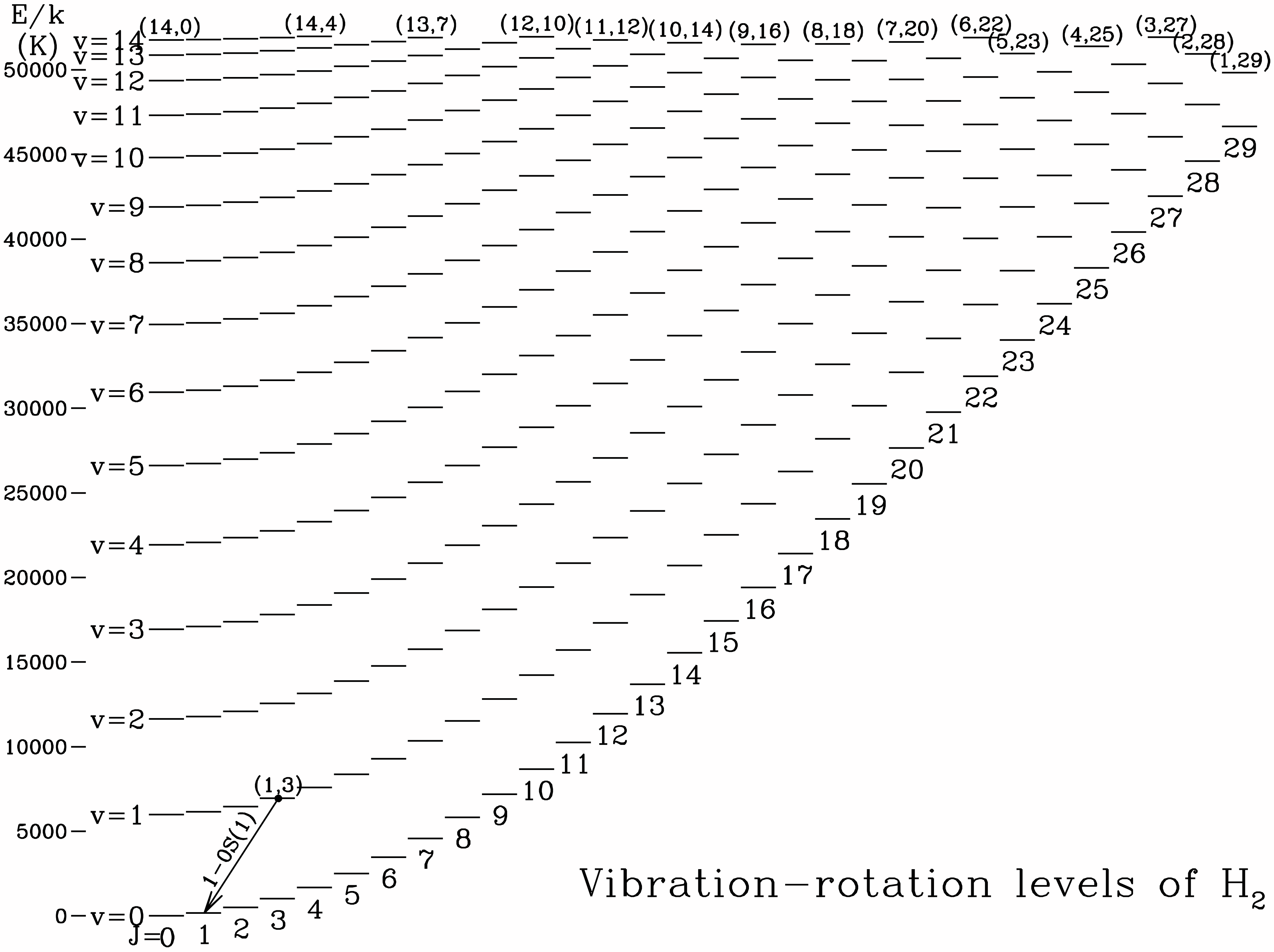
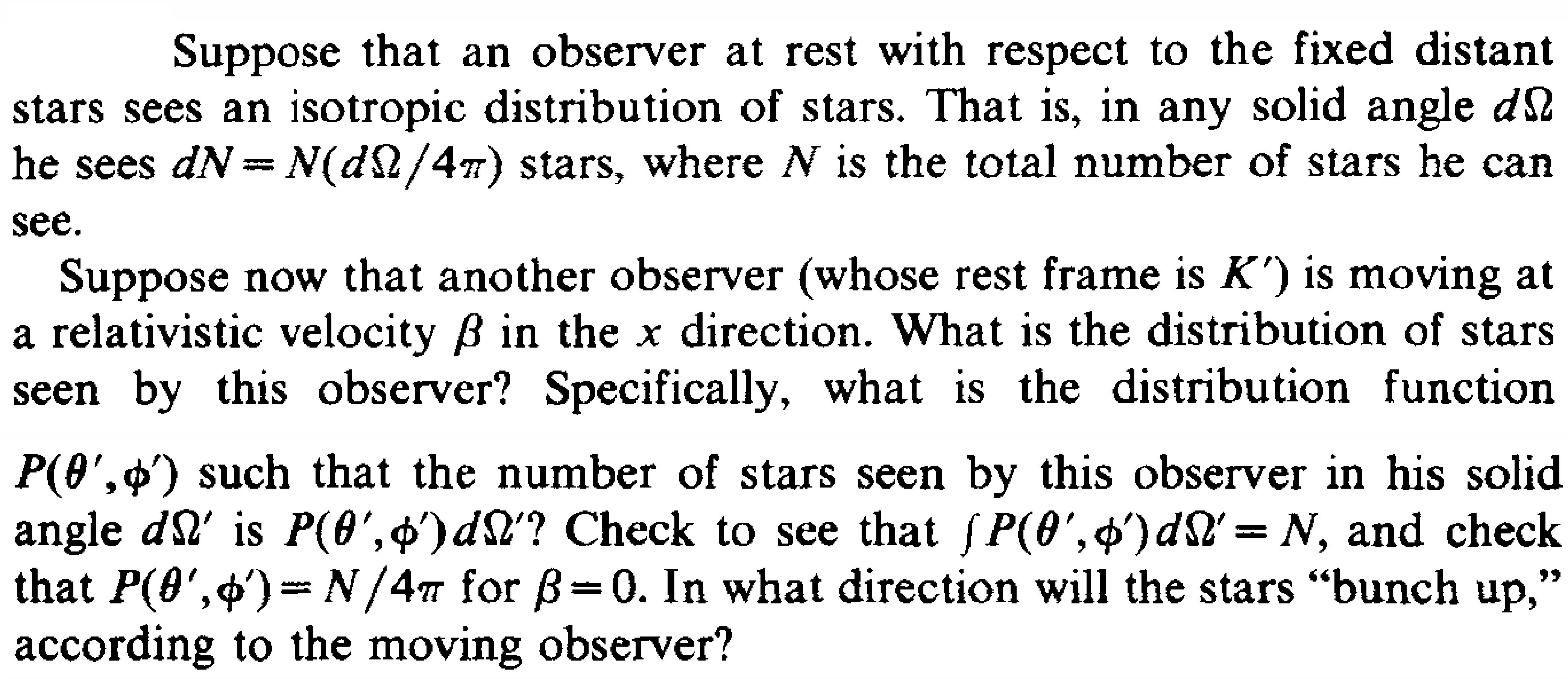


Figure 5.2 Vibration–rotation energy levels of the ground electronic state of H_2 with $J \leq 29$. The $(v, J) = (1, 3)$ level and 1–0S(1) $\lambda = 2.1218\,\mu$m transition are indicated.

Home Works
Due 5PM Dec. 20

Problem 1

- (Rybicki & Lightman problem 4.2)

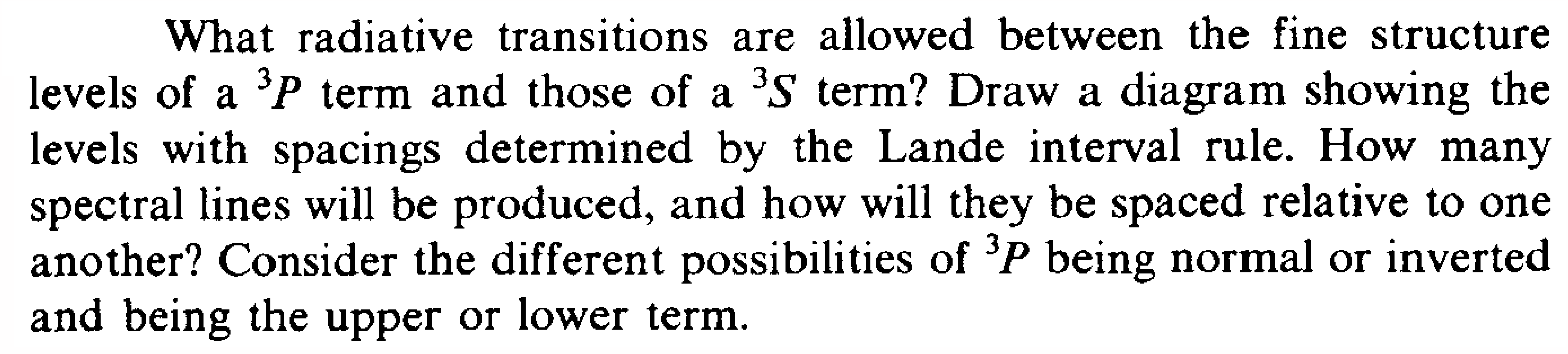


Suppose that an observer at rest with respect to the fixed distant stars sees an isotropic distribution of stars. That is, in any solid angle $d\Omega$ he sees $dN = N(d\Omega/4\pi)$ stars, where N is the total number of stars he can see.

Suppose now that another observer (whose rest frame is K') is moving at a relativistic velocity β in the x direction. What is the distribution of stars seen by this observer? Specifically, what is the distribution function $P(\theta',\phi')$ such that the number of stars seen by this observer in his solid angle $d\Omega'$ is $P(\theta',\phi')\,d\Omega'$? Check to see that $\int P(\theta',\phi')\,d\Omega' = N$, and check that $P(\theta',\phi') = N/4\pi$ for $\beta = 0$. In what direction will the stars "bunch up," according to the moving observer?

Problem 2

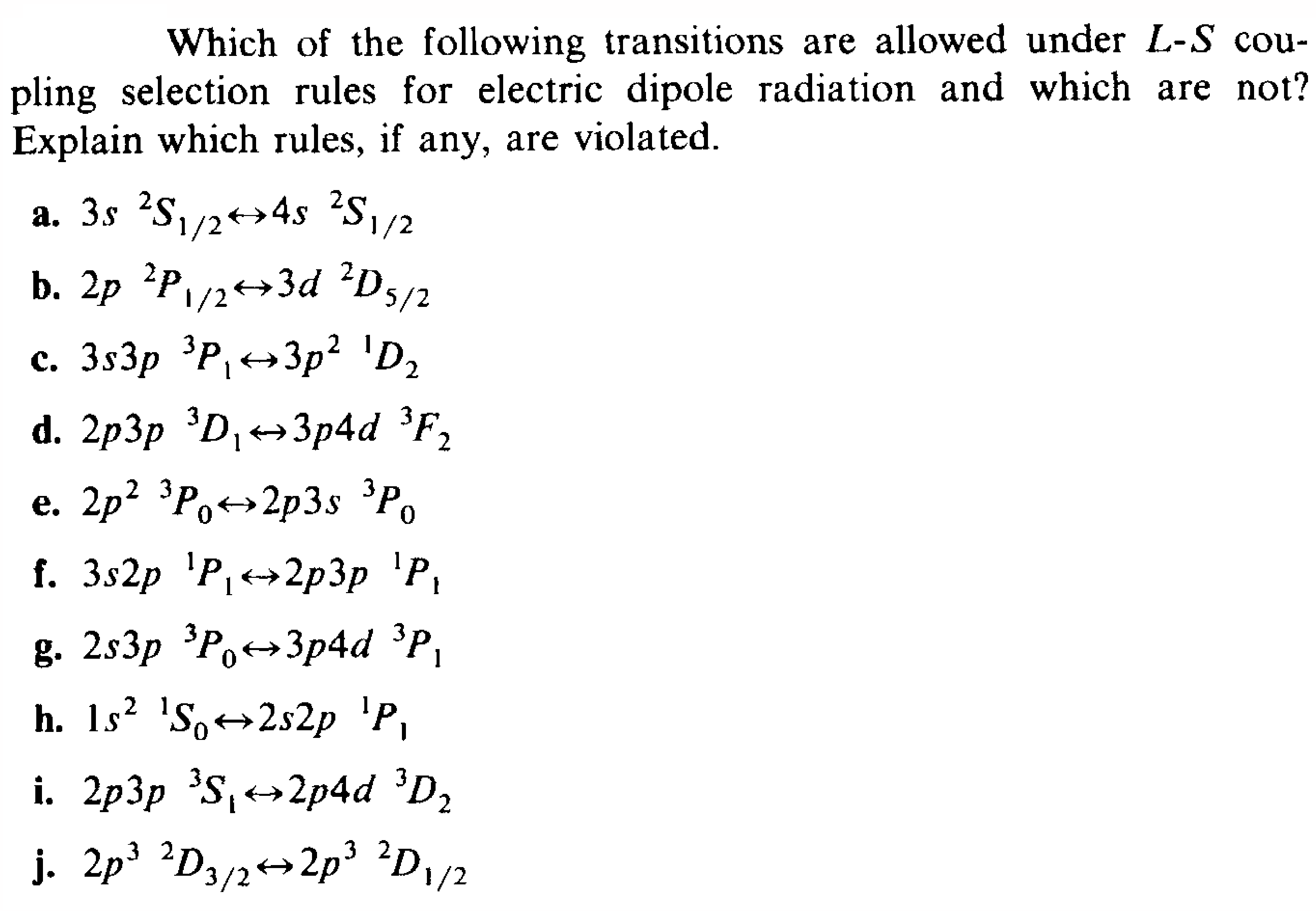
- (Rybicki & Lightman problem 10.1)



What radiative transitions are allowed between the fine structure levels of a ^3P term and those of a ^3S term? Draw a diagram showing the levels with spacings determined by the Lande interval rule. How many spectral lines will be produced, and how will they be spaced relative to one another? Consider the different possibilities of ^3P being normal or inverted and being the upper or lower term.

Problem 3

- (Rybicki & Lightman problem 10.2)



Which of the following transitions are allowed under L-S coupling selection rules for electric dipole radiation and which are not? Explain which rules, if any, are violated.

a. $3s\ ^2S_{1/2} \leftrightarrow 4s\ ^2S_{1/2}$

b. $2p\ ^2P_{1/2} \leftrightarrow 3d\ ^2D_{5/2}$

c. $3s3p\ ^3P_1 \leftrightarrow 3p^2\ ^1D_2$

d. $2p3p\ ^3D_1 \leftrightarrow 3p4d\ ^3F_2$

e. $2p^2\ ^3P_0 \leftrightarrow 2p3s\ ^3P_0$

f. $3s2p\ ^1P_1 \leftrightarrow 2p3p\ ^1P_1$

g. $2s3p\ ^3P_0 \leftrightarrow 3p4d\ ^3P_1$

h. $1s^2\ ^1S_0 \leftrightarrow 2s2p\ ^1P_1$

i. $2p3p\ ^3S_1 \leftrightarrow 2p4d\ ^3D_2$

j. $2p^3\ ^2D_{3/2} \leftrightarrow 2p^3\ ^2D_{1/2}$

Problem 4

Kirchhoff Revisited.

(a) Consider a central spherical blackbody at temperature T_{c}, surrounded by a concentric, non-scattering shell that is thermally emitting at T_{s}. For a slightline that passes from the central object through the shell, solve for I_ν as a function of $\tau_\nu(s)$. Write your solution in the form of $I_\nu = B_\nu(T_{\mathrm{c}}) + \Delta_\nu$, i.e., find $\Delta_\nu = I_\nu - B_\nu(T_{\mathrm{c}})$. For $T_{\mathrm{c}} > T_{\mathrm{s}}$, find I_ν and Δ_ν in the limits $\tau_\nu \ll 1$, $\tau_\nu \approx 1$, and $\tau_\nu \gg 1$, and comment. How will these change if $T_{\mathrm{c}} < T_{\mathrm{s}}$?

(b) Now consider the case in which the absorption coefficient α_ν is nonzero for a narrow region ("line") centered at ν_0 with width $\Delta\nu \ll \nu_0$. Also let the width have $\Delta\nu \ll kT_{\mathrm{s}}/h, kT_{\mathrm{c}}/h$, i.e., the line feature is narrow compared to the frequency scales over which the Planck spectra change. Using your solution for I_ν, explain how the spectrum I_ν will look for $T_{\mathrm{c}} > T_{\mathrm{s}}$ and for $T_{\mathrm{c}} < T_{\mathrm{s}}$.

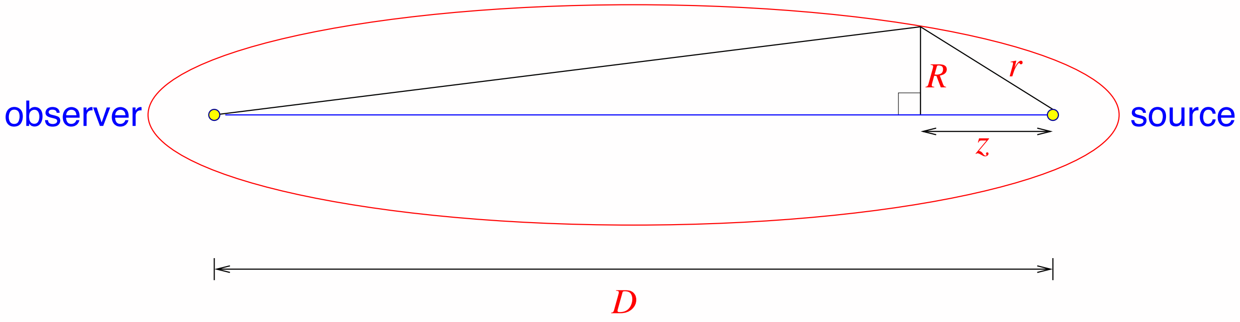
In the optical and infrared, the Sun's spectrum shows a continuum with absorption lines, but in the UV and X-rays it shows a continuum with emission lines. Interpret these physically on the basis of your results.

Problem 5

- Light Echoes

Consider an observer and a transient source, separated by a distance D. Assume the environment around the source contains scattering sources, possibly inhomogeneous, but with small optical depth so that at most one scattering event will occur. The unscattered light will be seen as the transient outburst, and the scattered radiation will be the light echo.

As seen in the diagram below, at a given time, a point on the echo will be measured at a projected distance R from the source.



(a) If the source is observed at a time t after the transient outburst is seen, show that the scattering sources lie on an *ellipse*, for which the source and the observer are each one focus. Also show that the major axis of the ellipse has length $D + ct$. *Hint*: the major axis is also the sum distances from the each focus to any point on the ellipse.

To identify the location of the scattering source at projected distance R, we must find its longitudinal distance z from the source (see diagram). Consider the "parabolic" approximation in which $D \gg r, z, R$. Show that in this approximation, we have

$$z = \frac{R^2}{2ct} - \frac{ct}{2}$$

which relates z to the observables R and t.

(b) For the case of SN 1987, the distance is $D \approx 50$ kpc. In the http://www.aao.gov.au/images/captions/aat066.html, there is a link to `a series of six images`. Look at the image from $t = 913$ days after the outburst. Estimate R for the two circles, and calculate z for each. What is the geometry of the scattering surfaces that produced the rings? Are they located in front of or behind the supernova?