

Astrophysical Exercises: Ionization Structure of an H II Region

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1. Physical Background

An HII region is the ionized volume of a gas cloud or the interstellar medium around a hot star. The gas is ionized by the ultraviolet radiation ($\lambda < 91$ nm or photon energy $E > 13.56$ eV) emitted by the star. In a state of equilibrium, depending on the number of these photons, the gas is ionized upto a certain radius R_S , called the Strömgren radius. We want to write a computer program that calculates the run of ionization in such an HII region. We assume that the star (with radius R_*) has a spectrum of a blackbody with temperature T_* , and is placed into a (infinitely) large cloud of pure hydrogen gas (density n particles per m^3). Thus the gaseous nebula will be spherically symmetric, and it suffices to calculate the ionization as a function of distance from the central star only, i.e. we consider a one dimensional problem. Starting at the inner radius R_i of the nebula which is at (or close by) the stellar surface, we go out further in radial steps, calculating at each radius the balance of photoionizations and recombinations of hydrogen and the attenuation of the starlight by the absorption by hydrogen atoms between the stellar surface and the radius under consideration. We break off the computation, if the outer limit of the ionized zone is reached, i.e. when $n(\text{H}^+)/n(\text{H}^0) = \xi$ is sufficiently small, for instance 0.001, or the region is optically thick to the ionizing photons, e.g. $\tau(91\text{nm}) > 100$.

2. The Equations

2.1 Ionization balance

Since we assumed equilibrium, so at every radius in the nebula the rate of photoionizations must be equal to the recombination rate:

$$n(\text{H}^0) \int_{\nu_{\text{H}}}^{\infty} \frac{4\pi J_{\nu}}{h\nu} a(\nu) d\nu = n(\text{H}^+) n_e \alpha_{\text{B}} \quad (1)$$

where $n(\text{H}^0)$, $n(\text{H}^+)$, n_e are the number densities of neutral and ionized hydrogen and electrons. $\nu_{\text{H}} = 3.29 \cdot 10^{15} \text{Hz}$ is the frequency of the hydrogen ionization threshold. $J_{\nu}(\nu, r)$ is the mean intensity of the radiation field, per unit frequency interval, and which is both a function of frequency ν and distance r from the central star. Far away from the star, we can approximate:

$$J_\nu(\nu, r) = \left(\frac{R_*}{2r}\right)^2 B_\nu(\nu, T_*) \exp(-\tau(\nu, r)) \quad (2)$$

The first factor describes the geometrical dilution of the radiation field as one moves away from the star, the second is the star's spectrum, which we assume to be a black body:

$$B_\nu(\nu, T) = \frac{2h\nu^3/c^2}{\exp(h\nu/kT) - 1} \quad (3)$$

The third factor describes the attenuation of starlight by the intervening neutral hydrogen, i.e. the loss of those photons which have already been used up for ionization. $\tau(\nu, r)$ is the optical thickness of this intervening layer of gas:

$$\tau(\nu, r) = \int_{R_i}^r \kappa(\nu, r') dr' \quad (4)$$

which is the integrated opacity

$$\kappa(\nu, r) = n(\text{H}^0)(r)a(\nu) \quad (5)$$

From quantum mechanics one can calculate the photoabsorption cross section (in m^2) for hydrogen:

$$a(\nu) = 6.3 \cdot 10^{-22} (\nu/\nu_{\text{H}})^{-3}$$

From this one also computes the recombination coefficient $\alpha_{\text{B}}(T_e)$ which is a function of the temperature T_e of the electrons, as shown in this table (units are $\text{m}^3 \text{s}^{-1}$):

T_e	5000	10000	20000	K
α_{B}	4.54	2.60	1.43	10^{-19}

There is a small trick here: in principle the radiation field not only consists of stellar photons (Eq. 2), but also those emitted by the nebular gas itself after recombinations directly to the ground state of the hydrogen atom. It is a good approximation to assume that these diffuse photons are absorbed "on the spot"; then one can show that these photoionizations are balanced by the recombinations to the ground state, and thus cancel each other in Eq. 1. This is why we need to consider here only the sum of all recombinations to excited levels α_{B} . Though we shall consider at first only isothermal nebulae ($T_e = 12000 \text{ K}$), it is a nice exercise to write an interpolation program for the above table ...

2.2 Charge Neutrality

Since the plasma is always neutral, in every volume the sum of charges of all ions is equal to the number of electrons. For a pure hydrogen gas, we simply have:

$$n_{ion} = n(\text{H}^+) = n_e \quad (6)$$

2.3 Conservation of Particles

As there are no nuclear reactions involved here, the number density of hydrogen in all forms must be constant:

$$n(\text{H}^0) + n(\text{H}^+) = n(\text{H}) = n(r) \quad (7)$$

and equal to the local hydrogen density $n(r)$. For simplicity, we shall initially assume that this density is independent of radius r , but it is worth experimenting with other laws!

3. Method of Solution

3.1 Radial and Frequency Grids

In our mathematical description of the HII region, the physical quantities are variables, the physical laws between them functions. However, in a numerical program these cannot be described symbolically, as we do when solving an equation analytically, but all physical quantities are represented by their values at discrete points in time and space. Thus the HII region will be described by the number densities of ions at certain radii $\{r_i | i = 1, N_r\}$, the spectrum of the central star by the intensity at a finite number of frequencies $\{\nu_k | k = 1, N_\nu\}$, and the radiation field by the mean intensity given at these radii and frequencies, and so on. The results of our computations will obviously be better, if we use grids as fine as possible. But as a doubling of the number of frequencies and radii will result in a four-fold increase of the number of manipulations to be done, the computing time will go up. Thus one has to choose wisely between the accuracy and speed.

There is no general rule how to make this decision, only tests can show how you can get what you need. For our problem, the frequency grid will remain fixed during the whole computation, and a good choice would be about 50 to 200 points distributed logarithmically within the relevant frequency limits. The radial grid will depend on the star and the gas density, and since the ionization changes drastically in the transition zone between ionized and neutral part, an automatic grid is the best choice. You might like to try out a fixed radial grid with a given grid spacing.....

3.2 Local Ionization Equilibrium

The central part of the program — and this is where one often begins with writing the code, is the set of local equations for the ionization. At any radius r we solve Eqs. 1, 6, and 7 by a fix point iteration:

1. compute the photoionization integral $\beta = \int_{\nu_H}^{\infty} 4\pi J_{\nu} a(\nu) d\nu / h\nu$. Of course, there is no such thing as ∞ in a numerical program; we have to choose a frequency sufficiently high ($\nu_{max} \approx 2 \cdot 10^{16}$ Hz) to ensure that the main contributions to the integral are within the limits, and the integral is evaluated with sufficient accuracy. The trapezoidal rule for the numerical integration is accurate enough, but of course any higher order formula, such as Simpson's or Gauss' methods can be employed.
2. choose a start value for n_e : This is either
 - a) $n_e = n$ for the first radius $r_1 = R_i$
 - b) $n_e = n_e(r_i)$ if the local ionization is not yet stable (see Sect. 3.4) below.
 - c) $n_e(r_i) = n_e(r_{i-1})$ for any radius r_i use the value obtained at the previous radius r_{i-1} .
3. with $\xi = \beta / (n_e \alpha_B)$ compute the densities $n(\text{H}^0) = n / (1 + \xi)$ and $n(\text{H}^+) = n\xi / (1 + \xi)$.
4. compute a new value for $n_{e,new} = \sqrt{n_{ion} n_e}$
5. if the absolute relative difference $|n_{e,new} / n_e - 1|$ is still larger than a given tolerance (say 0.0001), we go back to Step (3), using the new electron density. This iteration is a well behaved one (no oscillations, no extremely slow convergence — but you better have a look for yourself and check the convergence behaviour). It should converge with less than 10 steps. Since this iteration is done for every radius, and is nested within another iteration (see below), make sure that the program cannot enter an eternal loop without your notice.

3.3 How to Estimate the Next Radial Grid Point

To make our adaptive radial grid, we use the fact that the degree of ionization $\xi = n(\text{H}^+) / n(\text{H}^0)$ decreases monotonically as the distance from the star increases. If we demand that ξ changes from one radius to the next one by about a factor δ (let us say 0.8),

$$\xi(r_{i+1}) = \xi(r_i) \delta \quad (8)$$

we can estimate the next radius by linear interpolation from the present and the previous radius:

$$(r_{i+1} - r_i) = \lg(\delta) \frac{r_i - r_{i-1}}{\lg(\xi(r_i) / \xi(r_{i-1}))} \quad (9)$$

To do this, one needs to know the ionization in two points, i.e. the method cannot be applied to determine the second radius. This is done differently, by setting $r_2 = 1.01 r_1$, for example.

Of course this is not the only way to determine the next radial grid point; for example one can use the fact that the optical depth at the ionization threshold frequency

increases monotonically with radius. Also, one may use higher order extrapolation formulae. Though they may seem more accurate, they usually have the danger of "swinging" outside the range of reasonable values, if no precautions are taken.

3.4 Optical Depth

Before we can solve the ionization equations at the next radial grid point, we must know the optical depth (at all frequencies) of the radius r_{i+1} , as it enters the radiation field. This is done in two steps:

First we estimate from the previous radii the absorption coefficient at any frequency by linear extrapolation

$$\kappa_{i+1}^e = \kappa_i + (\kappa_i - \kappa_{i-1}) \frac{r_{i+1} - r_i}{r_i - r_{i-1}} \quad (10)$$

and the optical depth by integration using the trapezoidal rule

$$\tau^e(r_{i+1}) = \tau(r_i) + \frac{1}{2}(\kappa_{i+1}^e + \kappa_i)(r_{i+1} - r_i) \quad (11)$$

With these values the radiation field at r_{i+1} is computed and the ionization equations are solved (see Sect. 3.2). From this one gets improved values for the absorption coefficients

$$\kappa_{i+1}(\nu) = n(\text{H}^0)(r_{i+1})a(\nu) \quad (12)$$

with which one improves the optical depths

$$\tau(r_{i+1}) = \tau(r_i) + \frac{1}{2}(\kappa_{i+1} + \kappa_i)(r_{i+1} - r_i) \quad (13)$$

This is done until the value of the ionization $\xi(r_{i+1})$ has stabilized within a given tolerance, say $|\Delta\xi/\xi|$ of successive iteration steps less than 0.001. The iteration is very quickly convergent. Note that this iteration incorporates the iteration for local ionization balance, and one should take again care to prevent the occurrence of infinite loops.

As before, the extrapolation (Eq. 10) does not work for the step from the first to the second radius. Here we simply use $\kappa_2^e = \kappa_1$ and the optical depth $\tau_2^e = (r_2 - R_1)\kappa_1$.

3.5 Structure of the Program

1. Input routines for the model parameters, setting up the frequency grid, initializing constants, setting up the stellar spectrum, ...
2. Start at the inner radius: compute the mean intensities, set optical depths to zero
3. Solve the ionisation balance (see Sect. 3.2)
4. Calculate local absorption coefficients (Eq. 5).
5. Improve optical depths (Eq. 13)

6. Check for stability of ξ (This is not necessary for the first radius, since $\tau = 0$ for all frequencies. If ξ is not accurate enough, recalculate the mean intensities, and go back to Step 3)
7. Check whether the outer edge has been reached, either by sufficiently low ξ or sufficiently large τ . If that is the case, stop the calculation, print out results, ...
8. Compute the next radial grid point (Eq.9).
9. Estimate absorption coefficients and optical depths for next radius (Eqs.10, 11).
10. Compute the mean intensities; go back to Step 3.

4. Tests, Hints, and Kinks

0. Before actually writing the program, do make a flow chart diagram in order to understand the sequence of what is computed; a diagram of the program structure and the data structure to find out, how the loops and iterations are nested, which data from earlier parts you need at each section, which kind of vectors and arrays you are going to need. This may seem bureaucratic, boring or even old fashioned, but **don't start typing anything, before you are absolutely clear about what you plan to do**. Otherwise you may really end up wasting much time in trying to find the logical errors, loopholes, and cul-de-sacs of your hasty programming. Save yourself the frustration, disappointment, and anger!
1. General Program Planning: It is a good idea to lay out the program as general as possible. This makes it easier to include other effects, or to try out other situations. E.g. keep the number of frequency points, the upper and lower limits as parameters which are given values in the main program, rather than being specified everywhere the frequency grid is used. Checking the program for other kinds of stellar spectra can thus be done easily at any time. Or the grid parameters can be changed, whenever a model with high accuracy is to be computed.
2. Modular Construction: It is also a good idea to break up the program into mathematically or physically sensible units. This allows a better testing of these individual modules — and most of the time is spent in tracing an error — a more flexible use of them for other purposes, and their exchange against improved or alternative methods, improved data, other physical processes, etc. For example, if the frequency integration is contained in an independent unit, one simply exchanges this against a more sophisticated method, if need arises, but without the trouble of having to change the program at a dozen places. For testing, a simple main program has to be written which supplies the necessary input data to this unit.
3. Check Everything by Hand: Often, we underestimate our ingenuity to make small logical mistakes or simple typing errors, which may cause faulty results. The worst kind of mistakes are those which produce results that look as one would expect them to be. Take the trouble of check everything the program does, until you are sure it does only what you want it to do. In programs about physical

things, basic physics must be obeyed: conservation of particles, energy, etc. Also, all the simple and limiting cases which we do understand, must be reproduced accurately.

4. Be highly skeptic of anything the program produces.
5. Numerical Integration: For our purpose, trapezoidal rule is of sufficient accuracy, and simple to program. Please note that the end-points of the integration interval are treated differently than the inner points. Please verify that all integration routine do their job properly. This is done by integrating over a known function, so that the accuracy can be determined. Also, it is quite easy to compute the photoionization integral by hand, if one takes a very hot stellar spectrum. For $h\nu \gg kT_*$ one can use Wien's approximation of the blackbody spectrum $2h\nu^3 \exp(-h\nu/kT_*)/c^2$. How many photoionizations per second take place in a unit volume of the gas? Any guess?
6. Be Watchful of Iterations: Please check every iteration initially for its convergence behaviour. A good idea is to put a limit on the number of iterations to be performed. Also, a printout of everything happening for the last five iterations maybe helpful when trouble arises. Especially when several iterations are nested within each other, it is necessary to make sure that they do not end up in an infinite loop. Provide written messages if something goes not normal.
7. When you are making tests, and later running the program for various situations and parameters, try to keep a careful written record of what you do, noting input parameters and results. This will make it easier for you later to compare results with earlier ones, in case you have to hunt for an error that has crept in yesterday when you "just changed a few things, almost nothing — but the program doesn't work any more".

5. Some Tasks

The well known Strömgren radius R_S is the radius upto which the gas around the star is ionized. One computes it from the global balance of the number of ionizing photons \mathcal{N} the star emits per second and the total recombination rate in the ionized sphere:

$$4\pi R_*^2 \int_{\nu_H}^{\infty} \frac{\pi B_\nu(\nu, T_*)}{h\nu} d\nu = \mathcal{N} = 4\pi \int_{R_*}^{R_S} \alpha_B n_e n(\text{H}^+) r^2 dr = \frac{4\pi}{3} R_S^3 \alpha_B n_e^2 \quad (14)$$

Because this formula has the character of a global conservation law, the program should be able to reproduce it, for all nebular and stellar parameters. The deviation gives an indication of the overall accuracy of the program.

Consider these two models:

- (a) $R_* = 1 R_\odot$ and $n = 10^{10} \text{ m}^{-3}$
- (b) $R_* = 10 R_\odot$ and $n = 10^8 \text{ m}^{-3}$

both for a $T_* = 40000$ K star. How large are the Strömngren radii? Now compare the ionization structure, i.e. the run of ξ with radius, but measured in units of the Strömngren radius.

6. Extension: Dust

In the infrared many HII regions show a strong continuum which is interpreted as emission from warm dust particles of temperatures $T_D = 100...1000$ K. Since this emission comes from the same spatial extend as the optical and radio emission of the ionized gas, the dust particles must be distributed throughout the ionized region, and therefore will be able to absorb also ionizing photons. With the program we can easily investigate how the presence of dust changes the structure of the HII region, and how many of the photons are absorbed, if we add to the atomic absorption coefficient:

$$\kappa(\nu, r) = n(\text{H}^0)a(\nu) + \kappa_D(\nu, r) \quad (15)$$

the opacity by the dust $\kappa_D(\nu)$ which may be expressed as

$$\kappa_D(\nu) = n_D(r) \sigma_{abs}(\nu) \quad (16)$$

the product of a frequency dependant absorption cross section σ_{abs} and the local number density of the dust particles. For simplicity we shall assume that the dust to gas ratio (n_D/n) is constant everwhere in the HII region.

In the program, one only needs to setting up the frequency dependent $\kappa_D(\nu)$ before starting the computations. To do this, one needs to specify the opacity at some reference frequency, say ν_0 and the frequency dependance, e.g. constant or $\kappa_D/\kappa_D(\nu_H) \propto \nu$. This opacity is then just added to the local absorption coefficient of the gas. When one extrapolates the opacity to the next radial point, one should try out whether it is better to extrapolate the total opacity or just the part from the gas.

Here are some tasks:

- (a) For a fixed frequency dependence of κ_D one should investigate how the HII region changes when the dust to gas ratio is increased starting from zero: Strömngren radius, the volume of the ionized region. Which quantity is the important parameter which decides whether the HII region is dominated by dust or not? Hint: print out the optical depths of gas and dust separately.
- (b) Now try out various frequency dependances of κ_D and see how much the results from (a) are changed.
- (c) Now let's make it more realistic: A typical interstellar dust grain has a radius $r_D \approx 0.3 \mu\text{m}$, and the dust to gas ratio (by **mass**) in the interstellar medium amounts to $\rho_D/\rho_{\text{gas}} = 0.01$. Let us assume that the grains are spheres of a material like graphite (density 3000 kg m^{-3}). The absorption cross section shall be independent of frequency and very close to the geometrical cross section. The exciting stars in the Orion nebula are stars of spectral type O, with a temperature of about 40000 K and a luminosity of 10^6 times that of the Sun. The gas density in the nebula is about 100 atoms per cm^3 . Is the Orion nebula dominated by

dust or not? What fraction of the available stellar photons is absorbed by the dust?

- (d) The parameter space for our HII region models is three dimensional: T_* , R_* , n are the parameters. Can you indicate in which parts of this space the HII region (made of normal interstellar gas and dust, as above) are dust dominated and in which parts they are not?

7. Extension: Helium

After hydrogen, helium is the most abundant element in gas of "normal" chemical composition: by number of particles, the ratio is $\text{He}/\text{H} \approx 0.1$. So it can be quite important in the structure of an HII region or a planetary nebula. To incorporate it in our program, we have compute the ionisation of He^0 , He^+ , and He^{++} , and take into account the contributions to the number of electrons and to the absorption.

7.1 Ionisation Equilibrium

Now there are these equations:

$$n(\text{He}^+)n_e \alpha(\text{He}^+) = n(\text{He}^0) \int_{\nu_{\text{He}^0}}^{\infty} \frac{4\pi J_\nu}{h\nu} a(\text{He}^0) d\nu \quad (17a)$$

$$n(\text{He}^{++})n_e \alpha(\text{He}^{++}) = n(\text{He}^+) \int_{\nu_{\text{He}^+}}^{\infty} \frac{4\pi J_\nu}{h\nu} a(\text{He}^+) d\nu \quad (17b)$$

from which one computes $n(\text{He}^+)/n(\text{He}^0)$ and $n(\text{He}^{++})/n(\text{He}^+)$. With $n(\text{He}^0) = 1.0$ one gets the other ionic densities, which then are renormalized to the number density $nA(\text{He})$ of helium in all forms, in order to satisfy the conservation equation of particles:

$$n(\text{He}^0) + n(\text{He}^+) + n(\text{He}^{++}) = nA(\text{He}) \quad (18)$$

$A(\text{He}) = 0.1$ is the helium fraction of the gas. $A(\text{H}) = 0.9$ These ionisation equations are solved parallel to those of hydrogen.

7.2 Contribution to Electron Density

When computing the number of electron, we now add those coming from helium:

$$n_{ion} = n(\text{H}^+) + n(\text{He}^+) + 2n(\text{He}^{++}) \quad (19)$$

$$n_{e,new} = \sqrt{n_{ion}n_e} \quad (20)$$

to modify the existing iteration.

7.3 Opacity

Depending on frequency, to the hydrogen opacity we add the appropriate helium absorption coefficients:

$$\kappa(\nu) = \begin{cases} n(\text{H}^0)a(\text{H}) & \text{for } \nu < \nu_{\text{He}^0} \\ n(\text{H}^0)a(\text{H}) + n(\text{He}^0)a(\text{He}^0) & \text{for } \nu_{\text{He}^0} \leq \nu < \nu_{\text{He}^+} \\ n(\text{H}^0)a(\text{H}) + n(\text{He}^0)a(\text{He}^0) + n(\text{He}^+)a(\text{He}^+) & \text{for } \nu_{\text{He}^+} \leq \nu \end{cases} \quad (21)$$

since He^0 and He^+ absorb only for frequencies above the thresholds ν_{He^0} and ν_{He^+} .

7.4 Changes to the Method

Note that the addition of helium makes it necessary to put in the threshold frequencies to the frequency grid, mark these points, and other organizational changes.

Now one has in addition to the transition zone $\text{H}^+ \rightarrow \text{H}^0$ two more zones $\text{He}^{++} \rightarrow \text{He}^+$ and $\text{He}^+ \rightarrow \text{He}^0$, where the radial points have to be placed with a finer spacing. When determining the next grid point, one applies the same procedure already used for hydrogen also to He^0 and He^+ separately. From these three guesses one selects the most suitable one, e.g. the one with the smallest spacing. One has to try out the best way, and also the most suitable values for $\delta(\text{He}^0)$ and $\delta(\text{He}^+)$, in order to find a compromise between accuracy and short computation times. It is only the transition zones where the corresponding optical depths are of the order of 1, that the grid has to be placed carefully. If the optical depth for the important ion is very low, grid spacing is rather uncritical. If it is high, then the density of the particular ion is very low, so it can be set to zero, and the next lower ion becomes important when deciding on how to place the grid points.

7.5 Atomic Data

Ionisation frequencies:

$$\nu_{\text{He}^0} = 5.9451 \cdot 10^{15} \text{Hz}$$

$$\nu_{\text{He}^+} = 1.3158 \cdot 10^{16} \text{Hz}$$

Photoionization cross sections (in m^2):

$$a(\text{He}^0) = 7.83 \cdot 10^{-22} (\nu_{\text{He}^0}/\nu)^2 (1.66 - 0.66(\nu_{\text{He}^0}/\nu))$$

$$a(\text{He}^+) = 1.5 \cdot 10^{-22} (\nu_{\text{He}^+}/\nu)^3$$

Recombination coefficients (in $\text{m}^3 \text{s}^{-1}$):

$$\alpha(\text{He}^+) = 4.3 \cdot 10^{-19} (T_e/10^4 \text{K})^{-0.672}$$

$$\alpha(\text{He}^{++}) = 1.09 \cdot 10^{-19} \sqrt{x} (0.4288 + 0.5 \ln x + 0.469x^{-1/3})$$

with $x = h\nu_{\text{He}^+}/(kT_e)$

7.6 Some Tasks

Compute a series of nebulae around stars with different temperatures from 20000 to 200000 K. How do the Strömgen radii of H, He, and He^+ change their positions relative to each other? Can you say when the respective Strömgen formulae are not valid? Explain why.

8. Extension: The Intensities of Hydrogen and Helium Recombination Lines

When electrons recombine with ions of hydrogen and helium, they may leave the resultant atom in an excited state, from which it will decay to lower states by emitting photons of spectral lines, and finally arrive in the ground state. These recombination lines can be observed in the optical wavelength region, for example the Balmer series of hydrogen which corresponds to the transitions to the first excited level (the principal quantum number changes from $n = 3, 4, 5, \dots \rightarrow 2$). In the infrared there are the Paschen ($n \rightarrow 3$) and the Brackett series ($n \rightarrow 4$). From neutral helium there are several lines in the triplet and singlet series, and from ionized helium there is e.g. the Paschen α line at $\lambda 4686\text{\AA}$.

Since most nebulae are optically thin for most of these lines, the luminosity P_{line} of (i.e. the total power emitted by) an H II region in the line is simply the volume integral over the emissivity j_{line} :

$$P_{line} = 4\pi \int_{R_*}^{R_{neb}} j_{line} r^2 dr \quad (22)$$

since we assume spherical symmetry. As the collision of an electron with the respective ion is responsible for the emission process, the emissivity is proportional to the number densities of electrons and ions, for example

$$j_{\text{HeI } 4471} = \dots n(\text{He}^+) n_e$$

In the following table (from Osterbrock: Astrophysics of Gaseous Nebulae) the factors of proportionality $4\pi j / (n_{ion} n_e)$ is given for the some hydrogen and helium lines as a function of electron temperature T_e , for others the ratio of the emissivity to that of a principal line (such as $\text{H}\beta$, traditionally) are given. The emissivity depends also on electron density, but only very weakly, so that we may well neglect this. Please find nice fit formulae that reproduce the data from the table, so that you can compute the emissivities from any electron temperature.

	λ [Å]	$T_e =$ 5000	[K] 10000	20000	unit
$4\pi j_{\text{H}\beta}/n_+n_e$	4861	$2.22 \cdot 10^{-25}$	$1.24 \cdot 10^{-25}$	$6.59 \cdot 10^{-26}$	$\text{erg cm}^3 \text{ s}^{-1}$
$j_{\text{H}\alpha}/j_{\text{H}\beta}$	6563	3.00	2.85	2.74	
$j_{\text{H}\gamma}/j_{\text{H}\beta}$	4340	0.460	0.469	0.476	
$j_{\text{H}\delta}/j_{\text{H}\beta}$	0.253	0.259	0.264	
$4\pi j_{\text{HeI } 4471}/n_+n_e$	4471	$1.17 \cdot 10^{-25}$	$6.08 \cdot 10^{-26}$	$2.95 \cdot 10^{-26}$	$\text{erg cm}^3 \text{ s}^{-1}$
$j_{\text{HeI } 5876}/j_{4471}$	5876	3.01	2.76	2.58	
$4\pi j_{\text{HeII } 4686}/n_+n_e$	4686	$2.93 \cdot 10^{-24}$	$1.48 \cdot 10^{-24}$	$7.16 \cdot 10^{-25}$	$\text{erg cm}^3 \text{ s}^{-1}$

9. Extension: Other Elements

Elements heavier than helium such as carbon, nitrogen, oxygen, etc. have very low abundances, typically 10^{-4} of hydrogen. Thus one can neglect their contributions both to the electron density and the absorption coefficient. We only need to solve the ionisation balances for all the ions i of an element such as oxygen:

$$n_{i+1}n_e \alpha_i = n_i \int_{\nu_i}^{\infty} \frac{4\pi J_\nu}{h\nu} a_i(\nu) d\nu \quad (23)$$

As done with helium, one computes all the ionic densities and scales them so that the total number of oxygen ions is equal to the fraction of oxygen of the gas:

$$\sum_{i=0}^N n_i = n(O) = \frac{A(O)}{A(H)} n(H) \quad (24)$$

with the oxygen abundance $A(O)/A(H)$. The atomic data are

ν_i Frequency of the ionization threshold of O^{+i} .

$\alpha_i = A_i(T_e/10^4\text{K})^{-B_i}$

$$a_i(\nu) = \begin{cases} 0 & \text{for } \nu < \nu_i \\ a_i^o \left(\frac{\nu}{\nu_i}\right)^{-s_i} (\beta_i + (1 - \beta_i) \left(\frac{\nu_i}{\nu}\right)) & \text{for } \nu \geq \nu_i \end{cases}$$

i	ν_i	A_i	B_i	a_i^o	β_i	s_i
0	3.3	0.3	0.678	2.5	4.0	1
1	8.5	2.0	0.646	8.1	2.45	2
2	13.3	5.1	0.666	3.5	1.3	2
3	18.7	9.6	0.670	1.1	1.82	3
4	2.75	12.0	0.779	0.78	2.6	3
unit	10^{15}Hz	$10^{-18}m^3s^{-1}$		$10^{-22}m^2$		

10. Extension: Computing the Line Intensities

In the nebular gas there are a number ions which have energy levels that can be excited by collisions with the electrons. The excited ions will decay by spontaneous emission of photons, which escape from the nebula to form the emission lines we can observe. Let us consider a 2 level model of ion of species i with ground state 1 and excited state 2 with number density $n_{i,2}$ of ions in the excited state: in equilibrium there is a balance of the excitations and the deexcitations (spontaneous emission and also collisional deexcitation):

$$n_{i,1}C_{12} = n_{i,2}(A_{21} + C_{21}) \quad (25)$$

with the spontaneous transition probability A_{21} and the collisional rates C_{ik} . Of course, the conservation of number of ions demands:

$$n_{i,1} + n_{i,2} = n_i \quad (26)$$

where n_i is the number of ions of species i , in all energy levels, which had been computed earlier from the ionization balance in the last section.

Task: What this means is that ionization balance and excitation equilibrium can be separated into two independent problems. This is not self-evident, so better check this by computing all the rates between the energy levels, and compare them with the photoionization and recombination rates. Assume some reasonable model parameters and select a few representative distances from the central star. The collisional excitation rate is given by:

$$C_{12} = C_{21} \frac{g_2}{g_1} \exp(-E_{12}/kT_e) \quad (27)$$

g_1 and g_2 are the statistical weights of the ground and excited states; for simplicity but without losing much of the physical realism we may set $g_1 = g_2 = 1$. $E_{12} = h\nu_{12}$ is the energy difference between the levels, ν_{12} being the frequency of the emission line. The collisional deexcitation rate is given by

$$C_{21} = n_e \frac{8.629 \cdot 10^{-12} \Omega_{21}}{T_e^{1/2}} \frac{\Omega_{21}}{g_2} \quad (28)$$

The dimension of the C s is inverse time. Ω_{21} is an atomic constant for this transition, the collision strength. It has been computed from a quantum mechanical treatment of the collision process, we just take these results.

ion	λ_{12}	Ω_{21}	A_{21}
O ⁰	630	0.4	0.006
O ⁺	373	1.5	0.0004
O ⁺⁺	500	2.5	0.03
unit	nm		s ⁻¹

To compute the observable spectrum, one considers the emissivity j_{12} of the line per unit volume, which is just the energy released by the emission process:

$$4\pi j_{12} = n_{i,2} A_{21} h\nu_{12} \quad (29)$$

Since a gaseous nebula usually is transparent for all these emission lines, we compute the power P emitted in the line by the whole volume of the HII region:

$$\begin{aligned}
P_{12} &= \int 4\pi j_{12} dV_{ol} \\
&= A_{21} h\nu_{12} 4\pi \int_{R_i}^{R_s} n_{i,2}(r) r^2 dr
\end{aligned} \tag{30}$$

as we had assumed spherical symmetry. In principle these computations have to be done for all relevant energy levels and lines in all the ions. In the case of a two level ion one can calculate the number density $n_{i,2}$ of the excited ions directly from Eqs. 25 and 26.

11. Extension: Solving the Energy Balance

So far we have – for simplicity – assumed that the temperature of the electron gas is given somehow, and constant everywhere in the nebula. It is not difficult to compute the electron temperature from the thermal equilibrium between the heating by photoionization and cooling by emission of the continuum and lines. When the hydrogen atom (ionization energy $h\nu_H$) is ionized by a photon of energy $h\nu > h\nu_H$, the excess energy $h(\nu - \nu_H)$ is carried away by the photoelectron in the form of kinetic energy. This is distributed quickly by elastic collisions to the other electron, thus heating the electron gas:

$$H = n(\text{H}^0) \int_{\nu_H}^{\infty} \frac{4\pi J_\nu}{h\nu} (h\nu - h\nu_H) a(\nu) d\nu \tag{30}$$

is the heating rate (energy per time and volume units). On the other hand, the gas loses energy $h\nu_{jk}$ by the electron collisions exciting ions, which emit line photons. The total cooling rate

$$K = \sum_{jk} 4\pi j_{jk} + kT_e n_e n(\text{H}^+) \beta(T_e) \tag{31}$$

is the sum over all collisionally excited lines, and the second term describes losses by the emission of hydrogen recombination lines and continua:

$$\beta(T_e) = \alpha_B (1 + 0.16(T_e/10^4 K)) + \beta_{ff} \tag{32}$$

The losses by emission of thermal Bremsstrahlung (in the radio and infrared regions) are

$$\beta_{ff} = 1.42 \cdot 10^{-40} \sqrt{T_e} \tag{32}$$

11.1 Method of Solution

Since by now you are well experienced, it may be sufficient to give just a sketch of how this part is solved and put into the existing program: From the equilibrium condition $H = K$ the electron temperature T_e at each radius in the nebula is determined by a Newton-Raphson or Regula Falsi iteration to find the zero of the function $H(T_e) - K(T_e) = 0$. To do this, one computes the heating intergral H which is similar to the photoionization integral. The cooling function also has to be evaluated by computing the local emissivity which depends on T_e . With a guess value of $T_e = 10^4\text{K}$ or the electron temperature from the previous radial point, one starts the iteration, which continues, until the required accuracy is achieved.

This iteration must be successfully finished, before one goes to the next item, the computation of the local absorption coefficient. So this part goes after Step (3) in the program outline. However, since the recombination coefficients depend on electron temperature, the ionization balance will also shift after a new value for the temperature is found. So one has to solve ionization and energy balances consistently. One may well solve them together, iterating in 2 dimensions for (n_e, T_e) . However one can also just introduce yet another iteration, solving ionzation and thermal balance one after the other until all the values have stabilized. Do as you like.