AST1430 Assignment 3

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Perhaps if the days were substantially longer I may have been able to complete this assignment.

1 Emission of Ly α from an HII Region

This involves a lot of order-of-magnitude estimates.

Part 1

Estimate the neutral fraction for hydrogen in an HII region around an O6 star. The Stromgren sphere has a radius $r_s \sim 100\,\mathrm{pc}$ and a mean density of $1/\mathrm{cm}^3$. Note that an ionizing photon (Ly-continuum) has a mean-free-path of order the Stromgren radius.

Solution

Since we know that the mean-free-path is given by

$$\ell_{\rm mfp} = \frac{1}{n\sigma_{\nu}}$$

where n is the number density and σ_{ν} is the cross section, we can solve for the number density via

$$n = \frac{1}{\ell_{\rm mfp} \sigma_{\nu}}.$$

We're given that the mean-free-path is of order the Stromgren radius so $\ell_{\rm mfp}=100\,{\rm pc}$ and the ionization cross-section is given by

$$\sigma_{\nu} = 6 \times 10^{-18} \left(\frac{\nu}{\nu_0}\right)^3 \text{ cm}^2.$$

Assuming $\nu = \nu_0$ corresponds to the ionization frequency of hydrogen at 13.6 eV, the ionization cross section simplifies to $\sigma_{\nu} = 6 \times 10^{-18}$.

The ionization fraction of hydrogen X is then found via:

$$X = \frac{n_{\rm HI}}{n_{\rm H}}$$

$$X = \left(\frac{1}{\ell_{\rm mfp}\sigma_{\nu}}\right) \left(\frac{1}{n_{\rm H}}\right)$$

$$X = \frac{1}{(100\,{\rm pc})(6\times10^{-18}\,{\rm cm}^2)(1\,{\rm cm}^{-3})}$$

$$X = 0.0054$$

The neutral hydrogen fraction is therefore only

$$X = 0.54\%$$

meaning that 99.46% of the hydrogen atoms in the HII region are ionized.

Part 2

What is the mean-free-path for a Ly α photon ($n=2 \longleftrightarrow n=1$) in the same environment? The Einstein coefficient $A_{\text{Ly}\alpha} \approx 6 \times 10^8 \, \text{s}^{-1}$.

Solution

Recalling that the mean-free-path is expressed in terms of the absorption coefficient α_{ν} via,

$$\ell_{\rm mfp} = \frac{1}{\alpha_{\nu}},$$

we can used the expression for the absorption coefficient that we derived in the first assignment:

$$\alpha = \frac{c^2}{8\pi\nu^2} n_a A_{21} \frac{g1}{g2} \left[1 - \exp\left(-\frac{\Delta E}{k_B T}\right) \right] \phi(\nu). \tag{1}$$

Also recall that for Doppler-broadened line profiles,

$$\phi(\nu) = \frac{1}{\sqrt{\pi}\Delta\nu_D} \exp\left[-\left(\frac{\nu - \nu_0}{\Delta\nu_D}\right)^2\right],$$

where $\Delta \nu_D$ is the line width and is related to the Doppler parameter b (matter sound speed) as $\Delta \nu_D \approx (b/c)\nu_0$. So the absorption coefficient can be written as:

$$\alpha = \frac{c^2}{8\pi\nu^2} n_a A_{21} \frac{g1}{g2} \left[1 - \exp\left(-\frac{\Delta E}{k_B T}\right) \right] \frac{1}{\sqrt{\pi} \Delta \nu_D} \exp\left[-\left(\frac{\nu - \nu_0}{\Delta \nu_D}\right)^2\right]. \tag{2}$$

Since we are assuming $\nu = \nu_0$, this simplifies to

$$\alpha = \frac{c^2}{8\pi\nu^2} n_a A_{21} \frac{g_1}{g_2} \left[1 - \exp\left(-\frac{\Delta E}{k_B T}\right) \right] \frac{1}{\sqrt{\pi} \Delta \nu_D}.$$
 (3)

If we assume that the matter sound speed is 0.1c, $\Delta\nu_D \approx 0.1\nu_0$ which allows us to write the absorption coefficient as:

$$\alpha = \frac{c^2}{8\pi\nu^2} n_a A_{21} \frac{g1}{g2} \left[1 - \exp\left(-\frac{\Delta E}{k_B T}\right) \right] \frac{1}{\sqrt{\pi} 0.1 \nu_0}.$$
 (4)

Part 3

A Ly α photon can also freely escape the HII region if it gets absorbed by a (very) fast moving stom and gets re-emitted at a frequency that is optically thin. Assuming the line profile is thermally broadened with a temperature $T \sim 10^4 \,\mathrm{K}$ (typical of an HII region), how far away from the line centre does the new frequency have to be? Compared with diffusion by random walk (see above) through the HII region, is this process more likely?

Solution

Part 4

What is the fraction of neutral hydrogen that is in the n=2 state? To answer this question, we split it into two parts. Ionized hydrogen can recombime, with roughly similar probabilities, into the 2s and 2p state. This part looks at the 2s state. The transition between 2s and 1s is forbidden by dipole selection rules. However, an exotic process called the 2-photon process can happen and produces a transition probability of $A_{2\gamma} = 8.23 \, \mathrm{s}^{-1}$. Argue that for our HII region, this latter process dominates over collisional process in depopulating the 2s state. Table 3.12 of Osterbrock gives the collision strength between electron and H-atoms, $\Omega \approx 0.26$. Obtain the fraction of neutral hydrogen in the 2s state.

Solution

Part 5

On the other hand, the transition between 2p and n=1 is allowed. Estimate which of the following rates aree important for the 2p state: radiative recombination (+); electron collisional excitation from the n=1 and 2s states (+); radiative pumping by $\text{Ly}\alpha$ photons (+); spontaneous emission to the n=1 state (-); spontaneous emission to the 2s state (-);

electron collisional deexcitation to the n = 1 and 2s states (-). Take the relative numbers of Ly α and Ly-continuum photons to be their relative residence times in the HII region. What is the fraction of neutral hydrogen in the 2p state?

Solution

Part 6

Estimate the Einstein coefficient for a Balmer- α photon ($n = 2 \longleftrightarrow n = 3$), and compare your result with what you obtain by querying the NIST database. What is the integrated optical depth at its line centre?

Solution

Part 7

Compare the 2-photon process to those in sub-questiom 3, which one is a more likely fate for a Ly α photon? Relatedly, what do you think will be the dominant hydrogen lines from an HII region?

Solution

2 Largest Atom in Space

Part 1

Using L-S coupling, determine the spectroscopic terms for the ground configuration $(2s^22p^2)$ and excited configurations $(2s^22p3p, 2s^22p3s)$. Mark also possible J values. Which one is the ground state?

Solution

Ground configuration $(2s^22p^2)$

For the ground configuration $(2s^22p^2)$, $2s^2$ is a filled sub-shell and it therefore does not contribute to the angular momentum so we need only determine the spectroscopic terms for the paired electrons in the 2p orbital. First, we calculate the total number of possible microstates via

$$N = \frac{t!}{e!(t-e)!},$$

where $t = 2(2\ell + 1)$ and e is the number of available electrons. Since we have two paired electrons in the 2p orbital, $\ell = 1$, t = 6, and e = 2:

$$N = \frac{6!}{2!4!} = \frac{4! \cdot 5 \cdot 6}{2!4!} = \frac{5 \cdot 6}{2!} = 5 \cdot 3 = 15.$$

We draw out each of these 15 possible microstates (see Table 1).

Table 1: All possible electron configurations for the $(2s^22p^2)$ ground state.

		m_{ℓ}			
microstate	+1	0	-1	M_L	M_S
1	\uparrow	\uparrow		+1	+1
2		\uparrow	\uparrow	-1	+1
3	1		\uparrow	0	+1
4		\downarrow		+1	-1
5		\downarrow	\downarrow	-1	-1
6	\downarrow		\downarrow	0	-1
7	$\uparrow \downarrow$			+2	0
8	↑ ↓ ↑	\downarrow		+1	0
9	 		\downarrow	0	0
10		$\uparrow \downarrow$		0	0
11		\uparrow	\downarrow	-1	0
12	↓	\uparrow		+1	0
13			$\uparrow \downarrow$	-2	0
14	↓		\uparrow	0	0
15		\downarrow	\uparrow	-1	0

We can create a smaller table with each M_L and M_S and count up the number of such configurations (see Table 2) noting that $M_L \equiv \sum m_\ell$ and $M_S \equiv \sum m_s$ for L-S coupling.

Table 2: All possible spin and angular momentum quantum number configurations for the $(2s^22p^2)$ ground state.

		-	$\overline{M_S}$	
		+1	0	-1
	+2	0	1	0
	+1	1	2	1
M_L	0	1	3	1
	-1	1	2	1
	-2	0	1	0

The maximum spin and angular momenta in these configurations are $M_S = 1$ and $M_L = 1$ respectively, so S = 1 and L = 1. With L - S coupling, the spectroscopic terms for each configuration is given by

$$(2S+1)L_{J}$$

where S is the total spin angular momentum, (2S+1) is the spin multiplicity, L is the total orbital angular momentum which defines the orbital shape, and J is the total angular momentum with coupling between L and S. Since $^{(2S+1)}L$, this provides us with the 3P configuration. To find the possible J values, we know that

$$|L - S| \le J \le |L + S|,$$

where each value increases in integer increments. This gives us total angular momenta values of

$$|1-1| \le J \le |1+1|$$

 $0 \le J \le 2$
 $J = 0, 1, 2.$

Applying this to the ${}^{3}P$ configuration, we have the spectroscopic terms $3{}^{3}P_{0}$, $3{}^{3}P_{1}$ and $3{}^{3}P_{2}$.

We now remove these configurations from Table 2 which results in Table 3.

Table 3: Secondary spin and angular momentum quantum number configurations for the $(2s^22p^2)$ ground state.

			$\overline{M_S}$	
		+1	0	-1
	+2	0	1	0
	+1	0	1	0
M_L	0	0	2	0
	-1	0	1	0
	-2	0	1	0

Repeating the last step, the maximum spin and angular momenta in these configurations are $M_S = 0$ and $M_L = 2$ respectively, so S = 0 and L = 2. Since the spin multiplicity is ${}^{(2S+1)}L$, this provides us with the ${}^{1}D$ configuration. To find the possible J values,

$$|L - S| \le J \le |L + S||2 - 0| \le J \le |2 + 0||2 \le J \le 2J = 2.$$

Applying this to the 1D configuration, we have the spectroscopic term 1D_2 .

Repeating this step one last time, we obtain the last set of possible electron configurations in Table 4.

The maximum spin and orbital angular momenta are $M_S = 0$ and $M_L = 0$ implying that S = 0 and L = 0, respectively. Obtaining the possible J values,

$$|L - S| \le J \le |L + S|$$
$$|0 - 0| \le J \le |0 + 0|$$
$$0 \le J \le 0$$
$$J = 0.$$

Table 4: Secondary spin and angular momentum quantum number configurations for the $(2s^22p^2)$ ground state.

		-	$\overline{M_S}$	
		+1	0	-1
	+2	0	0	0
	+1	0	0	0
M_L	0	0	1	0
	-1	0	0	0
	-2	0	0	0

Thus, the final spectroscopic term is ${}^{1}S_{0}$.

To recap, all of the spectroscopic terms are: 3^3P_0 , 3^3P_1 , 3^3P_2 , 1D_2 and 1S_0 .

To find the ground state, we can use Hund's Rules which say that:

- 1. The term with maximum spin multiplicity (2S+1) has the lowest energy.
- 2. For a given multiplicity (2S + 1), the term with the largest value of the total orbital angular momentum L has the lowest energy.
- 3. For a given term, in an atom with outermost sub-shell half-filled or less, the level with the lowest value of the total angular momentum quantum number J = L + S lies lowest in energy. If the outermost shell is more than half-filled, the level with the highest value of J is lowest in energy.

Following these rules, the terms with the greatest spin multiplicity are ${}^{3}P_{0}$, ${}^{3}P_{1}$ and ${}^{3}P_{2}$. Since they all have the same orbital angular momentum L=0, we only need to find the term that satisfies the third of Hund's rules. Since each of these sub-shells only have 1 electron with a maximum electron occupancy of 6, they are all less than half filled so the term with the largest J has the lowest energy. The term ${}^{3}P_{0}$ is therefore the ground state.

Excited configuration $(2s^22p3p)$

In contrast with the previous ground configuration, this excited configuration does not have any paired electrons since there is one electron in the 2p sub-shell and another in the 3p sub-shells (the 2s sub-shell is full with two electrons so we can ignore it since it does not contribute to the angular momentum). We therefore do not need to go through the entire procedure as before to ensure the Pauli-exclusion principle is obeyed. Instead, we can simply use characteristics of L-S coupling to determine the spectroscopic terms.

The possible spin angular momentum values can be determined via

$$|s_1 - s_2| \le S \le |s_1 + s_2|,$$

where s_1 and s_2 are the spin values for the electrons in each sub-shells which gives us:

$$|1/2 - 1/2| \le S \le |1/2 + 1/2|$$

 $0 \le S \le 1$
 $S = 0, 1$.

We can also determine the possible orbital angular momentum values via

$$|\ell_1 - \ell_2| \le L \le |\ell_1 + \ell_2|,$$

where ℓ_1 and ℓ_2 are the orbital values for the electrons in each sub-shell which gives us:

$$|1-1| \le L \le |1+1|$$

 $0 \le L \le 2$
 $L = 0, 1, 2.$

Putting all of these together to determine the possible total angular momentum values J and their corresponding spectroscopic terms, we obtain Table 5.

Table 5: All possible configurations for the excited state $(2s^22p3p)$.

microstate	S	L	J	(2S+1)	spectroscopic terms
1	0	0	0	1	$^{1}S_{0}$
2	0	1	1	1	${}^{1}P_{1}$
3	0	2	2	1	$^{1}D_{2}$
4	1	0	1	3	${}^{3}S_{1}$
5	1	1	0,1,2	3	${}^{3}P_{0}, {}^{3}P_{1}, {}^{3}P_{2}$
6	1	2	1,2,3	3	$^{3}D_{1}, ^{3}D_{2}, ^{3}D_{3}$

Excited configuration $(2s^22p3s)$

The possible spin angular momentum values can be determined are

$$|s_1 - s_2| \le S \le |s_1 + s_2|$$

 $|1/2 - 1/2| \le S \le |1/2 + 1/2|$
 $0 \le S \le 1$
 $S = 0, 1$.

The possible orbital angular momentum values are

$$|\ell_1 - \ell_2| \le L \le |\ell_1 + \ell_2|$$

 $|1 - 0| \le L \le |1 + 0|$
 $1 \le L \le 1$
 $L = 1$.

Putting these together to determine the possible total angular momentum values J and their corresponding spectroscopic terms, we obtain Table 6.

Table 6: All possible configurations for the excited state $(2s^22p3s)$.

microstate	S	L	J	(2S+1)	spectroscopic terms
1	0	1	1	1	$^{1}P_{1}$
2	1	1	0,1,2	3	$^{3}P_{0}, ^{3}P_{1}, ^{3}P_{2}$

Part 2

A claim of the "largest atom in space" was reported by Stepkin et al. (2007, MNRAS, 374, 852). The authors detected CI absorption (jumping from, e.g., n = 1009 to n = 1013 state). Estimate the size of such an atom (e.g., $2s^22p1009p$), the orbital period for the outer electron, and the transition frequency.

Solution

The configuration of this atom is such that the outer electron is at an energy level of n = 1009. At such a high energy level (i.e., orbital radius), we can approximate the atom as a hydrogen atom allowing us to determine its size using a simple hydrogen model. Setting the Coulomb force equal to the centripetal force of the orbiting electron,

$$F_{\text{Coul}} = F_{\text{cent}}$$
$$\frac{k_e e^2}{r^2} = \frac{m_e v_e^2}{r},$$

where k_e is Coulomb's constant, e is the charge of the electron, m_e is the electron mass, v is the orbital speed and r is the orbital radius. Noting that the electron angular momentum is given by

$$L = n\hbar = m_e v_e r_e$$

allows us to substitute

$$v_e = \left(\frac{n\hbar}{m_e r_e}\right)$$

for the electron's orbital speed. Making this substitution,

$$\frac{k_e e^2}{r_e} = m_e v_e^2$$

$$\frac{k_e e^2}{r_e} = m_e \left(\frac{n\hbar}{m_e r_e}\right)^2$$

$$\frac{k_e e^2}{r_e} = \frac{m_e n^2 \hbar^2}{m_e^2 r_e^2}$$

$$k_e e^2 = \frac{n^2 \hbar^2}{m_e r_e}$$

$$r_e = \frac{n^2 \hbar^2}{k_e e^2 m_e}$$

$$r_e = \left(\frac{\hbar^2}{k_e e^2 m_e}\right) n^2$$

Noting that the term in parentheses is the Bohr radius a_0 , this allows us to write the electron orbital radius in terms of the hydrogen Bohr radius:

$$r_e = a_o n^2$$

This gives us an orbital size of

$$r_e = 0.054 \,\mathrm{mm},$$

where we have used $a_0 = 5.292 \times 10^{-11}$ m for the Bohr radius. The electron's orbital period of a circular orbit is given by

$$T_e = \frac{2\pi r_e}{v_e}$$

$$T_e = \frac{2\pi r_e}{\left(\frac{n\hbar}{m_e r_e}\right)}$$

$$T_e = 2\pi r_e \left(\frac{m_e r_e}{n\hbar}\right)$$

$$T_e = \frac{2\pi m_e r_e^2}{n\hbar}$$

$$T_e = \frac{2\pi (9.11 \times 10^{-31} \, \mathrm{kg})(0.054 \, \mathrm{mm})^2}{1009\hbar}$$

This gives us an orbital period of

$$T_e = 1.6 \times 10^{-7} \,\mathrm{s}^{-1}$$

To find the transition frequency, we can use the Rydberg formula for hydrogen:

$$\frac{1}{\lambda} = RZ \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

where $n_1 < n_2$ and we have scaled with the atomic number Z. Noting that Z = 6 for Carbon, $n_1 = 1009$ and $n_2 = 1013$, and solving for frequency:

$$\frac{\nu}{c} = 6R \left(\frac{1}{1009^2} - \frac{1}{1013^2} \right)$$
$$\nu = 6Rc \left(\frac{1}{1009^2} - \frac{1}{1013^2} \right).$$

This gives us the transition frequency of:

$$\nu = 152.8\,\mathrm{MHz}$$

Part 3

The presence of such atoms yields information about the local environment. If, for instance, collisional deexcitation is faster than the electron orbital period, no such atom can exist. Let the electron density of the observed region be $n_e = 0.02 \,\mathrm{cm}^{-3}$ and temperature be $T_e = 75 \,\mathrm{K}$. Estimate the collisional deexcitation lifetime for this atom. The quentum mechanical correction in this case is large, and you can take the collision strength $\Omega \sim n^4$ (and $g \sim 1$). Balancing the electron orbital period with the deexcitation lifetime yields the largest possible atom in this region.

Solution

Part 4

Consider atoms at states $n \sim 1000$. Estimate the lifetime for radiative decay (to a similar level), and the lifetime for collisional deexcitation. Are the atoms in LTE with respect to each other? Are they in LTE with atoms at states $n \sim 1$? Can the equivalent width in the observed absorption lines be used to infer the total carbon column density?

Solution

Part 5

How to these atoms get to such high levels? Substantiate your conclusion by estimating the relevant rates.

Solution

3 Oxygen Lines and Density of an HII Region

We consider two emission lines ([O II] λ 3728.80 Angstroms, [O II] λ 3726.04 Angstroms, both forbidden lines) that arise from two finely spaced upper states (call them a and b) decaying into the same ground state of OII (call it 1) from an HII region. Obtain the Einstein coefficients for these transitions, and the requisite g-factors, from the following website:

http://physics.nist.gov/PhysRefData/ASD/lines_form.html

The critical electron densities for the two transitions are, respectively, $n_{crit_{a1}}=1.6\times 10^4\,\mathrm{cm}^{-3}$ and $n_{crit_{b1}}=3\times 10^3\,\mathrm{cm}^{-3}$.

Consider the flux ratio of these two emission lines received at Earth. Let the HII region be optically thin to these photons. Ignore photon pumping.

Part 1

Derive, analytically, values for the line ratios when the electron density is extremely low, and when it is extremely high.

Solution

This system consists of two finely separated energy states a and b above a ground state designated 1.

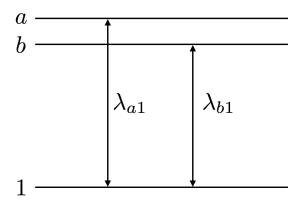


Figure 1:

First we obtain the Einstein coefficients and their respective g-coefficients for the two [O II] forbidden lines:

Before we derive the ratio of line fluxes F_{a1}/F_{b1} for the two given scenarios, we can obtain its general form. For a line transitioning from state $j \to i$, the line flux F_{ji} is determined by the number density of atoms in the upper state n_j , the volume of emitting gas V, the spontaneous emission Einstein coefficient A_{ji} ,, the transition wavelength λ_{ji} , and the distance r away:

$$\frac{\lambda_{ji} (\text{Å}) \quad A_{ji} (\text{s}^{-1}) \quad J \quad g_i \quad g_j \quad n_{\text{crit}} (\text{cm}^{-3})}{\text{O II}_{\text{a}} \quad 3728.80 \quad 2.86 \times 10^{-5} \quad 5/2 \quad 1 \quad 6 \quad 1.6 \times 10^4}$$

$$\text{O II}_{\text{b}} \quad 3726.04 \quad 1.86 \times 10^{-5} \quad 3/2 \quad 1 \quad 4 \quad 3 \times 10^3$$

Figure 2:

$$F_{ji} = n_j V A_{ji} \left(\frac{hc}{\lambda_{ii}} \right) \left(\frac{1}{4\pi r^2} \right).$$

Applying this to the [O II] transitions $a \to 1$ and $b \to 1$, we have

$$F_{a1} = n_a V A_{a1} \left(\frac{hc}{\lambda_{a1}}\right) \left(\frac{1}{4\pi r^2}\right)$$

and

$$F_{b1} = n_b V A_{b1} \left(\frac{hc}{\lambda_{b1}} \right) \left(\frac{1}{4\pi r^2} \right).$$

Taking their ratio, the emitting volume and distances cancel and we obtain:

$$\frac{F_{a1}}{F_{b1}} = \left(\frac{n_a}{n_b}\right) \left(\frac{A_{a1}}{A_{b1}}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right).$$

Since we know the Einstein coefficients and transition wavelengths, we need only find the number densities for each of the two scenarios.

Extremely low electron density

With an extremely low electron density, we can assume that the forbidden lines are in non-LTE so we cannot use the Boltzmann distribution. However we can use the equation for statistical equilibrium which balances excitation with de-excitation. For the general case of transition between states $1 \longleftrightarrow 2$:

$$n_1 n_e q_{12} + n_1 \bar{J} B_{12} = n_2 n_e q_{12} + n_2 B_{21} \bar{J} + n_2 A_{21}$$

where we recall that A_{21} , B_{21} and B_{12} are the Einstein coefficients for spontaneous emission, stimulated emission and stimulated absorption. Since we are in the optically thin regime, we can ignore B_{12} and B_{21} :

$$n_1 n_e q_{12} = n_2 n_e q_{12} + n_2 A_{21}.$$

Solving for n_2 :

$$n_1 n_e q_{12} = n_2 (n_e q_{12} + A_{21}) n_2 = \frac{n_1 n_e q_{12}}{n_e q_{12} + A_{21}}.$$

Recalling the definition of critical density for matter LTE, $n_{\rm crit} \equiv A/q$, the extremely low electron density regime that we're in suggests that:

$$n_e \ll n_{\rm crit} n_e \ll \frac{A_{21}}{q_{21}} n_e q_{a1} \ll A_{21}$$

which allows us to simplify the denominator of n_2 :

$$n_2 = \frac{n_1 n_e q_{12}}{A_{21}}.$$

Applying this to the number densities n_a and n_b for the [O II] transitions

$$n_a = \frac{n_1 n_e q_{1a}}{A_{a1}} n_b = \frac{n_1 n_e q_{1b}}{A_{b1}}$$

and taking their ratio:

$$\frac{n_a}{n_b} = \frac{\left(\frac{n_1 n_e q_{1a}}{A_{a1}}\right)}{\left(\frac{n_1 n_e q_{1b}}{A_{b1}}\right)}
\frac{n_a}{n_b} = \left(\frac{n_1 n_e q_{1a}}{A_{a1}}\right) \left(\frac{A_{b1}}{n_1 n_e q_{1b}}\right)
\frac{n_a}{n_b} = \left(\frac{n_1 n_e q_{1a}}{n_1 n_e q_{1b}}\right) \left(\frac{A_{b1}}{A_{a1}}\right)
\frac{n_a}{n_b} = \left(\frac{q_{1a}}{q_{1b}}\right) \left(\frac{A_{b1}}{A_{a1}}\right).$$

Substituting this into our general expression for the ratio of line fluxes and simplifying:

$$\frac{F_{a1}}{F_{b1}} = \left(\frac{n_a}{n_b}\right) \left(\frac{A_{a1}}{A_{b1}}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right).$$

$$\frac{F_{a1}}{F_{b1}} = \left(\frac{q_{1a}}{q_{1b}} \frac{A_{b1}}{A_{a1}}\right) \left(\frac{A_{a1}}{A_{b1}}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right).$$

$$\frac{F_{a1}}{F_{b1}} = \left(\frac{q_{1a}}{q_{1b}}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right).$$

We now need to find the excitation coefficients q_{1a} and q_{1b} which can be done using the relation for their ratio and the definition of critical density for matter LTE, $q \equiv A/n_{\rm crit}$:

$$\begin{aligned} \frac{q_{ij}}{q_{ji}} &= \left(\frac{g_j}{g_i}\right) \exp\left(\frac{-\Delta E_{ji}}{k_B T}\right) \\ q_{ij} &= q_{ji} \left(\frac{g_j}{g_i}\right) \exp\left(\frac{-\Delta E_{ji}}{k_B T}\right) \\ q_{ij} &= \left(\frac{A_{ji}}{n_{\text{crit}}}\right) \left(\frac{g_j}{g_i}\right) \exp\left(\frac{-\Delta E_{ji}}{k_B T}\right). \end{aligned}$$

Applying this to the [O II] transitions:

$$q_{1a} = \left(\frac{A_{a1}}{n_{\text{crit,a1}}}\right) \left(\frac{g_a}{g_1}\right) \exp\left(\frac{-\Delta E_{a1}}{k_B T}\right)$$

$$q_{1a} = \left(\frac{A_{a1}}{n_{\text{crit,a1}}}\right) \left(\frac{g_a}{g_1}\right) \exp\left(\frac{-(hc/\lambda_{a1})}{k_B T}\right)$$

$$q_{1a} = \left(\frac{A_{a1}}{n_{\text{crit,a1}}}\right) \left(\frac{g_a}{g_1}\right) \exp\left(\frac{-hc}{k_B T \lambda_{a1}}\right)$$

and

$$q_{1b} = \left(\frac{A_{b1}}{n_{\text{crit,b1}}}\right) \left(\frac{g_b}{g_1}\right) \exp\left(\frac{-\Delta E_{b1}}{k_B T}\right)$$

$$q_{1b} = \left(\frac{A_{b1}}{n_{\text{crit,b1}}}\right) \left(\frac{g_b}{g_1}\right) \exp\left(\frac{-(hc/\lambda_{b1})}{k_B T}\right)$$

$$q_{1b} = \left(\frac{A_{b1}}{n_{\text{crit,b1}}}\right) \left(\frac{g_b}{g_1}\right) \exp\left(\frac{-hc}{k_B T \lambda_{b1}}\right).$$

Returning to our expression for the line flux ratio and plugging in q_{1a} and q_{1b} , we obtain the solution for an extremely low electron density:

$$\begin{split} \frac{F_{a1}}{F_{b1}} &= \left(\frac{q_{1a}}{q_{1b}}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right) \\ \frac{F_{a1}}{F_{b1}} &= \left(\frac{\left(\frac{A_{a1}}{n_{\text{crit,a1}}}\right) \left(\frac{g_{a}}{g_{1}}\right) \exp\left(\frac{-hc}{k_{B}T\lambda_{a1}}\right)}{\left(\frac{A_{b1}}{n_{\text{crit,b1}}}\right) \left(\frac{g_{b}}{g_{1}}\right) \exp\left(\frac{-hc}{k_{B}T\lambda_{b1}}\right)} \right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right) \\ \frac{F_{a1}}{F_{b1}} &= \left(\frac{A_{a1}}{n_{\text{crit,a1}}}\right) \left(\frac{g_{a}}{g_{1}}\right) \exp\left(\frac{-hc}{k_{B}T\lambda_{a1}}\right) \cdot \left(\frac{n_{\text{crit,b1}}}{A_{b1}}\right) \left(\frac{g_{1}}{g_{b}}\right) \exp\left(\frac{hc}{k_{B}T\lambda_{b1}}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right) \\ \frac{F_{a1}}{F_{b1}} &= \left(\frac{A_{a1}}{A_{b1}}\right) \left(\frac{g_{a}}{g_{b}}\right) \left(\frac{n_{\text{crit,b1}}}{n_{\text{crit,a1}}}\right) \exp\left(\frac{-hc}{k_{B}T\lambda_{a1}}\right) \exp\left(\frac{hc}{k_{B}T\lambda_{b1}}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right) \\ \frac{F_{a1}}{F_{b1}} &= \left(\frac{A_{a1}}{A_{b1}}\right) \left(\frac{g_{a}}{g_{b}}\right) \left(\frac{n_{\text{crit,b1}}}{n_{\text{crit,a1}}}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right) \exp\left(\frac{-hc}{k_{B}T\lambda_{a1}} + \frac{hc}{k_{B}T\lambda_{b1}}\right) \\ \frac{F_{a1}}{F_{b1}} &= \left(\frac{A_{a1}}{A_{b1}}\right) \left(\frac{g_{a}}{g_{b}}\right) \left(\frac{n_{\text{crit,b1}}}{n_{\text{crit,a1}}}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right) \exp\left(\frac{hc}{k_{B}T}\left(\frac{1}{\lambda_{b1}} - \frac{1}{\lambda_{a1}}\right)\right). \end{split}$$

Plugging in values,

$$\frac{F_{a1}}{F_{b1}} = \left(\frac{2.86 \times 10^{-5}}{1.86 \times 10^{-5}}\right) \left(\frac{6}{4}\right) \left(\frac{3 \times 10^{3} \, \text{cm}^{-3}}{1.6 \times 10^{4} \, \text{cm}^{-3}}\right) \left(\frac{3726.04 \, \text{A}}{3728.8 \, \text{A}}\right) \exp\left(\frac{hc}{k_{B}(10^{4} \, \text{K})} \left(\frac{1}{3726.04 \, \text{A}} - \frac{1}{3728.8 \, \text{A}}\right)\right)$$

$$F_{a1} = 0.43$$
.

Extremely high electron density

Recall that we need to find the number densities of each energy level to complete our solution from the generic case. For an extremely high electron density, we can assume that both line transitions are in LTE which allows us to use the Boltzmann equation for the relative population of number densities with respect to the ground state:

$$\frac{n_a}{n_1} = \left(\frac{g_a}{g_1}\right) \exp\left(\frac{-\Delta E_{a1}}{k_B T}\right)
\frac{n_a}{n_1} = \left(\frac{g_a}{g_1}\right) \exp\left(\frac{-(hc/\lambda_{a1})}{k_B T}\right)
\frac{n_a}{n_1} = \left(\frac{g_a}{g_1}\right) \exp\left(\frac{-hc}{k_B T \lambda_{a1}}\right)$$

and

$$\frac{n_b}{n_1} = \left(\frac{g_b}{g_1}\right) \exp\left(\frac{-\Delta E_{b1}}{k_B T}\right)
\frac{n_b}{n_1} = \left(\frac{g_b}{g_1}\right) \exp\left(\frac{-(hc/\lambda_{b1})}{k_B T}\right)
\frac{n_b}{n_1} = \left(\frac{g_b}{g_1}\right) \exp\left(\frac{-hc}{k_B T \lambda_{b1}}\right).$$

Taking their ratios:

$$\frac{\binom{n_a}{n_1}}{\binom{n_b}{n_1}} = \frac{\binom{g_a}{g_1} \exp\left(\frac{-hc}{k_B T \lambda_{a1}}\right)}{\binom{g_b}{g_1} \exp\left(\frac{-hc}{k_B T \lambda_{b1}}\right)}$$

$$\frac{n_a}{n_1} \cdot \frac{n_1}{n_b} = \binom{g_a}{g_1} \exp\left(\frac{-hc}{k_B T \lambda_{a1}}\right) \cdot \binom{g_1}{g_b} \exp\left(\frac{hc}{k_B T \lambda_{b1}}\right)$$

$$\frac{n_a}{n_b} = \binom{g_a}{g_b} \exp\left(\frac{-hc}{k_B T \lambda_{a1}} + \frac{hc}{k_B T \lambda_{b1}}\right)$$

$$\frac{n_a}{n_b} = \binom{g_a}{g_b} \exp\left(\frac{hc}{k_B T \lambda_{a1}} + \frac{1}{\lambda_{b1}}\right).$$

Substituting this into our general equation for the ratio of line fluxes, we obtain the solution for an extremely high electron density:

$$\frac{F_{a1}}{F_{b1}} = \left(\frac{n_a}{n_b}\right) \left(\frac{A_{a1}}{A_{b1}}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right)
\frac{F_{a1}}{F_{b1}} = \left(\frac{A_{a1}}{A_{b1}}\right) \left(\frac{g_a}{g_b}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right) \exp\left(\frac{hc}{k_B T \lambda_{a1}} \left(\frac{1}{\lambda_{b1}} - \frac{1}{\lambda_{a1}}\right)\right).$$

Plugging in values,

$$\frac{F_{a1}}{F_{b1}} = \left(\frac{2.86 \times 10^{-5}}{1.86 \times 10^{-5}}\right) \left(\frac{6}{4}\right) \left(\frac{3726.04 \,\mathrm{A}}{3728.8 \,\mathrm{A}}\right) \exp\left(\frac{hc}{k_B (10^4 \,\mathrm{K})} \left(\frac{1}{3726.04 \,\mathrm{A}} - \frac{1}{3728.8 \,\mathrm{A}}\right)\right)$$

$$F_{a1} = 2.31$$
.

Part 2

How does the flux ratio vary when the density varies from, say, $1 \,\mathrm{cm}^{-3}$ to $10^5 \,\mathrm{cm}^{-3}$? How does your result depend on the temperature of the HII region?

Solution

With an electron density of $1 \,\mathrm{cm}^{-3}$, we are in the non-LTE regime since $n_e \ll n_{\mathrm{crit,a1}}$ and $n_e \ll n_{\mathrm{crit,b1}}$. We can therefore use the expression for the ratio of line fluxes derived in part 1 for non-LTE (i.e., extremely low electron density):

$$\frac{F_{a1}}{F_{b1}} = \left(\frac{A_{a1}}{A_{b1}}\right) \left(\frac{g_a}{g_b}\right) \left(\frac{n_{\text{crit,b1}}}{n_{\text{crit,a1}}}\right) \exp\left(\frac{hc}{k_B T} \left(\frac{1}{\lambda_{b1}} - \frac{1}{\lambda_{a1}}\right)\right)$$

$$\frac{F_{a1}}{F_{b1}} = 0.43$$
.

Conversely, with an electron density of $10^5 \,\mathrm{cm}^{-3}$, we are in the LTE regime since $n_e \gg n_{\mathrm{crit,a1}}$ and $n_e \gg n_{\mathrm{crit,b1}}$. We can therefore use the expression for the ratio of line fluxes derived in part 1 for LTE (i.e., extremely high electron density):

$$\frac{F_{a1}}{F_{b1}} = \left(\frac{A_{a1}}{A_{b1}}\right) \left(\frac{g_a}{g_b}\right) \left(\frac{\lambda_{b1}}{\lambda_{a1}}\right) \exp\left(\frac{hc}{k_B T \lambda_{a1}} \left(\frac{1}{\lambda_{b1}} - \frac{1}{\lambda_{a1}}\right)\right).$$

$$\frac{F_{a1}}{F_{b1}} = 2.31$$
.

Therefore the line flux ratio varies from 0.4 to 2.3 when the density varies from $1 \,\mathrm{cm}^{-3}$ (NLTE) to $10^5 \,\mathrm{cm}^{-3}$ (LTE).

4 Spectral Energy Distribution of a Protoplanetary Disk

We produce a theoretical prediction for the spectral energy distribution (SED) of a minimum-mass-solar nebula (one that is needed to account for all planet masses) around a sun-like star. The (gas+dust) surface mass density (measured perpendicular to the disk plane) of such a disk goes with radius as $\Sigma = 1700(r/{\rm AU})^{-3/2}\,{\rm g/cm^2}$, out of which 1% is dust. Dust grains have a size distribution of $dN/ds = c(r)s^{-3.5}$ everywhere, with a minimum size of $s_{\rm min}$ and a maximum size of $s_{\rm max}$. You can assume $s_{\rm min} \sim 0.01\,\mu{\rm m}$ and $s_{\rm max}$ is sitting somewhere between $100\,\mu{\rm m}$ and $100\,{\rm km}$.

Part 1

Consider the mass opacity $(\kappa_{\nu} = n\sigma_{\nu}/\rho)$ in the disk. Derive its dependence on s_{max} and ν for the two limits: $s_{\text{max}} \gg \lambda$ and $s_{\text{max}} \ll \lambda$. (Hint: For the former case you have to consider opacity in the $s_{\text{max}} \gg \lambda$ and $s_{\text{max}} \ll \lambda$ ranges separately. λ is the photon wavelength.)

Solution

Starting with the definition of mass opacity

$$\kappa_{\nu} = \frac{n\sigma_{\nu}}{\rho_{\rm disk}}$$

and re-writing the mass density of the disk in terms of the dust grains:

$$\kappa_{\nu} = \frac{n\sigma_{\nu}}{\frac{4}{3}\pi s^{3} n \rho_{\text{dust}}}$$
$$\kappa_{\nu} = \frac{\sigma_{\nu}}{\frac{4}{3}\pi s^{3} \rho_{\text{dust}}}.$$

The extinction cross section σ_{ext} can be used which is a combination of scattering and absorption:

$$\sigma_{\rm ext} = \sigma_{\rm abs} + \sigma_{\rm scat}$$
.

The extinction cross section σ_{ext} is given by the following for small grains

$$\sigma_{\rm ext}(s < \lambda) \approx \pi s^2 \left(\left(\frac{s}{\lambda} \right) + \left(\frac{s}{\lambda} \right) \right) = \pi s^2 \left(\left(\frac{s\nu}{c} \right) + \left(\frac{s\nu}{c} \right)^4 \right)$$

which is simplified for large grains to

$$\sigma_{\rm ext}(s > \lambda) \approx \pi s^2$$
.

Applying this to the mass opacity for a given dust grain size s and observing wavelength λ ,

$$\kappa_{\nu}(s < \lambda) \approx \frac{\pi s^{2} \left(\left(\frac{s\nu}{c} \right) + \left(\frac{s\nu}{c} \right)^{4} \right)}{\frac{4}{3} \pi s^{3} \rho_{\text{dust}}}$$
$$\kappa_{\nu}(s < \lambda) \approx \frac{3 \left(\left(\frac{s\nu}{c} \right) + \left(\frac{s\nu}{c} \right)^{4} \right)}{4s \rho_{\text{dust}}}$$

and

$$\kappa_{\nu}(s > \lambda) \approx \frac{\pi s^2}{\frac{4}{3}\pi s^3 \rho_{\text{dust}}}$$

$$\kappa_{\nu}(s > \lambda) \approx \frac{3}{4s \rho_{\text{dust}}}.$$

To get the total mass opacity, κ_{ν} needs to be integrated over all dust grain sizes s:

$$\kappa_{\nu} = \int \kappa_{\nu}(s < \lambda) \frac{dN}{ds} ds + \int \kappa_{\nu}(s > \lambda) \frac{dN}{ds} ds$$

$$\kappa_{\nu} = \int \frac{3\left(\left(\frac{s\nu}{c}\right) + \left(\frac{s\nu}{c}\right)^{4}\right)}{4s\rho_{\text{dust}}} \frac{dN}{ds} ds + \int \pi s^{2} \frac{dN}{ds} ds$$

Making the substitution

$$\frac{dN}{ds} = c(r)s^{-3.5}$$

for the dust grain size distribution, we get the following general expression for the mass opacity:

$$\kappa_{\nu} = \int_{s_{\min}}^{\lambda} \frac{3\left(\left(\frac{s\nu}{c}\right) + \left(\frac{s\nu}{c}\right)^{4}\right)}{4s\rho_{\text{dust}}} c(r) s^{-3.5} ds + \int_{\lambda}^{s_{\max}} \frac{3}{4s\rho_{\text{dust}}} c(r) s^{-3.5} ds$$

where the integration limits reflect the fact that small grains have sizes $s_{\min} < s < \lambda$ and large grains have sizes $\lambda < s < s_{\max}$.

Following through with integration:

$$\begin{split} \kappa_{\nu} &= \frac{3c(r)}{4\rho_{\rm dust}} \int_{s_{\rm min}}^{\lambda} \frac{\left(\left(\frac{s\nu}{c}\right) + \left(\frac{s\nu}{c}\right)^4\right)}{s} s^{-3.5} ds + \frac{3c(r)}{4\rho_{\rm dust}} \int_{\lambda}^{s_{\rm max}} \frac{1}{s} s^{-3.5} ds \\ \kappa_{\nu} &= \frac{3c(r)}{4\rho_{\rm dust}} \int_{s_{\rm min}}^{\lambda} \frac{1}{s} \left(\left(\frac{s\nu}{c}\right) + \left(\frac{s\nu}{c}\right)^4\right) s^{-3.5} ds + \frac{3c(r)}{4\rho_{\rm dust}} \int_{\lambda}^{s_{\rm max}} s^{-1} s^{-3.5} ds \\ \kappa_{\nu} &= \frac{3c(r)}{4\rho_{\rm dust}} \int_{s_{\rm min}}^{\lambda} \left(\left(\frac{s\nu}{c}\right) \frac{s^{-3.5}}{s} + \left(\frac{s\nu}{c}\right)^4 \frac{s^{-3.5}}{s}\right) ds + \frac{3c(r)}{4\rho_{\rm dust}} \int_{\lambda}^{s_{\rm max}} s^{-4.5} ds \\ \kappa_{\nu} &= \frac{3c(r)}{4\rho_{\rm dust}} \int_{s_{\rm min}}^{\lambda} \left(\left(\frac{\nu}{c}\right) s \frac{s^{-3.5}}{s} + \left(\frac{\nu}{c}\right)^4 s^4 \frac{s^{-3.5}}{s}\right) ds + \frac{3c(r)}{4\rho_{\rm dust}} \int_{\lambda}^{s_{\rm max}} s^{-4.5} ds \\ \kappa_{\nu} &= \frac{3c(r)}{4\rho_{\rm dust}} \int_{s_{\rm min}}^{\lambda} \left(\left(\frac{\nu}{c}\right) s^{-3.5} + \left(\frac{\nu}{c}\right)^4 s^{-0.5}\right) ds + \frac{3c(r)}{4\rho_{\rm dust}} \int_{\lambda}^{s_{\rm max}} s^{-4.5} ds \\ \kappa_{\nu} &= \frac{3c(r)}{4\rho_{\rm dust}} \left\{\left(\frac{\nu}{c}\right) \int_{s_{\rm min}}^{\lambda} s^{-3.5} ds + \left(\frac{\nu}{c}\right)^4 \int_{s_{\rm min}}^{\lambda} s^{-0.5} ds \right\} + \frac{3c(r)}{4\rho_{\rm dust}} \int_{\lambda}^{s_{\rm max}} s^{-4.5} ds \\ \kappa_{\nu} &= \frac{3c(r)}{4\rho_{\rm dust}} \left\{\left(\frac{\nu}{c}\right) \left[\frac{s^{-2.5}}{-2.5}\right]_{s_{\rm min}}^{\lambda} + \left(\frac{\nu}{c}\right)^4 \left[\frac{s^{0.5}}{0.5}\right]_{s_{\rm min}}^{\lambda} \right\} + \frac{3c(r)}{4\rho_{\rm dust}} \left[\frac{s^{-3.5}}{-3.5}\right]_{\lambda}^{s_{\rm max}} \\ \kappa_{\nu} &= \frac{3c(r)}{4\rho_{\rm dust}} \left\{\left(\frac{\nu}{c}\right) \left[\frac{s^{-2.5}}{2.5}\right]_{s_{\rm min}}^{\lambda} + \left(\frac{\nu}{c}\right)^4 \left[\frac{s^{0.5}}{0.5}\right]_{s_{\rm min}}^{\lambda} \right\} + \frac{3c(r)}{4\rho_{\rm dust}} \left[\frac{s^{-3.5}}{-3.5}\right]_{\lambda}^{s_{\rm max}} \right\} \\ \kappa_{\nu} &= \frac{3c(r)}{4\rho_{\rm dust}} \left\{\left(\frac{\nu}{c}\right) \left[\frac{s^{-2.5}}{2.5}\right]_{\lambda}^{s_{\rm min}} + \left(\frac{\nu}{c}\right)^4 \left[\frac{s^{0.5}}{0.5}\right]_{s_{\rm min}}^{\lambda} + \left[\frac{s^{-3.5}}{3.5}\right]_{s_{\rm max}}^{\lambda} \right\} \\ \kappa_{\nu} &= \frac{3c(r)}{4\rho_{\rm dust}} \left\{\frac{1}{2.5} \left(\frac{\nu}{c}\right) \left[s^{-2.5} - \lambda^{-2.5}\right] + \frac{1}{0.5} \left(\frac{\nu}{c}\right)^4 \left[\lambda^{0.5} - s_{\rm min}^{0.5}\right] + \frac{1}{3.5} \left[\lambda^{-3.5} - s_{\rm max}^{-3.5}\right] \right\} \\ \kappa_{\nu} &= \frac{3c(r)}{4\rho_{\rm dust}} \left\{\frac{2}{5} \left(\frac{\nu}{c}\right) \left[s_{\rm min}^{-5/2} - \lambda^{-5/2}\right] + 2\left(\frac{\nu}{c}\right)^4 \left[\lambda^{1/2} - s_{\rm min}^{1/2}\right] + \frac{2}{7} \left[\lambda^{-7/2} - s_{\rm max}^{-7/2}\right] \right\}. \end{cases}$$

Therefore, in the limit that $s_{\rm max} \gg \lambda$, the mass opacity scales as $\kappa_{\nu} \propto s_{\rm max}^{-7/2}$ and in the limit that $s_{\rm max} \ll \lambda$, the mass opacity scales as $\kappa_{\nu} \propto s_{\rm max}^{-5/2}$.

Part 2

Outside of what radius is the disk optically thin (vertically) to optical light, and thin to submm (say, 0.1 cm) radiation, respectively? Typical disks have sizes < 1000 AU.

Solution

Part 3

Write down the thermal emission from a ring at radius r in the optically thick limit. Integrate over the disk $(r_{\text{mim}} \text{ to } r_{\text{max}})$ to obtain the frequency slope of the integrated flux F_{ν} at the submm wavelength. Are you in the Rayleigh-Jeans tail? Do your results depend on dust mass and/or dust sizes? For disk temperature, assume a simple law of $T \propto 250 \,\text{K}(r/\text{AU})^{-1/2}$, independent of grain size.

Solution

In the optically thick limit, the thermal emission is that of a blackbody at temperature T:

$$I_{\nu} = B_{\nu}(T) = \frac{2h\nu}{c^2} \frac{1}{\exp(h\nu/k_B T) - 1}.$$

Assuming temperature scales with radius as $T \propto 250 \,\mathrm{K}(r/\mathrm{AU})^{-1/2}$,

$$I_{\nu} = B_{\nu}(T) = \frac{2h\nu}{c^2} \frac{1}{\exp\left(\frac{h\nu}{250k_BT}\sqrt{\frac{r}{\text{AU}}}\right) - 1}.$$

Part 4

Now repeat the exercise in the optically thin limit. Obtain the slope of the integrated spectrum, F_{ν} , as well as any dependence on s_{max} . (Hint: When you integrate the flux over radius, be sure to include the radius dependence of c(r). Also, differentiate between the case where $s_{\text{max}} \gg \lambda$ and $s_{\text{min}} \ll \lambda$.)

Solution

Part 5

Grains in the disk can grow by conglomeration. What happens to the SED when s_{max} increases from $100 \,\mu\text{m}$ to $100 \,\text{km}$?

Now you are ready to observe (as Andrews & Williams 2007 did).

Solution