Notes on approximations

The goal here is to understand, given statistical equilibrium, the behavior of the level populations as a function of radius for *spherically symmetric*, *pure hydrogen* gas illuminated by a *source radiating as a blackbody* at some fixed (position-indepedent) temperature T_s. The gas itself might have a radial temperature dependence which can affect its electron recombination rates. We assume that collisional transition rates are negligible.

Note that Johnson & Klinglesmith, with help from White 1961, wrote down the formal solution for the case with three bound levels plus continuum, and for a more arbitrary source spectrum. Here, with our restriction of the source to a blackbody, and by factoring out the optically thin solution, we obtain formuale more suitable for gaining physical intuition.

Two bound levels

Let the levels have energies E_1 and E_2, $E_2 > E_1$, with statistical weights g_1 and g_2. Also let $\nu_{12} = (E_2 - E_1)/h$. Statistical equilibrium at each position gives

$$n_2 A_{21} = n_1 \bar{J}_\nu B_{12} - n_2 \bar{J}_\nu B_{21} \tag{1}$$

where, as usual, $\bar{J}_\nu$ is equal to J_ν integrated over the line profile.

We rearrange to get

$$\frac{n_1}{n_2} = \frac{A_{21} + \bar{J}_\nu B_{12}}{\bar{J}_\nu B_{21}} \tag{2}$$

This equation, along with the total conservation equation $n_1 + n_2 = n_H$ and a manner of obtaining J_ν, specify the level populations completely. In general it is not easy to solve because $\bar{J}_\nu$ can depend on the level populations - in the formal soluiton for J in terms of the source function S, S depends on the level populations.

We will factor J as follows

$$J_\nu(r) = W(r) s_\nu B_\nu(T_s) \tag{3}$$

where W is the geometrical dilution factor

$$W(r) = \frac{1}{2}\left[1 - \sqrt{1 - \left(\frac{r_p}{r}\right)^2}\right] \tag{4}$$

and s_ν is any further enhancement/dehancement of the radiation field with respect to a diluted blackbody at each frequency. When the gas is optically thin, $s_\nu \to 1$ for all ν.

We will also consider the line to be sufficiently narrow such that $\bar{J}_\nu = J_{\nu_{12}}$ to a high degree of accuracy. Then we have

$$\frac{n_1}{n_2}(r) = \frac{A_{21} + s_{\nu_{12}} W(r) B_{\nu_{12}}(T_s) B_{12}}{s_{\nu_{12}} W(r) B_{\nu_{12}}(T_s) B_{21}} \tag{5}$$

One must be careful here not to confuse the Einstein coefficients with the Planck function evaulated at ν_{12} in the above expression.

After writing out the Planck function, using the relations between the Einstein coefficients, and going through some algebra, we get

$$\frac{n_1}{n_2}(r) = \left[\frac{g_1}{g_2} e^{\zeta_{12}}\right]\left[\frac{1 + e^{-\zeta_{12}}\left(s_{\nu_{12}} W(r) - 1\right)}{s_{\nu_{12}} W(r)}\right] \tag{6}$$

where

$$\zeta_{12} \equiv \frac{h\nu_{12}}{kT_s} \tag{7}$$

We see that if $sW \gg \exp(h\nu_{12}/kT_s)$ (which automatically implies $sW \gg 1$), then the ratio of the level populations approaches the ratio of the g's. That is, all states at all energy levels are occupied with nearly equal probability, because the radiation field is so energetic. As sW goes down, the ratio n_1/n_2 increases montonically.

Two bound levels plus continuum

The photoionization rate from level i, with photoionization cross-section $\sigma_i(\nu)$, is given by

$$\int_{\nu_{ci}}^{\infty} \frac{\sigma_i(\nu) J_\nu}{h\nu} d\nu \equiv \mathcal{I}_i \tag{8}$$

where ν_{ci} is the minimum frequency for photo-ionizing from level i to the continuum.

Then statistical equilibrium for the $n = 2$ level gives

$$n_2 A_{21} + n_2 \mathcal{I}_2 = n_1 \bar{J}_\nu B_{12} - n_2 \bar{J}_\nu B_{21} + n_e n_p \alpha_2 \tag{9}$$

Statistical equilibrium for the continuum gives

$$n_1 \mathcal{I}_1 + n_2 \mathcal{I}_2 = n_e n_p \left(\alpha_1 + \alpha_2\right) \tag{10}$$

Considering the equilibrium for $n = 1$ gives no new information. Of course, we still have the total conservation condition $n_1 + n_2 + n_p = n_H$. We're considering pure hydrogen for the moment, so $n_p = n_e$. We can use the continuum equation to write the product $n_e n_p$ in terms of other quantities, use the Einstein relations and go through the algebra to finally obtain

$$\frac{n_1}{n_2} = \frac{g_1}{g_2} e^{\zeta_{12}} \left[\frac{1 + e^{-\zeta_{12}}(s_{\nu_{12}} W - 1) + \frac{\mathcal{I}_2}{A_{21}} \left(1 - e^{-\zeta_{12}}\right) \frac{\alpha_1}{\alpha_1 + \alpha_2}}{s_{\nu_{12}} W + \frac{\mathcal{I}_1}{A_{21}} \frac{g_1}{g_2} \left(e^{\zeta_{12}} - 1\right) \frac{\alpha_2}{\alpha_1 + \alpha_2}} \right] \tag{11}$$

As a consistency check, we see that this reduces to the two-level solution without continuum when both $\mathcal{I}_1$ and $\mathcal{I}_2$ are zero. Now, as T_s varies, there exists a maximum value for n_2, instead of the monotonic behavior we saw without the continuum.

Three bound levels plus continuum

Statistical equilibrium for the $n = 2$ level gives

$$n_2 A_{21} + n_2 \bar{J}_\nu B_{21} + n_2 \bar{J}_\nu B_{23} + n_2 \mathcal{I}_2 = n_3 A_{32} + n_1 \bar{J}_\nu B_{12} + n_3 \bar{J}_\nu B_{32} + n_e n_p \alpha_2 \tag{12}$$

For the $n = 3$ level:

$$n_3 A_{32} + n_3 A_{31} + n_3 \bar{J}_\nu B_{31} + n_3 \bar{J}_\nu B_{32} + n_3 \mathcal{I}_3 = n_1 \bar{J}_\nu B_{13} + n_2 \bar{J}_\nu B_{23} + n_e n_p \alpha_3 \tag{13}$$

For the continuum:

$$n_1 \mathcal{I}_1 + n_2 \mathcal{I}_2 + n_3 \mathcal{I}_3 = n_e n_p \left(\alpha_1 + \alpha_2 + \alpha_3\right) \tag{14}$$

The $n = 1$ level euilibrium equation gives no new information. The condition $n_1 + n_2 + n_3 + n_p = n_H$, and hydrogen charge conservation $n_e = n_p$, close the system.

Our factoring of J_ν and the relations between the Einstein coefficients eventually let us write

$$\frac{n_1}{n_3} = \frac{1 + \frac{s_{\nu_{31}} W}{e^{\zeta_{31}} - 1} + \frac{\mathcal{I}_3}{A_{31}} \left(1 - \frac{\alpha_3}{\alpha_1 + \alpha_2 + \alpha_3}\right) + \frac{A_{32}}{A_{31}} \left(1 + \frac{s_{\nu_{32}} W}{e^{\zeta_{32}} - 1}\right)}{\frac{g_3}{g_1} \frac{s_{\nu_{31}} W}{e^{\zeta_{31}} - 1} + \frac{\mathcal{I}_1}{A_{31}} \left(\frac{\alpha_3}{\alpha_1 + \alpha_2 + \alpha_3}\right) + \frac{n_2}{n_1} \left[\frac{g_3}{g_2} \frac{A_{32}}{A_{31}} \frac{s_{\nu_{32}} W}{e^{\zeta_{32}} - 1} + \frac{\mathcal{I}_2}{A_{31}} \left(\frac{\alpha_3}{\alpha_1 + \alpha_2 + \alpha_3}\right)\right]} \tag{15}$$

and

$$\frac{n_1}{n_2} = \frac{1 + \frac{s_{\nu 21} W}{e^{\zeta_{21}}-1} + \frac{\mathcal{I}_2}{A_{21}}\left(1 - \frac{\alpha_2}{\alpha_1+\alpha_2+\alpha_3}\right) + \frac{g_3}{g_2}\frac{A_{32}}{A_{21}}\frac{s_{\nu 32} W}{e^{\zeta_{32}}-1}}{\frac{g_2}{g_1}\frac{s_{\nu 21} W}{e^{\zeta_{21}}-1} + \frac{\mathcal{I}_1}{A_{21}}\left(\frac{\alpha_2}{\alpha_1+\alpha_2+\alpha_3}\right) + \frac{n_3}{n_1}\left[\frac{A_{32}}{A_{21}}\left(1 + \frac{s_{\nu 32} W}{e^{\zeta_{32}}-1}\right) + \frac{\mathcal{I}_3}{A_{21}}\left(\frac{\alpha_2}{\alpha_1+\alpha_2+\alpha_3}\right)\right]} \tag{16}$$

So schematically, if

$$\frac{n_1}{n_3} = \frac{A}{B + C\frac{n_2}{n_1}} \qquad \frac{n_1}{n_2} = \frac{D}{E + F\frac{n_3}{n_1}} \tag{17}$$

then

$$\frac{n_1}{n_3} = \frac{AD - CF}{BD + CE} \qquad \frac{n_1}{n_2} = \frac{AD - CF}{AE + BF} \tag{18}$$

A note of caution: The presence of the terms such as $e^{\zeta_{32}} - 1$ in denominators will result in division by zero when two of the three levels are degenerate

Concluding remarks about the analytics

The main challenge we face when making use of these expressions for the level populations is their dependence on the exact structure of J_ν. This determines the values of the photoionization rates $\mathcal{I}_i$ and the line radiation enhancements $s_{\nu_{ij}}$.

In the optically thin limit all the $s_{\nu_{ij}} \to 1$ and the photoionization rates can be straightforwardly integrated numerically given expressions for the photoionization cross-sections.

When there is non-negligible optical depth to photoionization and the line transitions, the only way to proceed exactly is to simulatneously solve the transfer equation for J_ν along with the expressions for the level populations in terms of J_ν at each radius working outward, or using full Monte Carlo. The presence of electron scattering and/or bremsstrahlung complicates the soluiton even more.

Given certain guesses about the level populations, it might be possible to simplify the expressions for the population ratios by dropping terms and then check for self-consistency.

There might also be a way to make further progress on paper by assuming homolgous expansion and working with line escape probabilities.

Test problem

To put the preceding ideas into action, we set up a test problem with the following parameters: $T_s = 5 \times 10^4$ K, inner radius 3×10^{13} cm, outer radius 1×10^{14} cm, uniform gas density of 1 cm^{-3} (although this value does not matter, as long as the gas remains optically thin), and uniform gas temperature of 5×10^4 K.

The simplified hydrogen atomic strucutre consists of three bound levels, with principal quantum numbers n of 1, 2, and 3. An additional level representing unbound (continuum) electrons is also included in the model atom. The excitation energies for the bound levels are 0 eV, 10.20 eV, and 12.09 eV for the n = 1, 2, and 3 levels, respectively. The statistical weights for the levels are 2, 8, and 18, respectively. The einstein A coefficients for those three levels are 4.696e8 Hz, 5.572e7 Hz, and 4.408e7 Hz, respectively. The photoionization cross sections are taken to follow a ν^{-3} law, as in Rybicki & Lightman Equation 10.56, and the Gaunt factors are set to 1. The recombination rate coefficients α_n can then be computed using the Milne relation, as in Rybicki & Lightman Equation 10.62, and assuming that free electrons follow a Maxwellian velocity distribution at the specified temperature. For the parameters listed above, the recombination coefficients are found to be 5.83e-14, 2.02e-14, and 9.67e-15 cm^3 s^{-1}, respectively.

Figure 1 shows the results of the test problem. The solid lines correspond to the ratios $\frac{n_1}{n_2}$ and $\frac{n_1}{n_3}$ as analytically derived from equations (15) and (16), as a function of radius. The points are the

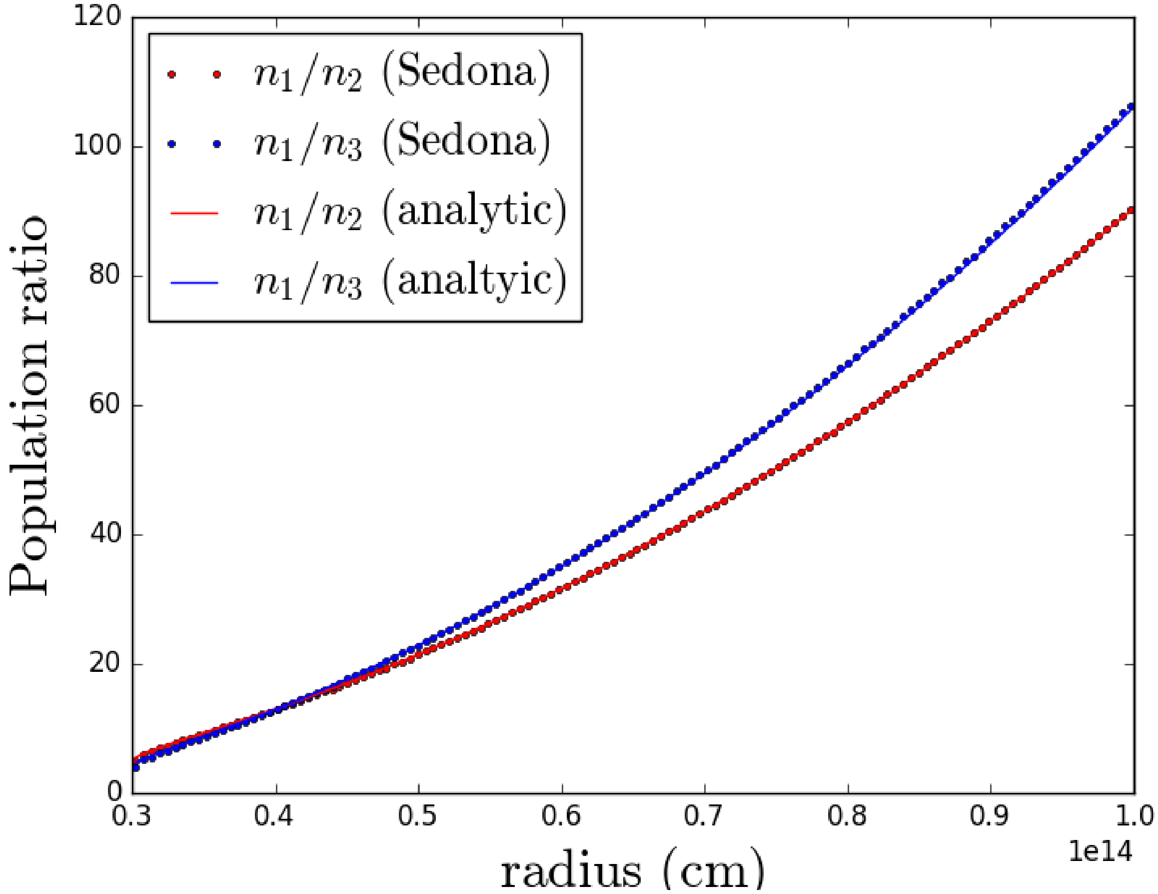

Figure 1: Level population ratios as a function of radius for the NLTE test problem

output of the NLTE solver implemented in Sedona. We find that the Sedona values match the analytic function to within 1% error over most of the computational domain, although the error rises to above 5% at the innermost radial zones.