

# (AGN)<sup>2</sup>

Week 2 and 3  
March 18 (Monday), 2024

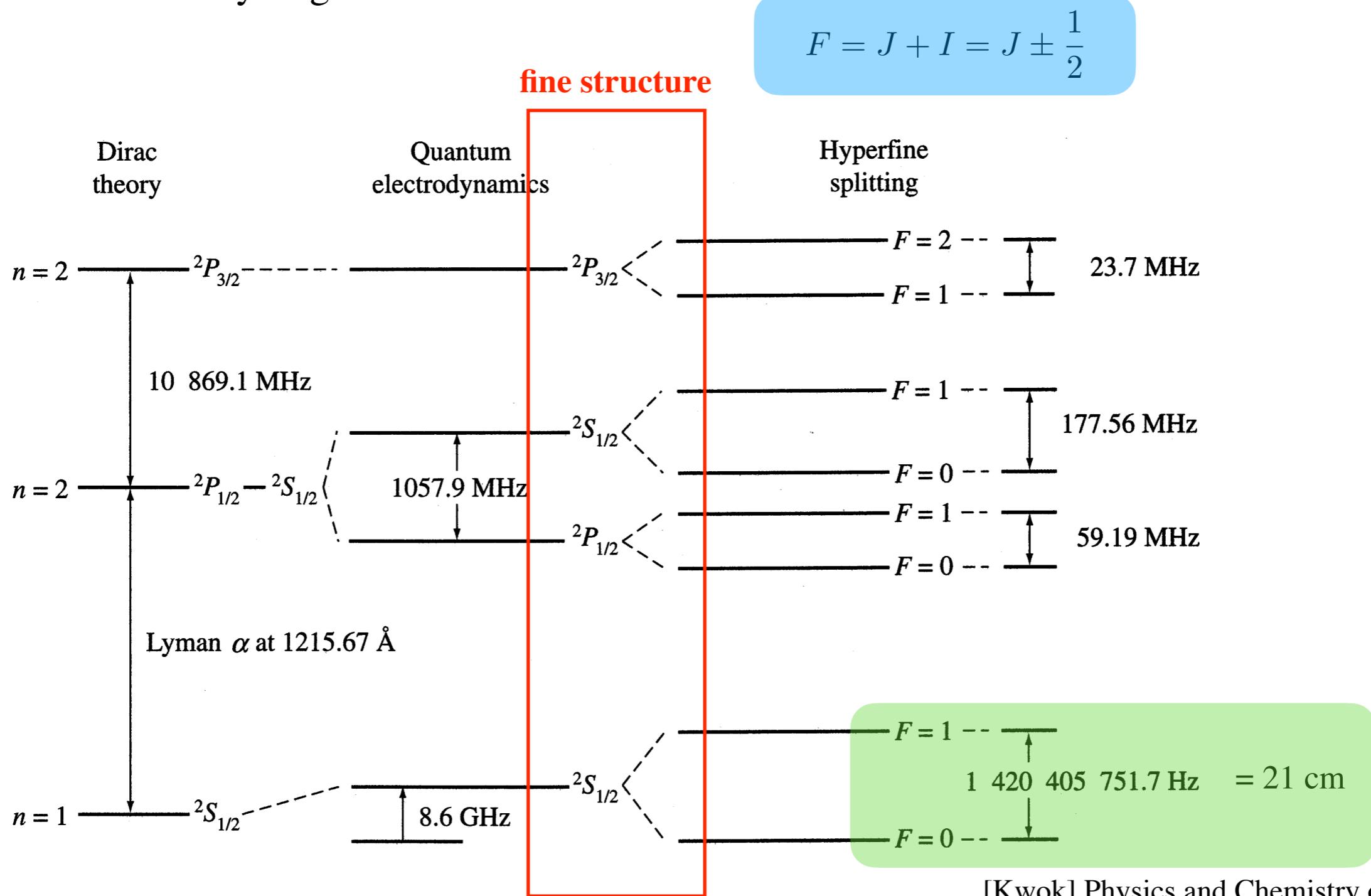
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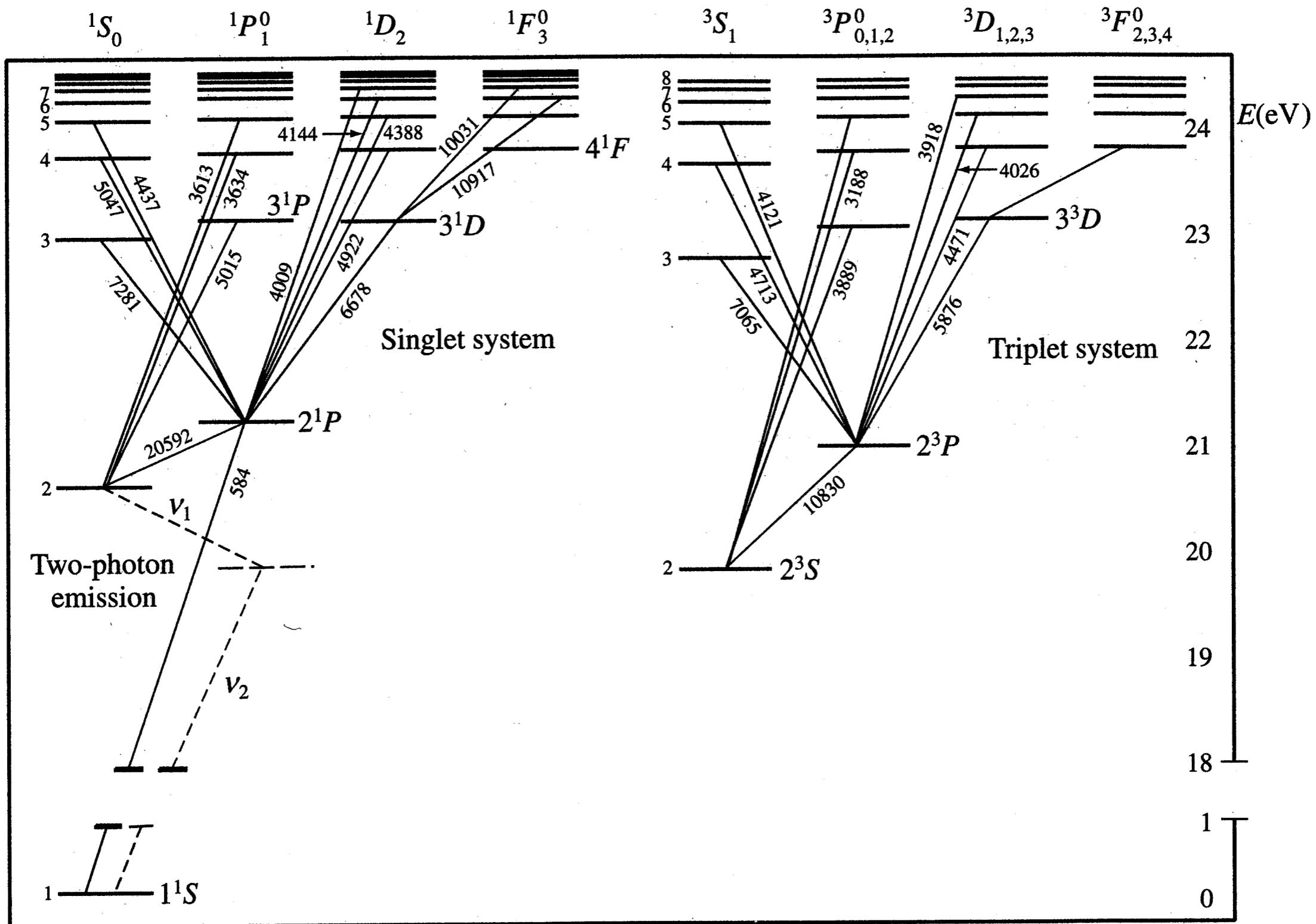
# Hydrogen Atom : Fine Structure / Hyperfine Structure

- Hyperfine Structure in the H atom

Coupling the nuclear spin  $I$  to the total electron angular momentum  $J$  gives the final angular momentum  $F$ . For hydrogen this means



# Helium Energy Levels (Grotrian diagram)



The states can be divided into two separate groups because of the selection rule  $\Delta S = 0$ .

# H II regions & Planetary Nebulae

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- Three processes govern the physics of H II regions:
  - ***Photoionization Equilibrium***: the balance between photoionization and recombination. This determines the spatial distribution of ionic states of the elements in the ionized zone.
  - ***Thermal Balance*** between heating and cooling. Heating is dominated by photoelectrons ejected from hydrogen and helium with thermal energies of a few eV. Cooling is mostly dominated by electron-ion impact excitation of metal ion followed by emission of “forbidden” lines from low-lying fine structure levels. It is these cooling lines that give H II regions their characteristic spectra.
  - ***Hydrodynamics***, including shocks, ionization and photodissociation fronts, and outflows and winds from the embedded stars.

# Photoionization

- The (nonrelativistic) quantum mechanics of hydrogen-like ions (with only one electron) give an analytic expression for the ground-state photoionization (photoelectric) cross section.

$$\sigma_{\text{pi}}(\nu) = \sigma_0 \left( \frac{Z^2 I_{\text{H}}}{h\nu} \right)^4 \frac{e^{4-4 \arctan(x)/x}}{1 - e^{-2\pi/x}}, \quad x \equiv \sqrt{\frac{h\nu}{Z^2 I_{\text{H}}} - 1} \quad \text{for } h\nu > Z^2 I_{\text{H}}$$

- The cross section at threshold is

$$\sigma_0 \equiv \frac{2^9 \pi}{3e^4} \alpha \pi a_0^2 Z^{-2} = 6.304 \times 10^{-18} Z^{-2} \text{ cm}^{-2} \quad \begin{matrix} \text{fine-structure constant} \\ (\alpha \equiv e^2/hc = 1/137.04, e = 2.71828...) \end{matrix}$$

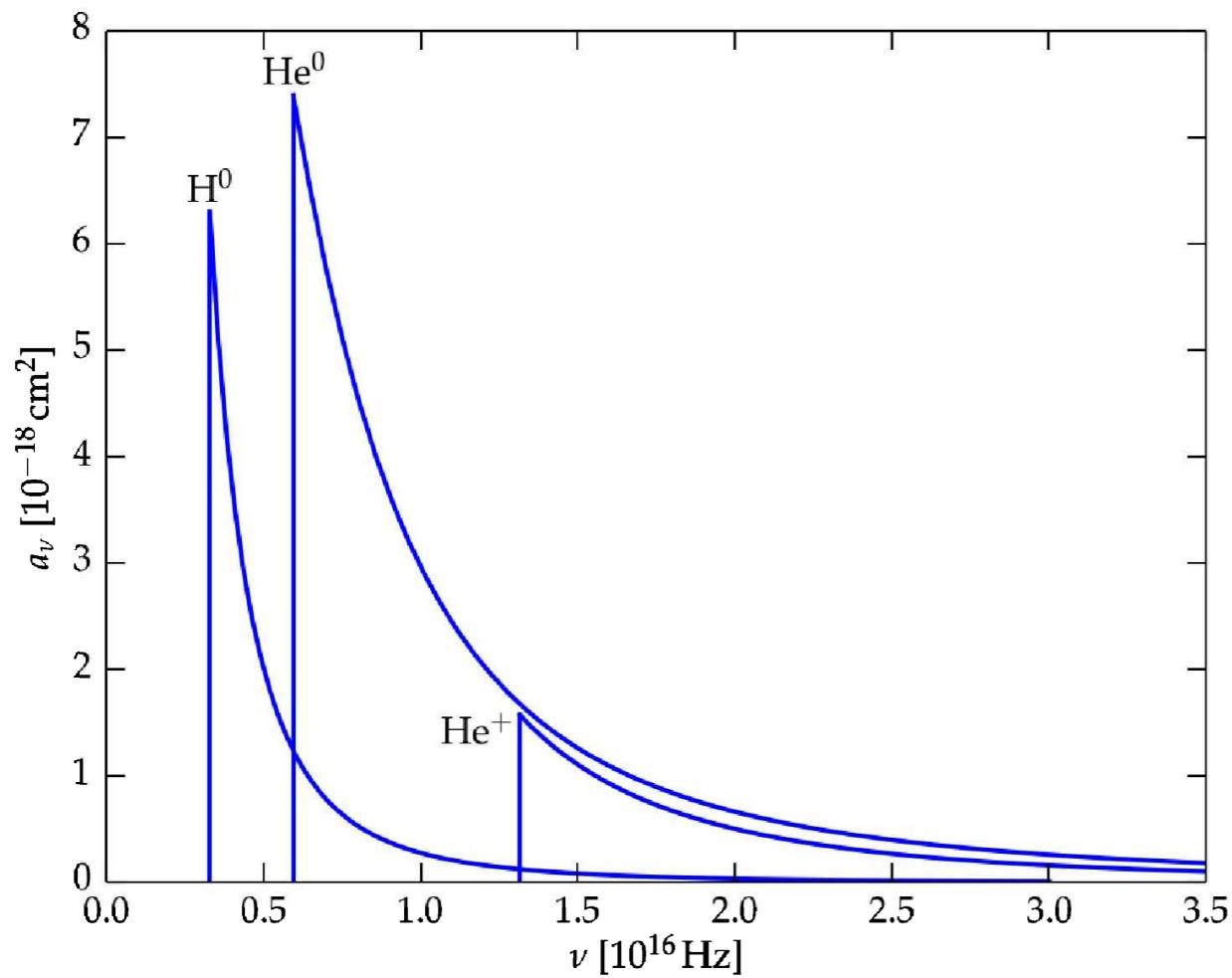
- The photoionization cross section is reasonably approximated by a power-law:

$$\sigma_{\text{pi}}(\nu) \approx \sigma_0 \left( \frac{h\nu}{Z^2 I_{\text{H}}} \right)^{-3} \quad \text{for } Z^2 I_{\text{H}} \lesssim h\nu \lesssim 100 Z^2 I_{\text{H}}$$

- At high energies, the asymptotic behavior is:

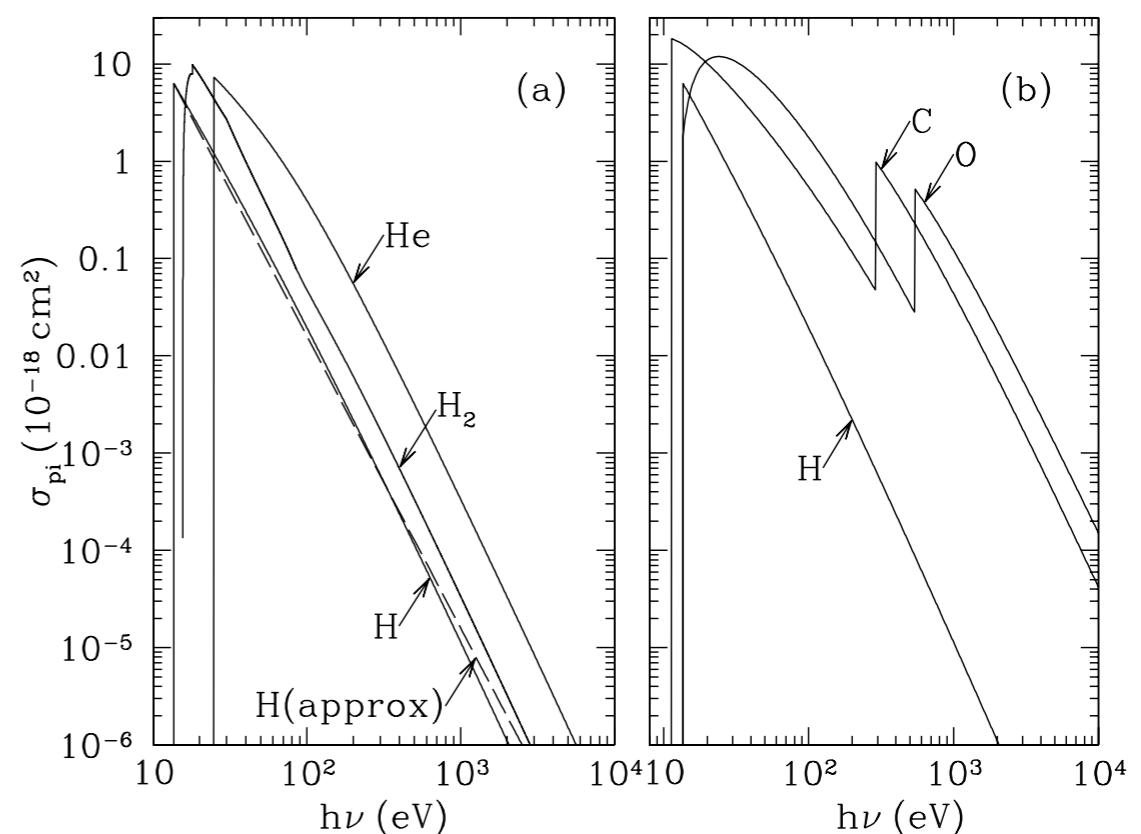
$$\sigma_{\text{pi}}(\nu) \approx \frac{2^8}{3Z^2} \alpha (\pi a_0^2) \left( \frac{h\nu}{Z^2 I_{\text{H}}} \right)^{-3.5} \quad \text{for } h\nu \gg Z^2 I_{\text{H}}$$

The hydrogen photoionization cross section becomes equal to the Thomson (Compton) Scattering cross section for  $h\nu \approx 2.5 \text{ keV}$ ; above this energy photoionization of H is dominated by Thomson scattering rather than photoelectric absorption.

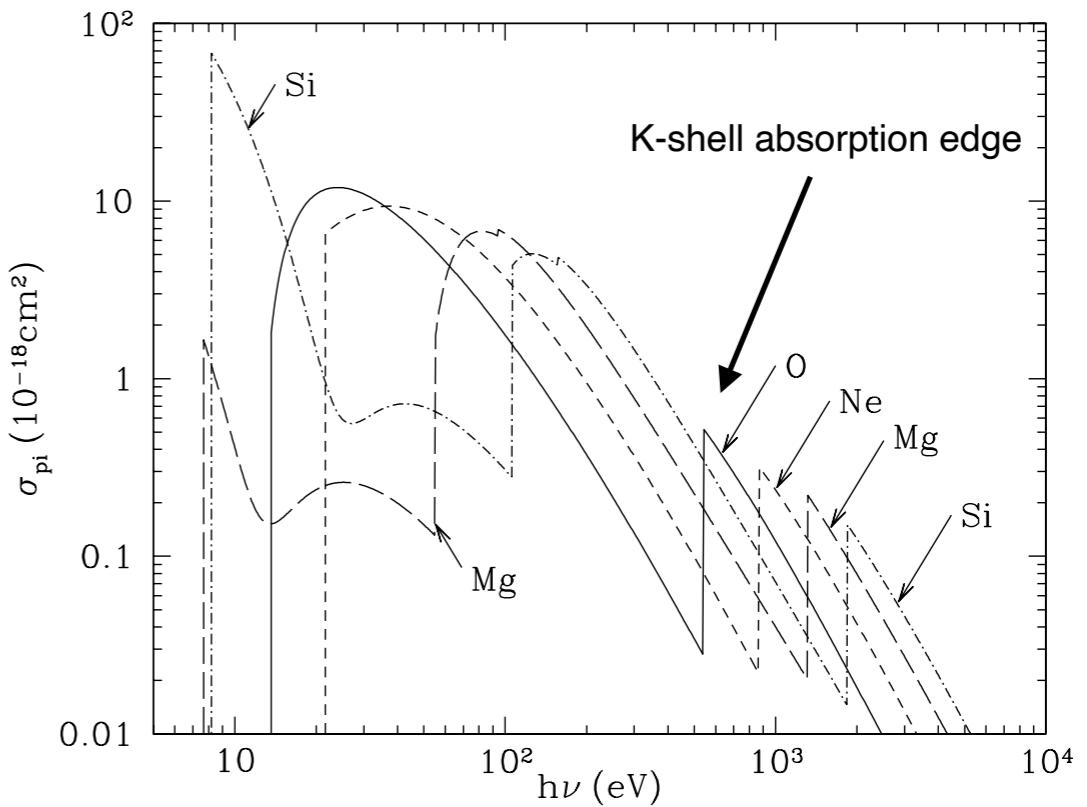


Photoionization cross section for hydrogen( $H^0$ ),  
hydrogenic helium ( $He^+$ ), and neutral helium ( $He^0$ ).  
[Fig. 4.1 in Ryden]

- For atoms with three or more electrons, the energy dependence of the photoionization cross section is considerably more complicated because there is more than one available channel.
  - Convenient analytic fits to the contribution of individual shells to photoionization cross section are given by Verner & Yakovlev (1995) and Verner et al. (1996).



[Fig. 13.1 in Draine]



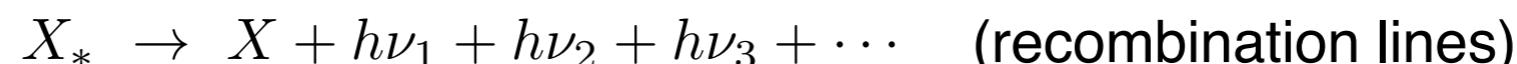
[Fig. 13.2 in Draine]

# Recombination

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- ***Radiative recombination***

- ▶ Radiative recombination is the process of capture of an electron by an ion where the excess energy of the electron is radiated away in a photon.
- ▶ The electron is captured into an excited state. The recombined but still excited ion radiates several photons in a radiative cascade, as it returns to the ground state:

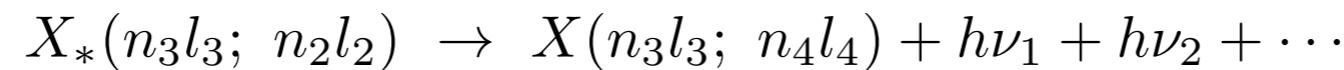
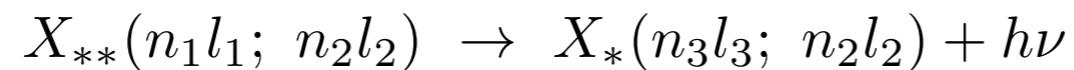
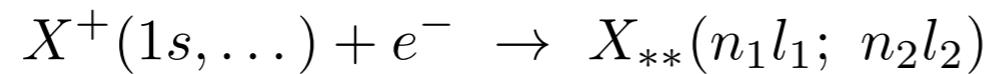


- ▶ The photon in the first line represents a **recombination continuum** ( $h\nu$ ) photon. However, photons ( $h\nu_1, h\nu_2, h\nu_3$ ) represent quantized transitions and are therefore termed **recombination lines**.
- ▶ ***The total effective recombination rate is the sum of the recombination rate to each state.***

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- ***Dielectronic recombination***

- For an electron that is initially free to be captured to a bound state of an atom or ion, the electron must lose energy.
  - ▶ Radiative recombination is relatively slow because it is necessary to create a photon to remove this energy as part of the capture process. This can take place only during the brief time that the free electron is appreciably accelerated by the electric field of ion.
  - ▶ However, if an ion has at least one bound electron, then it is possible for the incoming electron to transfer energy to a bound electron, promoting the bound electron to an excited state, and removing enough energy from the first electron that it too can be captured in an excited state. Then, the ion now have two electrons in excited state.
  - ▶ Dielectronic recombination (DR) is a resonant two-step process.
    - ▶ The first step is a double-electron process, often called dielectronic capture, through which one free electron is captured and another core electron is simultaneously excited forming a doubly excited state. One of the electron is in an autoionizing state,  $n_1l_1$ , and the other is in an excited state,  $n_2l_2$ . In the second step, the ion in a doubly excited state emits a photon and decays into a stable state below the ionization limit.

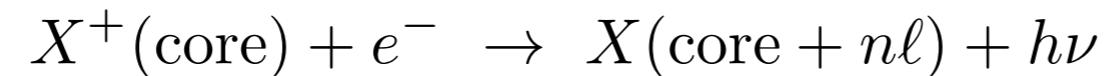


- ▶ Dielectronic recombination is important in high-temperature plasmas, where it often exceeds the radiative recombination rate.

# Radiative Recombination (RR)

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- The cross section for the radiative recombination can be obtained using the photoionization cross section and the *Milne relation*, which is derived from the principle of detailed balance.
- Consider an ion with its electron in some configuration that we will refer to as the “core”. In a low-density plasma, free electrons can undergo transitions to bound states by emission of a photon. The electron is captured into some specific state  $n\ell$  that will initially unoccupied.



- The RR rate coefficient for electron capture directly to level  $n\ell$ , with emission of a photon of energy  $h\nu = I_{n\ell} + E$  (where  $I_{n\ell}$  is the bounding energy required for ionization from level  $n\ell$  and  $E$  is the captured electron energy), is

$$\alpha_{n\ell}(T) \equiv \langle \sigma_{\text{rr},n\ell} v \rangle = \left( \frac{8kT}{\pi m_e} \right)^{1/2} \int_0^\infty \sigma_{\text{rr},n\ell}(E) \frac{E}{kT} e^{-E/kT} \frac{dE}{kT}$$

The integral indicates an average over the Maxwell distribution for electrons.

- The volumetric rate of RR, for instance for hydrogen, can be written as

$$\frac{dn_p}{dt} = -n_e n_p \alpha$$

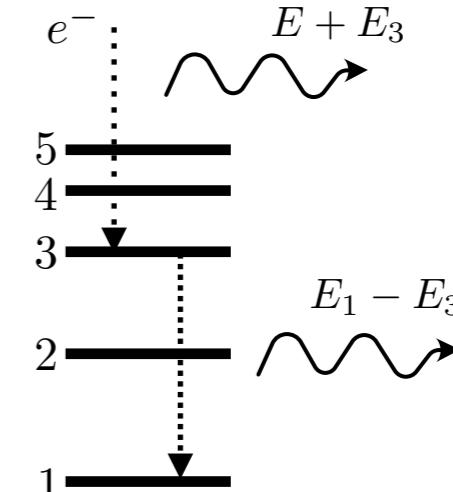
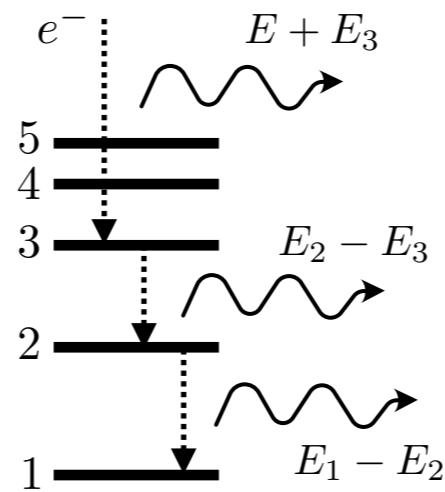
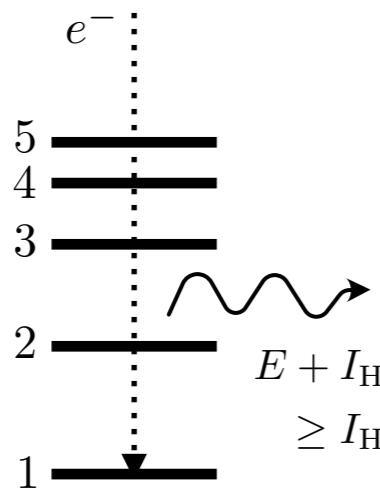
Notice that an electron of any energy can trigger a collisional de-excitation as well as RR.

- Properties of radiative recombination

- In general,  $\alpha_{n\ell}$  is a decreasing function of  $T$ , although it depends weakly on temperature. Therefore, ***it's easier to recombine with a slow electron than with a fast electron.***
- In general,  $\alpha_n = \sum_\ell \alpha_{n\ell}$  summed over all applicable values of  $\ell$ , is a decreasing function of  $n$ , implying that ***it's easier to recombine to a low energy level than to a high energy level.***

- **Recombination to the ground state:**

- If the recombination is to the ground state of hydrogen ( $n = 1$ ), the energy of the emitted photon is  $E + I_H \geq I_H$ . Thus, the emitted photon is guaranteed to have an energy of at least 13.6 eV, and will be capable of photoionizing any neutral hydrogen atom that it encounters. Thus, in regions that are optically thick to UV light at photon energies just above  $I_H$ , the emitted photon will be rapidly destroyed in photoionizing a nearby hydrogen atom.



# Case A and B (Radiative Recombination of Hydrogen)

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- ***On-the-spot approximation:***
  - In optically thick regions, it is assumed that every photon produced by radiative recombination to the ground state of hydrogen is immediately, then and there, destroyed in photoionizing other hydrogen atom.
  - In the on-the-spot approximation, recombination to the ground state has no net effect on the ionization state of the hydrogen gas.
- Baker & Menzel (1938) proposed two limiting cases:
  - ***Case A: Optically thin*** to ionizing radiation, so that every ionizing photon emitted during the recombination process escapes. For this case, we sum the radiative capture rate coefficient  $\alpha_{n\ell}$  over all levels  $n\ell$ .
  - ***Case B: Optically thick*** to radiation just above  $I_H = 13.60 \text{ eV}$ , so that ionizing photons emitted during recombination are immediately reabsorbed, creating another ion and free electron by photoionization. In this case, the recombinations directly to  $n = 1$  do not reduce the ionization of the gas: ***only recombinations to  $n \geq 2$  act to reduce the ionization.***
- ***Case B in photoionized gas:*** Photoionized nebulae around OB stars (H II regions) usually have large enough densities of neutral H. For this situation, case B is an excellent approximation.
- ***Case A in collisionally ionized gas:*** Regions where the hydrogen is collisional ionized are typically very hot ( $T > 10^6 \text{ K}$ ) and contain a very small density of neutral hydrogen. For these shock-heated regions, case A is an excellent approximation.

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- ***Radiative recombination rate coefficients:***

- In Case A, the relevant radiative recombination rate coefficient is found by summing over all energy levels of the hydrogen atom:

$$\alpha_{A,H}(T) \equiv \sum_{n=1}^{\infty} \sum_{\ell=0}^{n-1} \alpha_{n\ell}(T)$$

$$\approx 4.18 \times 10^{-13} T_4^{-0.721 - 0.021 \ln T_4} [\text{cm}^3 \text{s}^{-1}] \quad \text{for } 0.3 \lesssim T_4 \lesssim 3 \quad (T_4 \equiv T/10^4 \text{ K})$$

- In Case B, the relevant radiative recombination rate coefficient is found by summing over all energy levels other than the ground state:

$$\alpha_{B,H}(T) \equiv \sum_{n=2}^{\infty} \sum_{\ell=0}^{n-1} \alpha_{n\ell}(T) = \alpha_{A,H}(T) - \alpha_{1s}(T)$$

$$\approx 2.59 \times 10^{-13} T_4^{-0.833 - 0.034 \ln T_4} [\text{cm}^3 \text{s}^{-1}] \quad \text{for } 0.3 \lesssim T_4 \lesssim 3$$

- The percentage of radiative recombinations that go directly to the ground state is 30% at  $T = 3000 \text{ K}$  but increases to 46% at  $T = 30,000 \text{ K}$ . Thus, the distinction between Case A and Case B becomes increasingly important at higher temperatures.

$$\frac{\alpha_{1s,H}}{\alpha_{A,H}} = 1 - \frac{\alpha_{B,H}}{\alpha_{A,H}} = 1 - 0.0619 T_4^{-0.112 - 0.013 \ln T_4}$$

# Photoionization of He<sup>+</sup> to He<sup>++</sup>

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- The central stars of planetary nebulae are much hotter than even the hottest O3 stars, do radiate high-energy photons ( $h\nu > 54.5 \text{ eV}$ ) that produce He<sup>++</sup> zones, which are observed by the He II recombination spectra.
- The structure of the central He<sup>++</sup> zones is governed by equations that are very similar to those of pure H<sup>+</sup> zones.
- Three different recombination mechanisms producing photons that ionize H<sup>0</sup>
  - (1) (cascade) recombinations that populate  $2^2P^o$ , resulting in He II Ly $\alpha$  emission with 40.8 eV.
  - (2) (cascade) recombinations that populate  $2^2S$ , resulting in He II  $2^2S \rightarrow 1^2S$  two-photon emission for which  $h\nu' + h\nu'' = 40.8 \text{ eV}$  (the spectrum peaks at 20.4 eV, and on the average, 1.42 ionizing photons are emitted per decay)
  - (3) recombinations **directly** to  $2^2S$  and  $2^2P^o$ , resulting in He II Balmer-continuum emission, which has the same threshold as the Lyman limit of H ( $E \geq h\nu_0 = 13.6 \text{ eV}$ ).

$$\text{Note : } E_{n_2 \rightarrow n_1} = 13.6Z^2 \text{ eV} \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

- He II Ly $\alpha$  photons are scattered by resonance scattering, and diffuse only slowly away from their point of origin before they are absorbed.
- He II Balmer-continuum photons are concentrated close to the H<sup>0</sup> ionization threshold and have a short mean free path.

**Table 2.6**Generation of H ionizing photons in the  $\text{He}^{++}$  zone

Number generated per H recombination	$T = 10,000 \text{ K}$	$20,000 \text{ K}$
$n(\text{He}^{++})q(\text{He}^+\text{L}\alpha)/n(\text{H}^+)\alpha_B(\text{H}^0)$	0.64	0.66
$n(\text{He}^{++})q(\text{He}^+ \text{ 2 photon})/n(\text{H}^+)\alpha_B(\text{H}^0)$	0.36	0.42
$n(\text{He}^{++})q(\text{He}^+\text{B}\alpha\text{ c})/n(\text{H}^+)\alpha_B(\text{H}^0)$	0.20	0.25

NOTE: Numerical values are calculated assuming that  $n(\text{He}^{++})/n(\text{H}^+) = 0.15$ .

- The number of ionizing photons generated in the  $\text{He}^{++}$  zone by (1) and (3) is nearly balance the recombinations of  $\text{H}^+$  in this zone (see Table 2.6). They maintain the ionization of  $\text{H}^0$  in the  $\text{He}^+$  zone. The stellar radiation with  $13.6 \text{ eV} < h\nu < 54.4 \text{ eV}$  is not significantly absorbed by the  $\text{H}^0$  in the  $\text{He}^{++}$  zone. That with  $h\nu > 54.5 \text{ eV}$  is absorbed only by the  $\text{He}^+$ .
- The He II two-photon continuum is an additional source of ionizing photons of H; most of these photons escape from the  $\text{He}^{++}$  zone. Therefore, it must be added to the stellar radiation field with  $h\nu > 54.5 \text{ eV}$  in the  $\text{He}^+$  zone.
- Stromgren radius  $r_3$  of the  $\text{He}^{++}$  zone

$$Q(\text{He}^+) = \int_{4\nu_0}^{\infty} \frac{L_\nu}{h\nu} d\nu = \frac{4\pi}{3} r_3^3 n(\text{He}^{++}) n_e \alpha_B(\text{He}^+, T)$$

- Stellar temperatures  $T \geq 10^5 \text{ K}$  are required for  $r_3/r_1 \approx 1$ .

# Coulomb Focusing

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- [https://casper.astro.berkeley.edu/astrobaki/index.php/Coulomb\\_Focusing](https://casper.astro.berkeley.edu/astrobaki/index.php/Coulomb_Focusing)
- [https://www.youtube.com/watch?v=LXGBGNR5JxI&ab\\_channel=AaronParsons](https://www.youtube.com/watch?v=LXGBGNR5JxI&ab_channel=AaronParsons)

# Ionization of Helium

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- Now, what about helium?
  - Out of every 1000 atoms, there are on average 912 hydrogen atoms, 87 helium atoms and one heavy atom.
    - ▶ Looking at the photoionization cross sections for  $H^0$ ,  $He^0$ ,  $He^{+1}$ , we see that above the 24.6 eV threshold for ionizing  $He^0$ , the photoionization cross section for helium is larger than that for hydrogen.

$$\begin{aligned}\sigma_{\text{pi},He^0} &\approx 6.5 \sigma_{\text{pi},H^0} \quad \text{at } h\nu \sim 24.6 \text{ eV} \\ &\approx 14 \sigma_{\text{pi},H^0} \quad \text{at } h\nu \sim 54.5 \text{ eV}\end{aligned}$$

- ▶ Thus, the photoionization cross section for He is  $\sim 10$  times that of H, while the number density of He is  $\sim 0.1$  times that of H.
- ▶ This implies that if we suddenly turn on a hot star, ***the initial photons in the range  $24.6 \text{ eV} < h\nu < 54.4 \text{ eV}$  will be about as likely to photoionize a helium atom as a hydrogen atom.***
- ▶ ***In the range of  $13.6 \text{ eV} < h\nu < 24.6 \text{ eV}$ , on the other hand, nearly all the photons go to ionize H;*** scarcer atoms (metals like O and C) account for only a tiny fraction of the ionizations.

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- ***Radiative Recombination of Helium***



$$\alpha_A(T) \approx 4.13 \times 10^{-13} Z(T_4/Z^2)^{-0.7131-0.0115 \ln(T_4/Z^2)} \quad [\text{cm}^3 \text{s}^{-1}] \quad (30 \text{ K} < T/Z^2 < 3 \times 10^4 \text{ K})$$

$$\alpha_B(T) \approx 2.54 \times 10^{-13} Z(T_4/Z^2)^{-0.8163-0.0208 \ln(T_4/Z^2)} \quad [\text{cm}^3 \text{s}^{-1}]$$



$$\alpha_{1s^2, \text{He}} = 1.54 \times 10^{-13} T_4^{-0.486} \quad [\text{cm}^3 \text{s}^{-1}] \quad (0.5 < T_4 < 2)$$

$$\alpha_{B, \text{He}} = 2.72 \times 10^{-13} T_4^{-0.789} \quad [\text{cm}^3 \text{s}^{-1}]$$

Here,  $\alpha_{1s^2, \text{He}}$  is the recombination rate to the ground state  $1s^2 \ ^1S_0$ ,  
and  $\alpha_{B, \text{He}}$  is the recombination rate coefficient to all states except the ground state.

Note:  $\alpha_{B, \text{H}} \approx \alpha_{B, \text{He}}$  and  $\alpha_{A, \text{H}} \approx \alpha_{A, \text{He}}$ .

- ***Effective recombination rate coefficient for Helium***

- Note that ***the stellar LyC photons with  $h\nu > 24.6 \text{ eV}$  are capable of photoionizing not only neutral helium atoms but also neutral hydrogen atoms***
- The recombinations directly to the ***ground state  $1s^2 1S_0$***  of neutral helium produce photons with  $h\nu > 24.6 \text{ eV}$ . ***The recombination continuum photons are capable of photoionizing not only neutral helium atoms but also neutral hydrogen atoms; the fraction of these that ionize hydrogen*** is

$$\begin{aligned} y &= \frac{n_{\text{H}^0} \sigma_{\text{pi}, \text{H}^0}(E)}{n_{\text{H}^0} \sigma_{\text{pi}, \text{H}^0}(E) + n_{\text{He}^0} \sigma_{\text{pi}, \text{He}^0}(E)} \\ &= \left[ 1 + \frac{n_{\text{He}^0}}{n_{\text{H}^0}} \frac{\sigma_{\text{pi}, \text{He}^0}(E)}{\sigma_{\text{pi}, \text{H}^0}(E)} \right]^{-1}, \quad \text{where } E \approx 24.6 \text{ eV} + kT \end{aligned}$$

$$\sigma_{\text{pi}, \text{He}^0}/\sigma_{\text{pi}, \text{H}^0} > 6.0 \text{ for } E > 24.6 \text{ eV}$$

$$y < 0.5 \text{ if } n_{\text{He}^0}/n_{\text{H}^0} > 0.16$$

In an optically thick gas, the effective radiative recombination rate coefficient for  $\text{He}^+ \rightarrow \text{He}^0$  is then

$$\alpha_{\text{eff}, \text{He}} = \alpha_{\text{B}, \text{He}} + y \alpha_{1s^2, \text{He}} = \alpha_{\text{A}, \text{He}} - (1 - y) \alpha_{1s^2, \text{He}}$$

$$\text{At } T = 10,000 \text{ K, } \alpha_{\text{B}, \text{He}} = 2.72 \times 10^{-13} \text{ [cm}^3 \text{s}^{-1}\text{]} \rightarrow \alpha_{\text{eff}, \text{He}} \approx 3.0 \times 10^{-13} \text{ [cm}^3 \text{s}^{-1}\text{]}$$

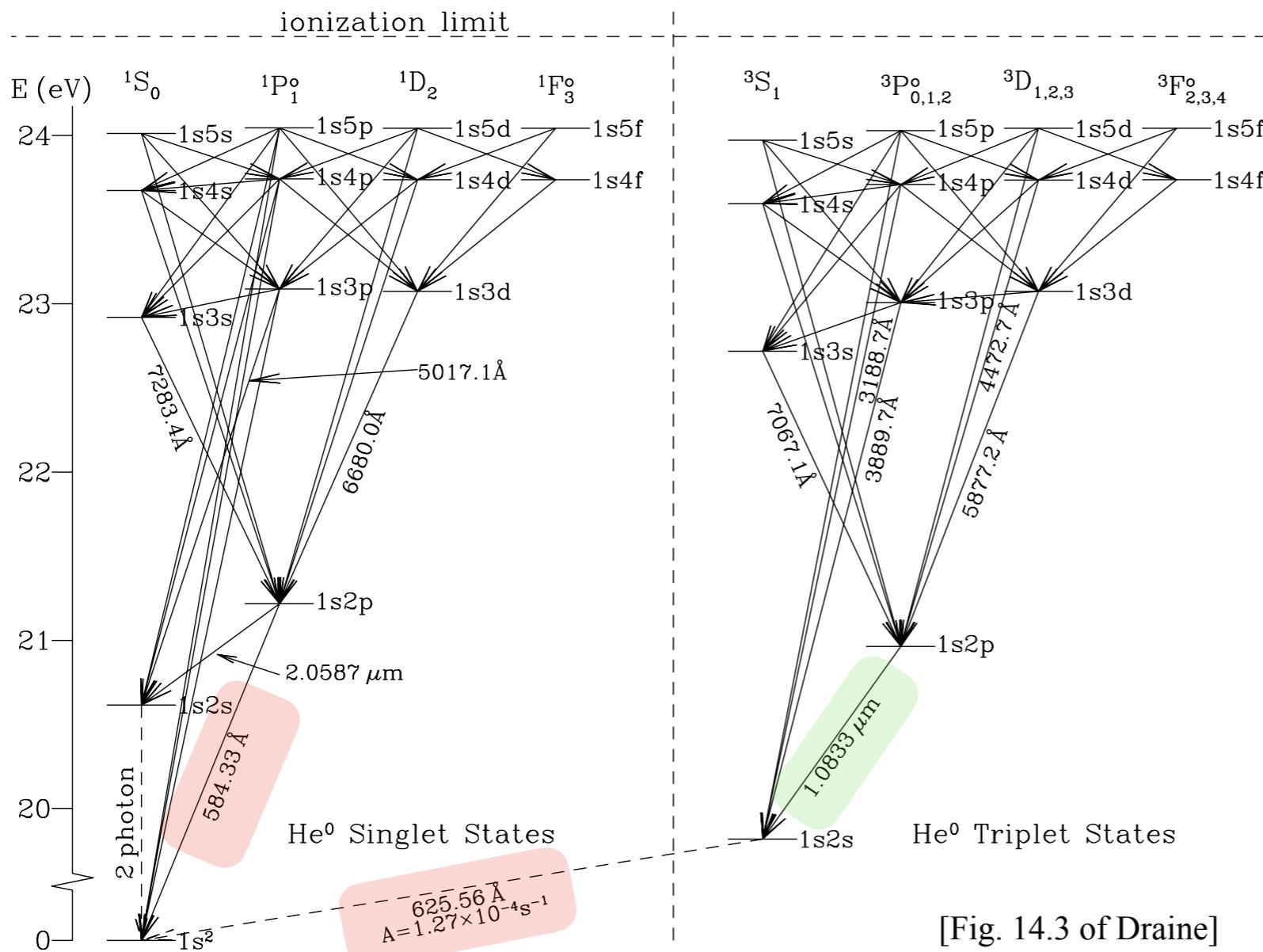
$$\alpha_{1s^2, \text{He}} = 1.54 \times 10^{-13} \text{ [cm}^3 \text{s}^{-1}\text{]} \approx 1.2 \alpha_{\text{B}, \text{H}}$$

$$y \approx 0.2$$

- This is not all. Consider now the recombination to ***excited levels*** of  $\text{He}^0$ , which are followed by a radiative cascade down. Most of photons produced by the cascades have  $h\nu > 13.6 \text{ eV}$ . ***A fraction of these photons are capable of photoionizing hydrogen. Let  $z$  be this fraction.*** However, note that ***this fraction is not relevant to the recombination of He, but contribute to the photoionization  $H$ .***

$$\begin{aligned} z &\approx 0.96 \text{ at low densities} \\ &\approx 0.67 \text{ at high densities} \end{aligned}$$

We take an intermediate value  $z \approx 0.8$ .



- See Section 14.3.2 and 15.5 of [Draine] for details.
- [Ryden] assumes that  $z = 1$ .

Note that  $1.08 \mu\text{m}$  is useful to probe the planetary atmosphere

[Fig. 14.3 of Draine]

- ***How many recombinations occur for He:*** Suppose that we have a Strömgren sphere with the cosmic abundance ratio of helium to hydrogen.  $f \equiv n_{\text{He}}/n_{\text{H}} \approx 0.096$ . Now define:

$$Q_0 \equiv \int_{I_{\text{H}}/h}^{\infty} \frac{L_{\nu}}{h\nu} d\nu, \quad Q_1 \equiv \int_{I_{\text{He}}/h}^{\infty} \frac{L_{\nu}}{h\nu} d\nu \quad (Q_1 < Q_0)$$

- In the very central region, the hydrogen would be fully ionized, and the helium would be all singly ionized. Even **the hottest O stars don't produce a significant number of photons with  $h\nu > 54.5 \text{ eV}$** ; hence, there will be no significant amount of doubly ionized  $\text{He}^{+2}$ .

- This will result in

$$\begin{aligned} n_p &= n_{\text{H}} \\ n_{\text{He}^+} &= n_{\text{He}} = f n_{\text{H}} \end{aligned} \quad \text{inside the Strömgren sphere.}$$

$$n_e = n_p + n_{\text{He}^+} = (1 + f)n_{\text{H}}$$

- The volumetric rate of the hydrogen recombination is

$$\frac{dn_p}{dt} = -\alpha_{\text{B,H}} n_e n_p = -\alpha_{\text{B,H}} (1 + f) n_{\text{H}}^2$$

- The volumetric rate of He recombination is

$$\frac{dn_{\text{He}^+}}{dt} = -\alpha_{\text{eff,He}} n_e n_{\text{He}^+} = -\alpha_{\text{eff,He}} f (1 + f) n_{\text{H}}^2$$

- Comparing the two equations, we see that

$$\begin{aligned}\frac{dn_{\text{He}^+}}{dt} &= \left( \frac{\alpha_{\text{eff}, \text{He}}}{\alpha_{\text{B}, \text{H}}} \right) f \frac{dn_p}{dt} \\ &\approx (1.2)(0.096) \frac{dn_p}{dt} \\ &\approx 0.11 \frac{dn_p}{dt}\end{aligned}$$

- Thus, for every helium recombination, we expect about 9 hydrogen recombinations.

- Remember the recombination paths, under the Case B condition:
  - $13.6 \text{ eV} < h\nu < 24.6 \text{ eV}$  : A stellar photon will ionize one H atom.
  - $h\nu > 24.6 \text{ eV}$  : For a fraction of  $y$  of the photoionization followed by the **direct recombinations to the ground state**, a stellar photon will ionize one H atom. For the remaining fraction  $(1 - y)$  of these, a stellar photon will ionize one He atom.
  - $h\nu > 24.6 \text{ eV}$  : For the photoionization followed by **the recombinations to excited states**, a stellar photon will ionize one H atom for a fraction of  $z$  of the recombination events.
- **Number of ionized atoms:** The number of ionized helium and hydrogen,  $N(\text{He}^+)$  and  $N(\text{H}^+)$ , within the ionized regions can be estimated by balancing recombinations and photoionizations:

$$\begin{aligned}
 N(\text{He}^+)n_e (\alpha_{\text{B},\text{He}} + y\alpha_{1s^2,\text{He}}) &= (1 - y)Q_1 \\
 N(\text{H}^+)n_e \alpha_{\text{B},\text{H}} &= (Q_0 - Q_1) + yQ_1 + N(\text{He}^+)n_e (z\alpha_{\text{B},\text{He}} + y\alpha_{1s^2,\text{He}})
 \end{aligned}$$

stellar LyC with  $h\nu > 24.5 \text{ eV}$  that ionize H

Contribution by the recombination to the ground state.

Contribution by the recombination to the excited state.

$$\rightarrow N(\text{H}^+)n_e \alpha_{\text{B},\text{H}} = Q_0 - N(\text{He}^+)n_e (1 - z) \alpha_{\text{B},\text{He}}$$

$$\longrightarrow \frac{N(\text{He}^+)}{N(\text{H}^+)} = \frac{(1 - y)\alpha_{\text{B},\text{H}}(Q_1/Q_0)}{\alpha_{\text{B},\text{He}} + y\alpha_{1s^2,\text{He}} - (1 - y)(1 - z)(Q_1/Q_0)\alpha_{\text{B},\text{He}}}$$

$$\frac{N(\text{He}^+)}{N(\text{H}^+)} \approx \frac{0.68(Q_1/Q_0)}{1 - 0.17(Q_1/Q_0)} \quad \text{for } z \approx 0.8, T = 8000 \text{ K, and } y = 0.2$$

- Condition for full ionization of the He in the H<sup>+</sup> Strömgren sphere:

$$\frac{N(\text{He}^+)}{N(\text{H}^+)} = \frac{n_{\text{He}}}{n_{\text{H}}} = 0.096 \rightarrow \frac{Q_1}{Q_0} \approx 0.15$$

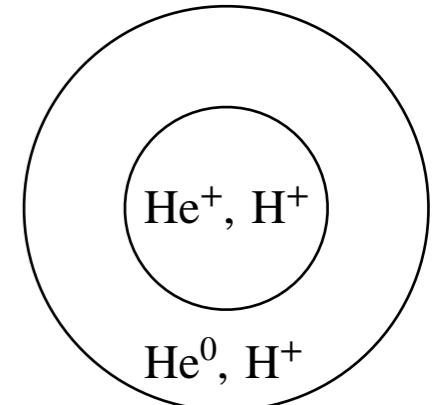
- ***Radius of the He<sup>+</sup> zone:***

$$N(\text{He}^+) = \frac{4\pi}{3} R_{\text{He}}^3 n_{\text{He}}$$

$$N(\text{H}^+) = \frac{4\pi}{3} R_{\text{H}}^3 n_{\text{H}}$$

$$R_{\text{He}} < R_{\text{H}} \quad \text{if } Q_1/Q_0 \lesssim 0.15$$

$$\begin{aligned} \frac{R_{\text{He}}}{R_{\text{H}}} &= \left[ \frac{n_{\text{H}}}{n_{\text{He}}} \frac{N(\text{He}^+)}{N(\text{H}^+)} \right]^{1/3} \\ &= \left[ \frac{7.08(Q_1/Q_0)}{1 - 0.17(Q_1/Q_0)} \right]^{1/3} \end{aligned}$$



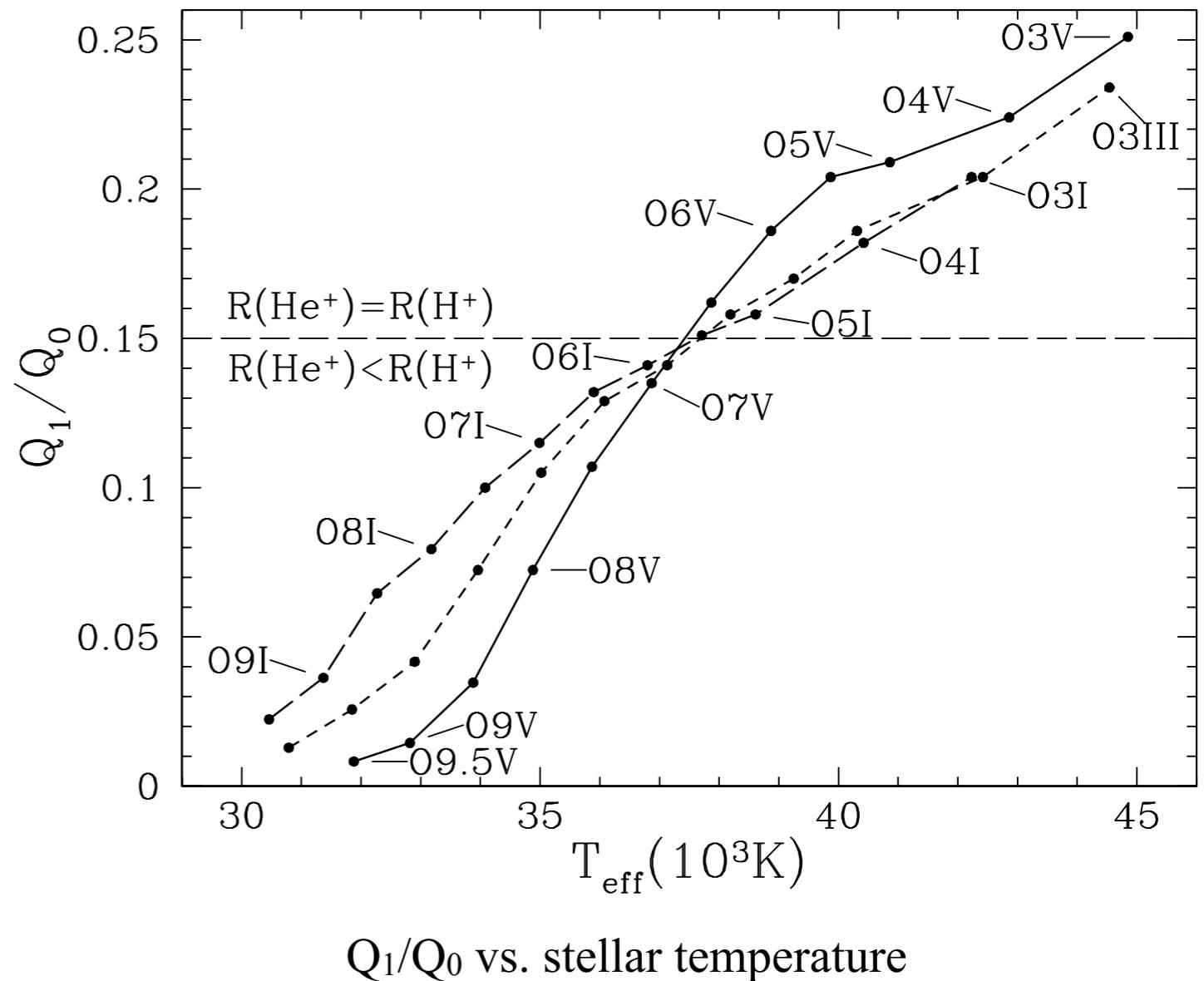
- On the main sequence, a star with spectral class O7, corresponding to effective temperature  $T_{\text{eff}} = 37,000 \text{ K}$ , will have a critical ratio  $Q_1/Q_0 \sim 0.14$ .
  - ▶ For cooler ionizing stars, the ionized helium sphere will have a radius that is smaller than the radius of the ionized hydrogen sphere.
  - ▶ For stellar temperature  $T_{\text{eff}} > 37,000 \text{ K}$ , the ionized helium sphere has the same size as the ionized hydrogen sphere, because of the limit on the abundance. The photons with  $h\nu > 24.6 \text{ eV}$  will be used up to ionize H.

Table 15.1 [Draine]

SpTp	$M/M_{\odot}$	$T_{\text{eff}}$ (K)	$\log_{10}(Q_0/\text{s}^{-1})^b$	$Q_1/Q_0^c$	$\log_{10}(L/L_{\odot})^d$
O3V	58.0	44850	49.64	0.251	5.84
O4V	46.9	42860	49.44	0.224	5.67
O5V	38.1	40860	49.22	0.209	5.49
O5.5V	34.4	39870	49.10	0.204	5.41
O6V	31.0	38870	48.99	0.186	5.32
O6.5V	28.0	37870	48.88	0.162	5.23
O7V	25.3	36870	48.75	0.135	5.14
O7.5V	22.9	35870	48.61	0.107	5.05
O8V	20.8	34880	48.44	0.072	4.96
O8.5V	18.8	33880	48.27	0.0347	4.86
O9V	17.1	32830	48.06	0.0145	4.77
O9.5V	15.6	31880	47.88	0.0083	4.68
O3III	56.0	44540	49.77	0.234	5.96
O4III	47.4	42420	49.64	0.204	5.85
O5III	40.4	40310	49.48	0.186	5.73
O5.5III	37.4	39250	49.40	0.170	5.67
O6III	34.5	38190	49.32	0.158	5.61
O6.5III	32.0	37130	49.23	0.141	5.54
O7III	29.6	36080	49.13	0.129	5.48
O7.5III	27.5	35020	49.01	0.105	5.42
O8III	25.5	33960	48.88	0.072	5.35
O8.5III	23.7	32900	48.75	0.0417	5.28
O9III	22.0	31850	48.65	0.0257	5.21
O9.5III	20.6	30790	48.42	0.0129	5.15
O3I	67.5	42230	49.78	0.204	5.99
O4I	58.5	40420	49.70	0.182	5.93
O5I	50.7	38610	49.62	0.158	5.87
O5.5I	47.3	37710	49.58	0.151	5.84
O6I	44.1	36800	49.52	0.141	5.81
O6.5I	41.2	35900	49.46	0.132	5.78
O7I	38.4	34990	49.41	0.115	5.75
O7.5I	36.0	34080	49.31	0.100	5.72
O8I	33.7	33180	49.25	0.079	5.68
O8.5I	31.5	32270	49.19	0.065	5.65
O9I	29.6	31370	49.11	0.0363	5.61
O9.5I	27.8	30460	49.00	0.0224	5.57

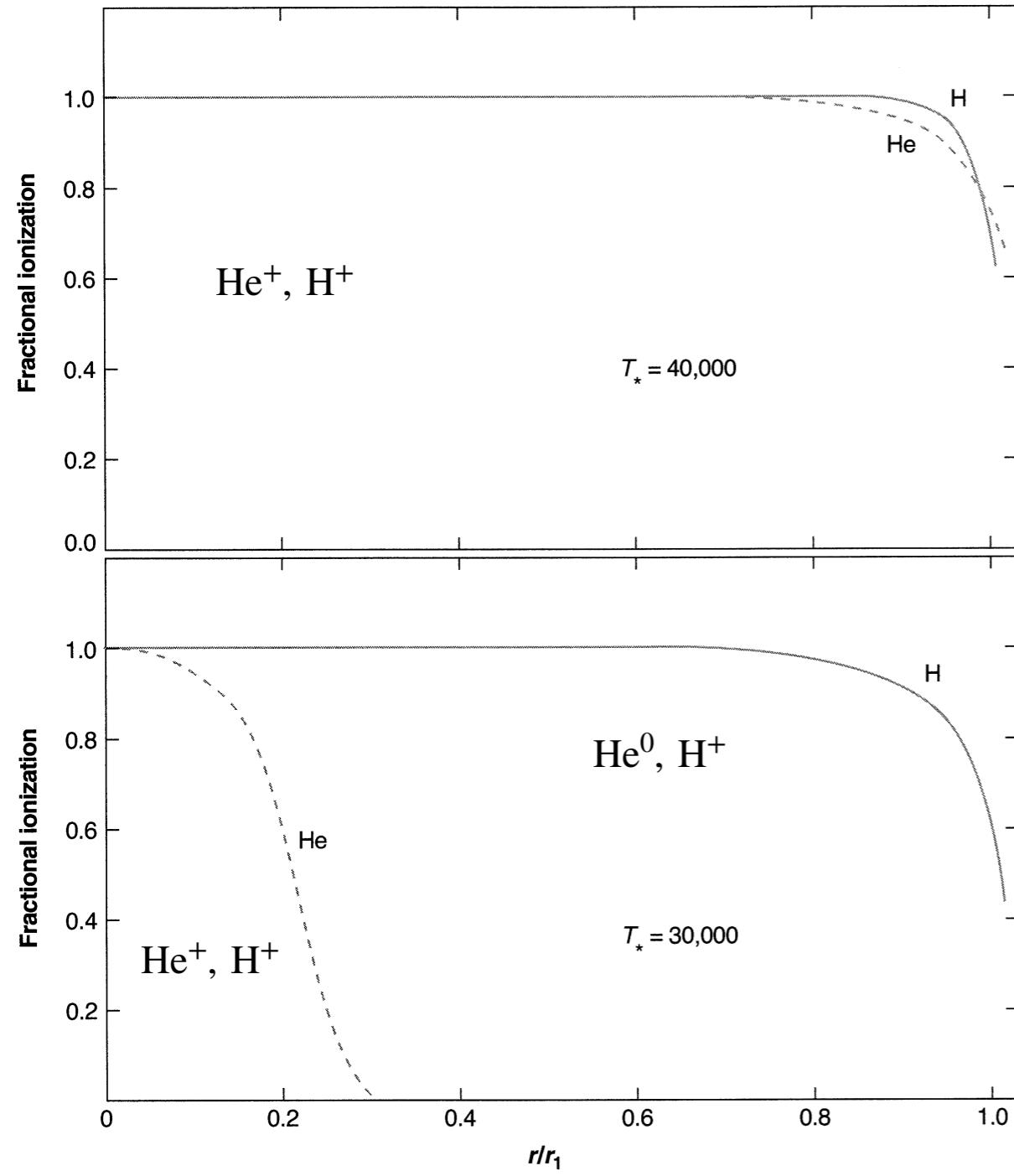
<sup>a</sup> After Martins et al. (2005).<sup>b</sup>  $Q_0$  = rate of emission of  $h\nu > 13.6 \text{ eV}$  photons.<sup>c</sup>  $Q_1$  = rate of emission of  $h\nu > 24.6 \text{ eV}$  photons.<sup>d</sup>  $L$  = total electromagnetic luminosity.

Figure 15.5 [Draine]



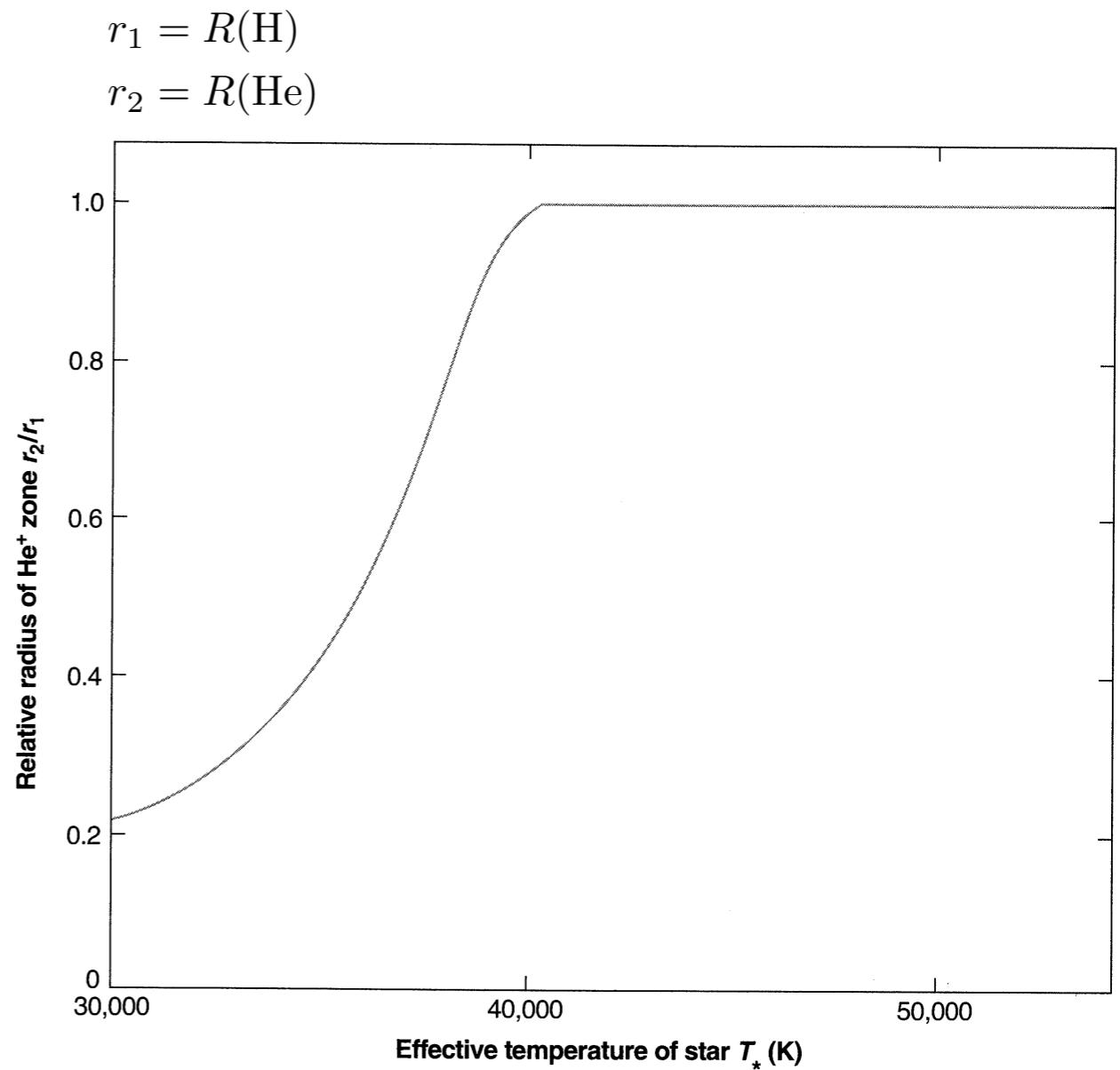
$Q_1/Q_0 > 0.15$  is required for He to be ionized throughout the H II region, corresponding to  $T_{\text{eff}} > 37,000 \text{ K}$ .

Figure 2.4 [Osterbrock]



Ionization structure of two homogeneous H + He models for H II regions.

Figure 2.5 [Osterbrock]



Relative radius of  $\text{He}^+$  zone as a function of effective temperature of exciting star.

# Collisional Excitation & De-excitation

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- **Collisional Rate (Two Level Atom)**

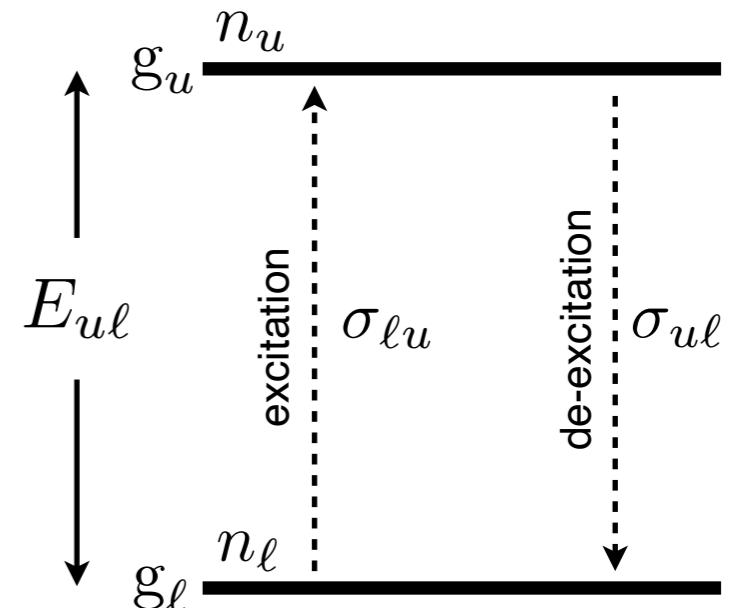
- ▶ The cross section  $\sigma_{\ell u}$  for collisional excitation from a lower level  $\ell$  to an upper level  $u$  is, in general, inversely proportional to the impact energy (or  $v^2$ ) above the energy threshold  $E_{u\ell}$  and is zero below.
- ▶ The collisional cross section can be expressed in the following form using a dimensionless quantity called the ***collision strength***  $\Omega_{\ell u}$ :

$$\begin{aligned}\sigma_{\ell u}(v) &= (\pi a_0^2) \left( \frac{hR_H}{\frac{1}{2}m_e v^2} \right) \frac{\Omega_{\ell u}}{g_\ell} \text{ cm}^2 \quad \text{for } \frac{1}{2}m_e v^2 > E_{u\ell} \\ &= \frac{h^2}{4\pi m_e^2 v^2} \frac{\Omega_{\ell u}}{g_\ell}\end{aligned}$$

or  $\sigma_{\ell u}(E) = \frac{h^2}{8\pi m_e E} \frac{\Omega_{\ell u}}{g_\ell} \quad \left( E = \frac{1}{2}m_e v^2 \right)$

where,  $a_0 = \frac{\hbar^2}{m_e e^2} = 5.12 \times 10^{13}$  cm, Bohr radius

$$R_H = \frac{m_e e^4}{4\pi \hbar^3} = 109,737 \text{ cm}^{-1}, \text{ Rydberg constant} \quad \left( \hbar = \frac{h}{2\pi} \right)$$



- ▶ The collision strength  $\Omega_{\ell u}$  is a function of electron velocity (or energy) but is often approximately constant near the threshold. Here,  $g_\ell$  and  $g_u$  are the statistical weights of the lower and upper levels, respectively.

- Advantage of using the collision strength is that (1) it removes the primary energy dependence for most atomic transitions and (2) they have the symmetry between the upper and the lower states.

**The principle of detailed balance** states that ***in thermodynamic equilibrium each microscopic process is balanced by its inverse.***

$$n_e n_\ell v_\ell \sigma_{\ell u}(v_\ell) f(v_\ell) dv_\ell = n_e n_u v_u \sigma_{u\ell}(v_u) f(v_u) dv_u$$

Here,  $v_\ell$  and  $v_u$  are related by.  $\frac{1}{2}m_e v_\ell^2 = \frac{1}{2}m_e v_u^2 + E_{u\ell}$ , and  $f(v)$  is a Maxwell velocity distribution of electrons. Using the Boltzmann equation of thermodynamic equilibrium,

$$\frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

we derive the following relation between the cross-sections for excitation and de-excitation are

$$g_\ell v_\ell^2 \sigma_{\ell u}(v_\ell) = g_u v_u^2 \sigma_{u\ell}(v_u) \quad \text{Here, } \frac{1}{2}m_e v_\ell^2 = \frac{1}{2}m_e v_u^2 + E_{u\ell} \rightarrow g_\ell \cdot (E + E_{u\ell}) \cdot \sigma_{\ell u}(E + E_{u\ell}) = g_u \cdot E \cdot \sigma_{u\ell}(E)$$

and the symmetry of the collision strength between levels. where  $E = \frac{1}{2}m_e v_u^2$

$$\Omega_{\ell u} = \Omega_{u\ell}$$

more precisely  $\Omega_{\ell u}(E + E_{u\ell}) = \Omega_{u\ell}(E)$

These two relations were derived in the TE condition. However, ***the cross-sections are independent on the assumptions, and thus the above relations should be always satisfied.***

► Collisional excitation and de-excitation rates

The ***collisional de-excitation rate per unit volume per unit time, which is thermally averaged,*** is

$$\begin{aligned} \left( \frac{dn_\ell}{dt} \right)_{u \rightarrow \ell} &= n_e n_u \int_0^\infty v \sigma_{u\ell}(v) f(v) dv \\ &= n_e n_u k_{u\ell} \quad [\text{cm}^{-3} \text{ s}^{-1}] \end{aligned}$$

$$k_{u\ell} \equiv \langle \sigma v \rangle_{u \rightarrow \ell}$$

$$\begin{aligned} k_{u\ell} &= \int_0^\infty v \sigma_{u\ell}(v) f(v) dv \\ &= \left( \frac{2\pi\hbar^4}{k_B m_e^3} \right)^{1/2} T^{-1/2} \frac{\langle \Omega_{u\ell} \rangle}{g_u} \\ &= \frac{8.62942 \times 10^{-6}}{T^{1/2}} \frac{\langle \Omega_{u\ell} \rangle}{g_u} \quad [\text{cm}^3 \text{ s}^{-1}], \end{aligned}$$

**effective collision strength:**

$$\langle \Omega_{u\ell} \rangle \equiv \int_0^\infty \Omega_{u\ell}(E) e^{-E/k_B T} d(E/k_B T)$$

and the ***collisional excitation rate per unit volume per unit time*** is

$$\left( \frac{dn_u}{dt} \right)_{\ell \rightarrow u} = n_e n_\ell k_{\ell u}$$

$$k_{\ell u} \equiv \langle \sigma v \rangle_{\ell \rightarrow u}$$

$$\begin{aligned} k_{\ell u} &= \int_{v_{\min}}^\infty v \sigma_{\ell u}(v) f(v) dv \quad \text{Here, } \frac{1}{2} m_e v_{\min}^2 = E_{u\ell} \\ &= \left( \frac{2\pi\hbar^4}{k_B m_e^3} \right)^{1/2} T^{-1/2} \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} \exp\left(-\frac{E_{u\ell}}{k_B T}\right) \end{aligned}$$

Here,  $k_{\ell u}$  and  $k_{u\ell}$  are the collisional rate coefficient for excitation and de-excitation coefficients in units of  $\text{cm}^3 \text{ s}^{-1}$ , respectively. We also note that ***the rate coefficients for collisional excitation and de-excitation are related by***

$$k_{\ell u} = \frac{g_u}{g_\ell} k_{u\ell} \exp\left(-\frac{E_{u\ell}}{k_B T}\right) \quad \langle \sigma v \rangle_{\ell \rightarrow u} = \frac{g_u}{g_\ell} \langle \sigma v \rangle_{u \rightarrow \ell} \exp\left(-\frac{E_{u\ell}}{k_B T}\right)$$

# Sum rule for collision strengths

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- Quantum mechanical sum rule for collision strengths for the case where one term consists of a singlet ( $S = 0$  or  $L = 0$ ) and the second consists of a multiplet: the collision strength of each fine structure level  $J$  is related to the total collision strength of the multiplet by

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

Here,  $(2J' + 1)$  is the statistical weight of an individual level in the multiplet, and  $(2S' + 1)(2L' + 1)$  is the statistical weight of the multiplet term.

We can regard the collision strength as “shared” amongst these levels in proportion to the statistical weights of the individual levels ( $g_J = 2J + 1$ ).

- The flux ratio between the lines in a multiplet is proportional to the ratio of their collision strengths, in a low density medium.*** Then, the flux ratio is determined by the ratio of their statistical weights.

- C-like ions ( $1s^2 2s^2 2p^2 \rightarrow 1s^2 2s^2 2p^2$ ) forbidden or inter combination transitions.

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

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

- Li-like ions ( $1s^2 2s^1 \rightarrow 1s^2 2p^1$ ) resonance transitions

ground state (singlet) -  ${}^2S_{1/2}$

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

# Collisionally-Excited Emission Line

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- Emission line flux
  - ▶ In the low density limit, the collisional rate between atoms and electrons is much slower than the (spontaneous) radiative de-excitation rate of the excited level. Thus, we can balance the collisional feeding into level  $u$  by the rate of radiative transition back down to level  $\ell$ . The level population is determined by

$$n_e n_\ell k_{\ell u} = A_{u\ell} n_u$$

$$\frac{n_u}{n_\ell} = \frac{n_e k_{\ell u}}{A_{u\ell}}$$

$$= \frac{n_e}{A_{u\ell}} \beta \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} T^{-1/2} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

where  $A_{u\ell}$  is the Einstein coefficient for spontaneous emission. The line emissivity is given by

$$4\pi j_{u\ell} = E_{u\ell} A_{u\ell} n_u = E_{u\ell} n_e n_\ell k_{\ell u}$$

$$= n_e n_\ell E_{u\ell} \frac{8.62942 \times 10^{-6}}{T^{1/2}} \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right) \quad [\text{erg cm}^{-3} \text{ s}^{-1}]$$

$$\simeq \beta \chi n_e^2 E_{\ell u} T^{-1/2} \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

Here,  $\beta = \left(\frac{2\pi\hbar^4}{km_e^2}\right)^{1/2} = 8.62942 \times 10^{-6}$   
 $\chi = n_\ell/n_e$

For low temperature, the exponential term dominates because few electrons have energy above the threshold for collisional excitation, so that the line rapidly fades with decreasing temperature.

At high temperature, the  $T^{-1/2}$  term controls the cooling rate, so the line fades slowly with increasing temperature.

- 
- ▶ In **high-density limit**, the level population are set by the Boltzmann equilibrium, and the line emissivity is

$$\begin{aligned} 4\pi j_{ul} &= E_{\ell u} A_{ul} n_u \\ \frac{n_u}{n_\ell} &= \frac{g_u}{g_\ell} \exp\left(-\frac{E_{ul}}{kT}\right) \\ &= n_\ell E_{\ell u} A_{ul} \frac{g_u}{g_\ell} \exp\left(-\frac{E_{\ell u}}{kT}\right) \\ &\simeq \chi n_e E_{\ell u} A_{ul} \frac{g_u}{g_\ell} \exp\left(-\frac{E_{\ell u}}{kT}\right) \end{aligned}$$

Here, **the line flux scales as  $n_e$  rather than  $n_e^2$ , but the line flux tends to a constant value at high temperature.**

- ▶ **Critical density** is defined as **the density where the radiative depopulation rate matches the collisional de-excitation for the excited state.**

$$\begin{aligned} A_{ul} n_u &= n_e n_u k_{ul} \\ n_{\text{crit}} &= \frac{A_{ul}}{k_{ul}} \end{aligned}$$

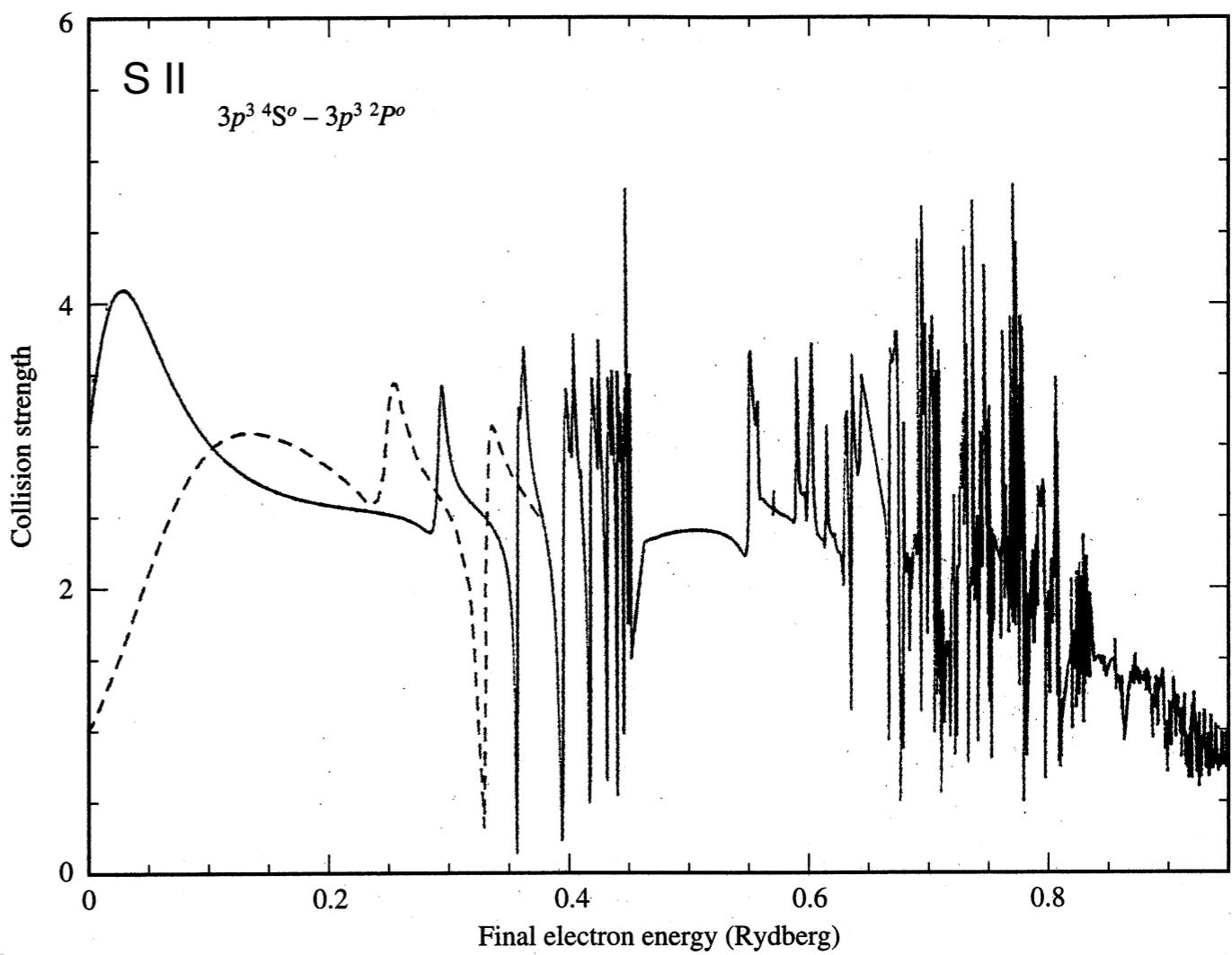
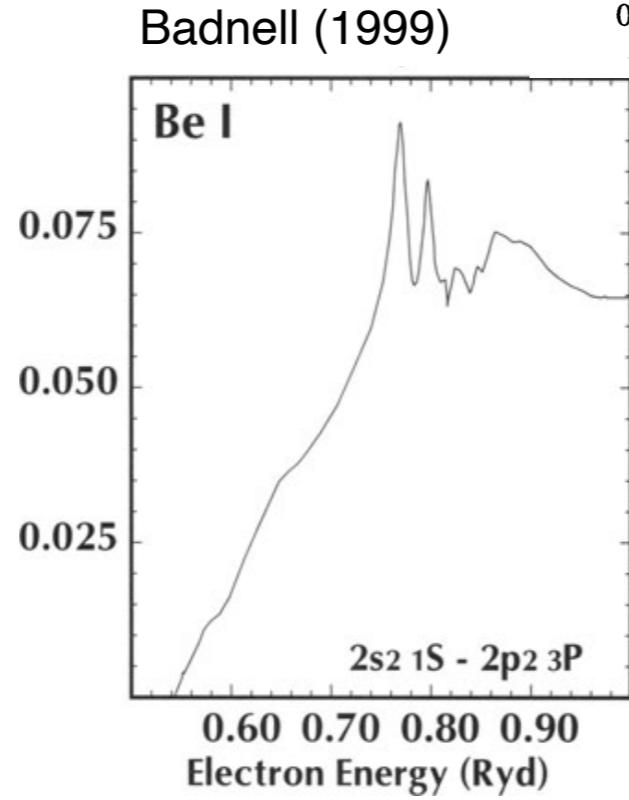
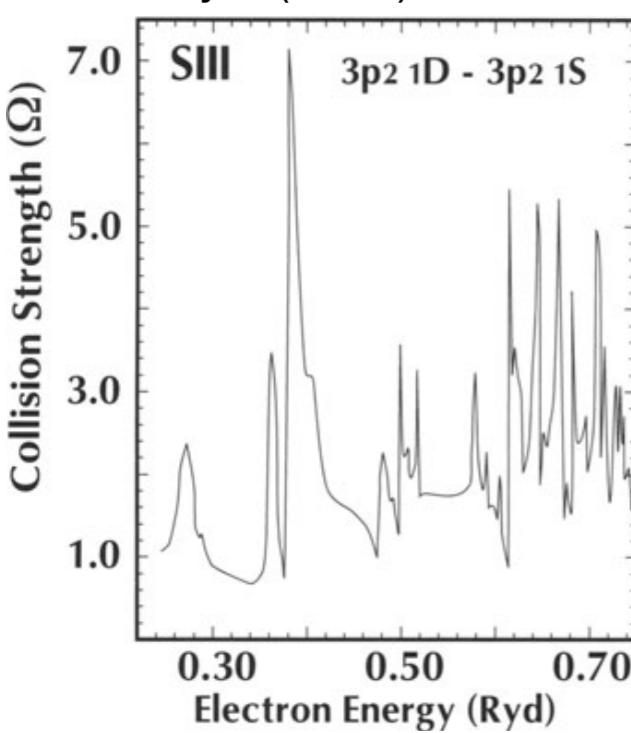
$$\begin{aligned} \rightarrow n_{\text{crit}} &= A_{ul} \frac{g_u}{\beta \langle \Omega_{ul} \rangle} T^{1/2} \\ &= 1.2 \times 10^3 \frac{A_{ul}}{10^{-4} \text{ s}^{-1}} \frac{g_u}{\langle \Omega_{ul} \rangle} \left( \frac{T}{10^4 \text{ K}} \right)^{1/2} [\text{cm}^{-3}] \end{aligned}$$

- ▶ At densities higher than the critical density, collisional de-excitation becomes significant, and the forbidden lines will be weaker as the density increases.

*At around the critical density, the “line emissivity vs density” plotted in log-log scale changes slope from +2 to +1.*

- Collision Strength

- Quantum mechanical calculations show that (1) the resonance structure in the collision strengths is important and (2) the collision strength increases with energy for neutral species.



The **effective collision strength**, which is thermally averaged, has a value in a range of

$$\langle \Omega_{ul} \rangle = \int_0^\infty \Omega_{ul}(E) e^{-E/k_B T} d(E/k_B T)$$

$$10^{-2} < \langle \Omega_{ul} \rangle < 10$$

See Table F.1 to F.5 in [Draine]

- As can be seen in Tables and the formula, collisional de-excitation is negligible for resonance and most forbidden lines in the ISM.

Collision strengths at T = 10<sup>4</sup> K

Table 4.1 in The Interstellar Medium [Lequeux]

Ion	$\ell$	u			$n_{H,\text{crit}}(u)$	
			$E_\ell/k$ (K)	$E_u/k$ (K)	$\lambda_{u\ell}$ (μm)	T = 100 K (cm <sup>-3</sup> )
C II	$^2P_{1/2}^o$	$^2P_{3/2}^o$	0	91.21	157.74	$2.0 \times 10^3$
CI	$^3P_0$	$^3P_1$	0	23.60	609.7	620
	$^3P_1$	$^3P_2$	23.60	62.44	370.37	720
O I	$^3P_2$	$^3P_1$	0	227.71	63.185	$2.5 \times 10^5$
	$^3P_1$	$^3P_0$	227.71	326.57	145.53	$8.4 \times 10^3$
Si II	$^2P_{1/2}^o$	$^2P_{3/2}^o$	0	413.28	34.814	$1.0 \times 10^5$
Si I	$^3P_0$	$^3P_1$	0	110.95	129.68	$4.8 \times 10^4$
	$^3P_1$	$^3P_2$	110.95	321.07	68.473	$9.9 \times 10^4$
						$3.5 \times 10^4$

Table 17.1 in [Draine]

- However, it is not true for the 21 cm hyperfine structure line of hydrogen.
    - The critical density for 21cm line is
- $$n_{\text{crit}} \sim 10^{-3} (T/100 \text{ K})^{-1/2} [\text{cm}^{-3}]$$

$$A_{u\ell} = 2.88 \times 10^{-15} [\text{s}^{-1}]$$
- The hyperfine levels are thus essentially in collisional equilibrium in the CNM.

Ion	Transition l-u	$\lambda$ μm	$A_{ul}$ s <sup>-1</sup>	$\Omega_{ul}$	$n_{\text{crit}}$ cm <sup>-3</sup>
C I	$^3P_0 - ^3P_1$	609.1354	$7.93 \times 10^{-8}$	–	(500)
	$^3P_1 - ^3P_2$	370.4151	$2.65 \times 10^{-7}$	–	(3000)
C II	$^2P_{1/2} - ^2P_{3/2}$	157.741	$2.4 \times 10^{-6}$	1.80	47 (3000)
	$^3P_0 - ^3P_1$	205.3	$2.07 \times 10^{-6}$	0.41	41
N II	$^3P_1 - ^3P_2$	121.889	$7.46 \times 10^{-6}$	1.38	256
	$^3P_2 - ^1D_2$	0.65834	$2.73 \times 10^{-3}$	2.99	7700
	$^3P_1 - ^1D_2$	0.65481	$9.20 \times 10^{-4}$	2.99	7700
N III	$^2P_{1/2} - ^2P_{3/2}$	57.317	$4.8 \times 10^{-5}$	1.2	1880
	$^3P_2 - ^3P_1$	63.184	$8.95 \times 10^{-5}$	–	$2.3 \times 10^4 (5 \times 10^5)$
O I	$^3P_1 - ^3P_0$	145.525	$1.7 \times 10^{-5}$	–	$3400 (1 \times 10^5)$
	$^3P_2 - ^1D_2$	0.63003	$6.3 \times 10^{-3}$	–	$1.8 \times 10^6$
	$^4S_{3/2} - ^2D_{5/2}$	0.37288	$3.6 \times 10^{-5}$	0.88	1160
O II	$^4S_{3/2} - ^2D_{3/2}$	0.37260	$1.8 \times 10^{-4}$	0.59	3890
	$^3P_0 - ^3P_1$	88.356	$2.62 \times 10^{-5}$	0.39	461
O III	$^3P_1 - ^3P_2$	51.815	$9.76 \times 10^{-5}$	0.95	3250
	$^3P_2 - ^1D_2$	0.50069	$1.81 \times 10^{-2}$	2.50	$6.4 \times 10^5$
	$^3P_1 - ^1D_2$	0.49589	$6.21 \times 10^{-3}$	2.50	$6.4 \times 10^5$
	$^1D_2 - ^1S_0$	0.43632	1.70	0.40	$2.4 \times 10^7$
	$^2P_{1/2} - ^2P_{3/2}$	12.8136	$8.6 \times 10^{-3}$	0.37	$5.9 \times 10^5$
Ne II	$^3P_2 - ^3P_1$	15.5551	$3.1 \times 10^{-2}$	0.60	$1.27 \times 10^5$
	$^3P_1 - ^3P_0$	36.0135	$5.2 \times 10^{-3}$	0.21	$1.82 \times 10^4$
Si II	$^2P_{1/2} - ^2P_{3/2}$	34.8152	$2.17 \times 10^{-4}$	7.7	$(3.4 \times 10^5)$
	$^4S_{3/2} - ^2D_{5/2}$	0.67164	$2.60 \times 10^{-4}$	4.7	1240
S II	$^4S_{3/2} - ^2D_{3/2}$	0.67308	$8.82 \times 10^{-4}$	3.1	3270
	$^3P_0 - ^3P_1$	33.4810	$4.72 \times 10^{-4}$	4.0	1780
S III	$^3P_1 - ^3P_2$	18.7130	$2.07 \times 10^{-3}$	7.9	$1.4 \times 10^4$
	$^2P_{1/2} - ^2P_{3/2}$	10.5105	$7.1 \times 10^{-3}$	8.5	$5.0 \times 10^4$
Ar II	$^2P_{1/2} - ^2P_{3/2}$	6.9853	$5.3 \times 10^{-2}$	2.9	$1.72 \times 10^6$
	$^3P_2 - ^3P_1$	8.9914	$3.08 \times 10^{-2}$	3.1	$2.75 \times 10^5$
Ar III	$^3P_1 - ^3P_0$	21.8293	$5.17 \times 10^{-3}$	1.3	$3.0 \times 10^4$
	$^6D_{7/2} - ^6D_{5/2}$	35.3491	$1.57 \times 10^{-3}$	–	$(3.3 \times 10^6)$
Fe II	$^6D_{9/2} - ^6D_{7/2}$	25.9882	$2.13 \times 10^{-3}$	–	$(2.2 \times 10^6)$