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 **n** (where **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, $I_\nu(\mathbf{n})\, dt\, dA\, d\nu\, d\Omega$ is the energy that a receiver with area dA, viewing a solid angle of the sky $d\Omega$ through a filter with bandpass $d\nu$ receives over a time dt
- 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 $n_{\gamma,\mathrm{LTE}} = \frac{1}{e^{h\nu/k_B T} - 1}$
- 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 $n_{\gamma,\mathrm{LTE}} = \frac{1}{e^{h\nu/k_B T} - 1}$
- 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: $$-\frac{g_u}{g_\ell} e^{-h\nu_{u\ell}/k_B T} \left(A_{u\ell} + \frac{C_{u\ell}}{e^{h\nu_{u\ell}/k_B T} - 1} \right) + \frac{C_{\ell u}}{e^{h\nu_{u\ell}/k_B T} - 1} = 0$$
- 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:

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

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

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*:

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

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

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

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:

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

- 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

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

Collisional term — dominates for $n \gg n_{\mathrm{crit},i}$

Radiative term — dominates for $n \ll n_{\mathrm{crit},i}$