Class 2: Theory of line emission

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Motivation: since line emission is our most powerful observational tool, we need to understand how it works in detail.

Outline

- Radiation fields and photon occupation numbers
- Radiative transition rates and Einstein coefficients
- Statistical equilibrium for multi-level atoms
- Critical densities for multi-level atoms

Quick primer on radiation fields

(We will assert rather than prove much of this, since it is covered in other courses)

- A general radiation field is described in terms of the *intensity*, which specifies how much energy at photon frequency ν is flowing in a particular direction $\mathbf{n}$ (where $\mathbf{n}$ is a unit vector); this quantity is generally written $I_\nu(\mathbf{n})$
- $I_\nu(\mathbf{n})$ has units of energy per time per area per frequency per solid angle; that is, $I_\nu(\mathbf{n})\, \mathrm{d}t\, \mathrm{d}A\, \mathrm{d}\nu\, \mathrm{d}\Omega$ is the energy that a receiver with area $\mathrm{d}A$, viewing a solid angle of the sky $\mathrm{d}\Omega$ through a filter with bandpass $\mathrm{d}\nu$ receives over a time $\mathrm{d}t$
- In local thermodynamic equilibrium at temperature T, the intensity is equal to the Planck function:

$$I_\nu(\mathbf{n}) = B_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/k_B T} - 1}$$

Photon occupation numbers

- In quantum statistical mechanics, it is more convenient to work with a related quantity: the *photon occupation number* $n_\gamma(\nu,\mathbf{n}) = (c^2 / 2h\nu^3)\, I_\nu(\mathbf{n})$
- In LTE, we therefore have $n_{\gamma,\mathrm{LTE}} = \dfrac{1}{e^{h\nu/k_B T} - 1}$
- Clearly n_γ is dimensionless, and it has a simple physical interpretation: it is the expected number a photons in a particular mode.
- In non-relativistic problems were generally don’t care about the direction of the photons, so we commonly work with the photon occupation number averaged over direction:

$$\langle n_\gamma \rangle (\nu) = \frac{1}{4\pi} \int n_\gamma(\nu, \mathbf{n})\, d\Omega$$

Radiative transitions and Einstein coefficients

Part I

- We now consider an atom / molecule of species X, which has a higher energy state u and a lower energy state l; these need not be its only states. The states have energies E_u and E_l, and degeneracies g_u and g_l
- Radiative transitions between these states occur via: (1) spontaneous emission of photons from particles in u, (2) absorption of photons by particles in state l, and (3) stimulated emission of photons by particles in state u
- The photons involved in these transitions have frequency $\nu_{ul} = (E_u - E_l) / h$
- Our goal is to write down rates at which processes (1), (2), and (3) occur

Radiative transitions and Einstein coefficients

Part II

- We have already written down spontaneous emission: $(dn_u / dt)_{se} = -A_{ul}\, n_u$

- The rates of absorption and stimulated emission must be proportional to the numbers of atoms in the initial state and the photon occupation numbers at the relevant frequencies: thus $(dn_u / dt)_{stim.e} = -C_{ul}\, n_u\langle n_\gamma\rangle(\nu_{ul})$ and $(dn_u / dt)_{abs} = -C_{lu}\, n_l\langle n_\gamma\rangle(\nu_{ul})$, where C_{ul} and C_{lu} are constants to be determined

- Thus the total rate of change in the number density in the upper state is

$$\frac{dn_u}{dt} = -n_u A_{u\ell} - C_{u\ell} n_u \langle n_\gamma\rangle(\nu_{u\ell}) + C_{\ell u} n_l \langle n_\gamma\rangle(\nu_{u\ell})$$

Radiative transition and Einstein coefficients

Part III

- To figure out the values of C_{ul} and C_{lu}, consider atoms at very low density, so collisions occur negligibly often. We place these atoms in a radiation field that is in LTE, so the photon occupation number is $n_{\gamma,\mathrm{LTE}} = \dfrac{1}{e^{h\nu/k_B T} - 1}$
- In steady state in LTE, the number densities of atoms in states *u* and *l* follow the Boltzmann distribution, $n_u / n_l = (g_u / g_l)\, e^{-h\nu_{ul} / kT}$
- If we substitute n_γ, n_u, and n_l into our equation for dn_u / dt, we get

$$-\frac{g_u}{g_\ell} e^{-h\nu_{u\ell}/k_B T} \left(A_{u\ell} + \frac{C_{u\ell}}{e^{h\nu_{u\ell}/k_B T} - 1} \right) + \frac{C_{\ell u}}{e^{h\nu_{u\ell}/k_B T} - 1} = 0$$

Radiative transitions and Einstein coefficients

Part IV

- Starting from: $-\frac{g_u}{g_\ell} e^{-h\nu_{u\ell}/k_BT} \left(A_{u\ell} + \frac{C_{u\ell}}{e^{h\nu_{u\ell}/k_BT} - 1} \right) + \frac{C_{\ell u}}{e^{h\nu_{u\ell}/k_BT} - 1} = 0$
- High temperature limit, $h\nu_{ul} \ll kT$: in this case exponential terms all approach 1, so denominators of C terms go to zero, and these terms dominate. Satisfying the equation in this limit requires $C_{lu} = (g_u / g_l)\, C_{ul}$
- Low temperature limit, $h\nu_{ul} \gg kT$: in this case exponential terms in denominator are large, so drop –1's. Also, drop $e^{-h\nu_{ul} / kT} C_{ul}$ comared to C_{lu}. Satisfying the equation in this limit requires $C_{lu} = (g_u / g_l)\, A_{ul}$

Radiative transitions and Einstein coefficients

Part V

- Final conclusion:

$$\frac{dn_u}{dt} = \underbrace{A_{u\ell}}_{\text{Einstein coefficient}} \left\{ -\left[\underbrace{1}_{\text{Spontaneous emission}} + \underbrace{\langle n_\gamma \rangle (\nu_{u\ell})}_{\text{Simulated emission}}\right] n_u + \underbrace{\frac{g_u}{g_\ell} \langle n_\gamma \rangle (\nu_{u\ell}) n_\ell}_{\text{Absorption}} \right\}$$

- Adding in collisions:

$$\frac{dn_u}{dt} = A_{u\ell} \left\{ -\left[1 + \langle n_\gamma \rangle (\nu_{u\ell})\right] n_u + \frac{g_u}{g_\ell} \langle n_\gamma \rangle (\nu_{u\ell}) n_\ell \right\}$$

$$+ \underbrace{k_{u\ell}}_{\text{Collision rate coefficient}} n \left(\underbrace{e^{h\nu_{u\ell}/k_B T} n_\ell}_{\text{Collisional excitation}} - \underbrace{n_u}_{\text{Collisional de-excitation}} \right)$$

Exercise

Consider a two-level atom, immersed in a set of both other atoms that it collides with, and photons.

Suppose that the radiation field and the background gas are both individually in thermal equilibrium, but at two different temperatures T_{gas} and T_{rad}, for example a molecular cloud where the gas is at 10 K, immersed in the cosmic microwave background at 2.7 K.

Show that, in statistical equilibrium, the ratio of atoms in the upper and lower states behaves as:

$$\lim_{n\to 0} \frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} e^{-h\nu_{u\ell}/k_B T_{\mathrm{rad}}} \qquad \lim_{n\to\infty} \frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} e^{-h\nu_{u\ell}/k_B T_{\mathrm{gas}}}$$

Multilevel atoms

Problem set up

- We now consider an atom X with an arbitrary number of energy states, which we number 0, 1, 2, … from lowest to highest energy. We let:
  - E_i = energy of state i
  - g_i = degeneracy of state i
  - $E_{ij} = E_i - E_j$ = energy difference between states
  - $\nu_{ij} = E_{ij} / h$ = frequency of photons associated with energy difference
  - A_{ij} = Einstein coefficient for transitions from i to j (= 0 for $i < j$)
  - $\langle n_{\gamma,ij} \rangle = \langle n_\gamma \rangle(\nu_{ij})$ = photon occupation number at frequency ν_{ij}
  - k_{ij} = collision rate coefficient for transitions from i to j
  - n = number density of colliding particles causing transitions
  - n_i = number density of atoms X in state i
  - $n_X = \sum n_i$ = total number density of atoms X in all quantum states
- Fundamental question: in statistical equilibrium, what are the values of n_i?

Multilevel atoms

Collision rates

- Rate at which collisions remove atoms from state *i*:

$$\left(\frac{dn_i}{dt}\right)_{\text{coll. out}} = -n_i n \sum_j k_{ij}$$

- Rate at which collisions put atoms from other states into state *i*:

$$\left(\frac{dn_i}{dt}\right)_{\text{coll. in}} = n \sum_j n_j k_{ji}$$

Multilevel atoms

Spontaneous emission rates

- Rate at which spontaneous emissions remove atoms from state *i*:

$$\left(\frac{dn_i}{dt}\right)_{\text{se. out}} = -n_i \sum_j A_{ij}$$

- Rate at which spontaneous emissions put atoms from other states into state *i*:

$$\left(\frac{dn_i}{dt}\right)_{\text{se. in}} = \sum_j n_j A_{ji}$$

Multilevel atoms

Stimulated emission and absorption rates

- Rate at which stimulated emissions and absorptions remove atoms from state *i*:

$$\left(\frac{dn_i}{dt}\right)_{\text{stim. emiss. out.}} = -n_i \sum_j A_{ij} n_{\gamma,ij} \qquad \left(\frac{dn_i}{dt}\right)_{\text{abs. out}} = -n_i \sum_j \frac{g_i}{g_j} A_{ij} n_{\gamma,ij}$$

- Rate at which stimulated emissions and absorptions put atoms into state *i*:

$$\left(\frac{dn_i}{dt}\right)_{\text{stim. emiss. in.}} = \sum_j n_j A_{ji} n_{\gamma,ij} \qquad \left(\frac{dn_i}{dt}\right)_{\text{abs. in}} = \sum_j \frac{g_i}{g_j} n_j A_{ji} n_{\gamma,ij}$$

Multilevel atoms

Putting it all together

- Statistical equilibrium amounts to saying that the sum of all the terms we have just written down is zero.T his is a linear system: we have some terms that are linearly proportional to n_i, and a bunch of terms that don't depend on it.

- This is best expressed as a matrix problem: **M·n** = **n**, where **n** is the vector of n_i values, and **M** is a matrix whose elements are:

$$M_{ij} = \frac{nk_{ji} + (1 + \langle n_{\gamma,ji} \rangle)\, A_{ji} + \frac{g_i}{g_j} \langle n_{\gamma,ij} \rangle A_{ij}}{\sum_\ell \left[nk_{i\ell} + (1 + \langle n_{\gamma,i\ell} \rangle)\, A_{i\ell} + \frac{g_\ell}{g_i} \langle n_{\gamma,\ell i} \rangle A_{\ell i} \right]}$$

- The solution is just the eigenvector of **M** that has an eigenvalue of 1. There are multiple packages (RADEX, DESPOTIC) that take data on collision rates and Einstein coefficients and solve this problem.

Critical densities for multi-level atoms

Part I

- With this formalism, we can now extend the definition of critical density to multi-level atoms. We consider a state *i* that is populated primarily from below, i.e., there are many more transitions from state *j* to *i* for *j* < *i* than *j* > *i*.

- In this case the rate equation becomes

$$\frac{dn_i}{dt} = \sum_{j<i} n_j n k_{ji} + \sum_{j<i} n_j \frac{g_i}{g_j} \langle n_{\gamma,ij} \rangle A_{ij} - n_i \sum_{j<i} \left[k_{ij} + \left(1 + \langle n_{\gamma,ij} \rangle\right) A_{ij} \right]$$

- In steady state, dn_i / dt = 0, we can solve immediately:

$$n_i = \frac{\sum_{j<i} n_j n k_{ji} + \sum_{j<i} n_j \frac{g_i}{g_j} \langle n_{\gamma,ij} \rangle A_{ij}}{\sum_{j<i} \left[n k_{ij} + \left(1 + \langle n_{\gamma,ij} \rangle\right) A_{ij} \right]}$$

Critical densities for multi-level atoms

Part II

- We now define the critical density in analogy to the two-level case, as the ratio of the radiative and collisional de-excitation rate coefficients:

$$n_{\mathrm{crit},i} = \frac{\sum_{j<i} \left(1 + \langle n_{\gamma,ij} \rangle\right) A_{ij}}{\sum_{j<i} k_{ij}},$$

- Putting this into the equation for the equilibrium solution, we have

$$n_i = \left(\frac{n}{n + n_{\mathrm{crit},i}}\right) \underbrace{\frac{\sum_{j<i} n_j k_{ji}}{\sum_{j<i} k_{ij}}}_{\substack{\text{Collisional term —} \\ \text{dominates for } n \gg n_{\mathrm{crit},i}}} + \left(\frac{n_{\mathrm{crit},i}}{n + n_{\mathrm{crit},i}}\right) \underbrace{\frac{\sum_{j<i} n_j \frac{g_i}{g_j} \langle n_{\gamma,ij} \rangle A_{ij}}{\sum_{j<i} \left(1 + \langle n_{\gamma,ij} \rangle\right) A_{ij}}}_{\substack{\text{Radiative term —} \\ \text{dominates for } n \ll n_{\mathrm{crit},i}}}$$

Exercise

Compute the critical densities of the following lines: CO $J = 1 \rightarrow 0$, $J = 3 \rightarrow 2$, CO $J = 5 \rightarrow 4$, and HCN $J = 1 \rightarrow 0$ for 10 K gas, now using the general definition of critical density we just provided.

How different are the results from the simplified estimates we made in class last time? Can you give an intuitive explanation for why they are as different or similar as you find?