

# Astrophysical Exercises: Time-dependent Ionization

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## 1. Physics Background

When young massive star reaches the Main Sequence, and hence an effective temperature of greater than about 20000 K, the energetic radiation from this hot stellar atmosphere is able to ionize any hydrogen gas that may be in the neighbourhood of the star. Thus hydrogen atoms are turned into protons plus a free electron. Depending on the density of the gas, some of the collisions of electrons with protons lead to a recombination into an atom. Thus there remains a certain small fraction of neutral gas. The steady flux of energetic photons from the star produces ions from atoms, while recombination does the inverse process. If one waits for a sufficient long time, an equilibrium will be formed. When this is reached, the ionized region extends up to a certain distance from the star - the Strömgren radius - and we speak of an HII-region. Massive stars evolve quickly and after a few million years they explode as a supernova. As such an explosion would upset the entire surroundings, the question what happens to the HII-region after the ionizing flux from the massive star vanishes, is quite academic ... However, there can be the situation where a massive star moves rather rapidly through the interstellar medium, thereby ionizing a certain region and then leaving it behind.

The same physical processes are at work in planetary nebulae, where a red giant star ejects part of its outer envelope, while the remnant star collapses to become a white dwarf and thereby rising strongly in temperature. But when the star's nuclear fuel finally runs out, the stellar temperature drops, and the surrounding nebula slowly recombines.

Eruptions of novae or events in the accretion disks of black holes and other compact objects - giving rise to eruptions in the X-rays - also affect the vicinity of the object in the same way.

Since observations of the emission of the gas permit - in principle - to determine the state of ionization of the gas, and since all relevant atomic data are well known, they can be used to infer the temperature of the central ionizing object. If we knew that the gas is in ionization equilibrium, we could thus follow the time evolution of the central object.

In this exercise, we shall consider a small test volume of gas, situated at some distance from a radiative source, whose temperature shall be a function of time. Let us compute the degree of ionization (of hydrogen) in this gas, and how it varies with time. Under which conditions can we safely assume that the gas is in ionization equilibrium? We may consider different types of objects, with different time histories, and with different physical parameters (gas density). Let us find out under which conditions planetary nebulae, HII-regions, active galactic nuclei, variable X-ray sources, and other objects may be interpreted with equilibrium models, and when this may no longer be a good assumption.

## 2. Photoionization

Let us first formulate the general case and write down the general equation: Assume we have a source of radiation, characterized by its radius  $R_*$  and the spectral flux  $F_\nu(\nu)$  at that radius. The spectrum could be that of a blackbody with a given temperature  $T_*$  or a power law, e.g. for X-ray sources. For later use, we shall think of the flux (or the temperature) - or even the radius - to be a function of time, but to avoid clumsy notation, we shall not indicate this dependence explicitly! Then the mean intensity of the radiation at a distance  $r$  from the star is given by

$$J_\nu(\nu, r) = \frac{\pi R_*^2}{4\pi r^2} F_\nu(\nu) \quad (1)$$

Note that the index  $\nu$  in  $J$  and  $F$  indicates that we consider these quantities per unit frequency, so that the unit of flux is  $\text{Wm}^{-2}\text{Hz}^{-1}$ . The first factor describes the geometrical dilution, as the star's entire radiation is distributed over the sphere of radius  $r$ . The number of ionizations per unit time and unit volume is the integral for all frequencies larger than the ionization threshold ( $\nu_0$ , for hydrogen  $h\nu = 13.56 \text{ eV}$ ) over the product of mean intensity and photoionization cross section  $a(\nu)$

$$\text{ION}(r) = n_0(r) \int_{\nu_0}^{\infty} \frac{4\pi J_\nu(\nu) a(\nu)}{h\nu} d\nu \quad (2)$$

where  $n_0(r)$  is the density of neutral atoms in the test volume at distance  $r$  from the star. For hydrogen the photoionization cross section is

$$a(\nu) = 6.3 \cdot 10^{-22} \text{m}^2 (\nu_0/\nu)^3 \quad (3)$$

Equation (1) holds true only, if we neglect any absorption between the star and the test volume. This is an approximation which we shall adopt to make things a bit easier: in principle we should take into account here that the gas between the star and the test volume also is partially neutral, and thus the photons that ionized it, are missing in the intensity at radius  $r$ . But as long as the medium is highly ionized,

we may use this approximation ... Then we realize that the integral in Equation (2) may be simplified

$$\text{ION}(r) = n_0(r) \frac{\pi R_*^2}{4\pi r^2} \int_{\nu_0}^{\infty} \frac{4\pi F_\nu(\nu) a(\nu)}{h\nu} d\nu \quad (4)$$

so that it depends no longer on the distance  $r$ , but only on the spectrum of the central source, and we shall define:

$$\mathcal{N} = \int_{\nu_0}^{\infty} \frac{4\pi F_\nu(\nu) a(\nu)}{h\nu} d\nu \quad (5)$$

which represents the number of photoionizations that the spectrum is capable of producing. For spherical star with a blackbody spectrum we have  $F_\nu(\nu) = \pi B_\nu(\nu, T_*)$  thus this number  $\mathcal{N}$  is a function of stellar temperature only.

The recombination rate depends on the densities of electrons  $n_e$  and ions  $n_+$

$$\text{REC} = n_e n_+ \alpha_B \quad (6)$$

with a recombination coefficient  $\alpha_B = 5.6 \cdot 10^{-19} \cdot T_4^{-0.6} \text{ m}^3 \text{ s}^{-1}$  where  $T_4 = T_e/10^4$  is the temperature of the electron gas, measured in  $10^4$  K. In most circumstances, this temperature is close to 10000 K, so  $T_4 \approx 1$ .

To formulate the basic equation, we note that the number density of hydrogen ion is increased by ionization and decreased by recombination:

$$\frac{dn_+}{dt} = \text{ION} - \text{REC}$$

which is written explicitly

$$\frac{dn_+}{dt} = n_0 \frac{\pi R_*^2}{4\pi r^2} \mathcal{N} - n_e n_+ \alpha_B$$

If we consider pure hydrogen gas, we have  $n_+ + n_0 = n$  with the total gas density  $n$ , but also all electrons come from the hydrogen ions:  $n_e = n_+$ . If we now define  $x = n_+/n$  as the ionized fraction, we get this equation

$$\frac{d(nx)}{dt} = n(1-x) \frac{\pi R_*^2}{4\pi r^2} \mathcal{N} - n^2 x^2 \alpha_B \quad (7)$$

If we also assume that the total gas density does not change in the test volume, we get

$$\frac{dx}{dt} = (1-x) \frac{\pi R_*^2}{4\pi r^2} \mathcal{N} - nx^2 \alpha_B \quad (7a)$$

Note that we would get the same equation, if we had started with an equation for the evolution of the density of hydrogen atoms. This is because we consider a gas with only one species, and because hydrogen has only two ionic states: neutral and

ionized. Therefore the state of the gas is completely described by a single variable, such as its ionized fraction  $x$ .

## 2.1 Ionization equilibrium

Equilibrium is described by the absence of any changes:  $dx/dt = 0$ . In our system this means that

$$(1 - x_{eq}) \frac{R_*^2}{4r^2} \mathcal{N} = nx_{eq}^2 \alpha_B \quad (8)$$

Solving this quadratic equation for  $x$  we get

$$x_{eq} = A/2 \times (\pm \sqrt{4/A + 1} - 1) \quad (9)$$

with  $A = \mathcal{N} \times R_*^2 / (4r^2 n \alpha_B)$ . Obviously, the solution with the plus-sign is the only physically possible.

## 2.2 Time-scales

What is the time one has to wait for the equilibrium to be reached? Inspection of Equation (7a) indicates from the term that depends most strongly on  $x$  - the recombination term - that the equilibrium is reached for times larger than  $n\alpha_B$ . However, this is not the usual exponential time-scale, because the recombination depends quadratically on  $x$ : Consider the case of ionized gas in which we suddenly switch off the ionizing source: the subsequent evolution is described by

$$\frac{dx}{dt} = -nx^2 \alpha_B \quad (10)$$

with the exact solution:

$$x(t) = \frac{x(0)}{1 + t/(x(0)n\alpha_B)} \quad (11)$$

Fully ionized gas would have  $x(0) = 1$ .

### 3. How to Compute it

The equation (7a) fully describes the behaviour of the gas in the test volume, given the flux of the central source, in particular its time history. Solving it is straight-forward: given the ionized fraction at some time, it permits us to compute how the fraction changes during the time step  $\Delta t$

$$x(t + \Delta t) = x(t) + \Delta t \times \frac{dx}{dt} \quad (12)$$

At the new time, we recompute the derivative, and so get the next step of evolution, and so on. Note that if the temperature or luminosity of the central source change with time, the ionization rate changes accordingly. Repeated application of this formula hence gives the complete evolution after an initial state and following the history of the source.

Obviously, the time step  $\Delta t$  should be sufficiently small to follow the changes of the ionization state as well as the history of the ionizing flux from the central source. One may adopt a time step small enough to capture both, but that choice may result in a very small value, and thus a long execution time, or one wastes computing time during times when no large changes happen. Also, a small time step may produce long files with results that you want to plot ... there is no point trying to plot a file with Gigabytes of data! If that happens, you should think of reducing the output by not printing out every times step. Some tests will show you what time step might be a good compromise between accuracy and execution time.

A better way is using an adaptive step width: If you demand that the change in  $x$  should always be smaller than a certain  $\epsilon$  you can compute from the current derivative the necessary time step  $\Delta t$ :

$$\epsilon = \Delta t \times \left| \frac{dx}{dt} \right|$$

Sometimes it is useful to add lower and upper bounds, to ensure that this automatic method does not get astray, for example by getting stuck with very small time steps.

However, you might find out that our straight-forward formulation of the equations is not a very satisfactory way of solving it numerically: the variable  $x$  has physically sensible values only in the intervall from 0 to 1, which are given by the law of conservation of particles ... but if the time step is too large, it is easily possible that our Equation 12 yields values larger than 1 or negative values, thus the numerical method has the potential to violate a fundamental law of physics, and to produce numbers that are physically nonsense. It may be possible to design an adaptive time step method that prevents this, but you might find that this becomes somewhat complicated.

It is much better to formulate the problem in such a way, that the physically sensible values cover the entire range of real numbers, so that the basic conservation law cannot be disobeyed. We can realize this by defining a new variable:

$$\xi = \ln\left(\frac{n_+}{n_0}\right) = -\ln\left(\frac{1}{x} - 1\right) \quad (13)$$

which gives  $-\infty$  for neutral gas and  $+\infty$  for completely ionized gas. This leads to the following version of Equation (7a):

$$\frac{d\xi}{dt} = \frac{1}{x(1-x)} \frac{dx}{dt} = \frac{R_*^2}{4xr^2} \mathcal{N} - \frac{nx\alpha_B}{(1-x)} \quad (14)$$

where  $x$  is computed from  $\xi$  with Equation 13. Adding an adaptive time step, as described above, results in an efficient and reliable method to solve the equation. We only need to give the tolerance  $\epsilon$  to suit our needs for accuracy and computational speed.

### 3.1 Some words about units

In this problem we deal with quantities that give large numbers when expressed in SI units, such as distances and luminosities, but also atomic quantities which give small numbers. However, numerical calculations such as integrations are best done when the computer deals with numbers close to unity. Also, it is not very practical to measure astronomical distances in meters! It is recommendable to use practical units for the input and output. For the numerical evaluation of the equations and formulae it is also practical to scale quantities so that we deal with reasonable numbers. For example, if we measure distances in parsec and the source radius in solar radii, we can express the geometrical dilution factor

$$\frac{\pi R_*^2}{4\pi r^2} = \left(\frac{R_*/R_\odot}{r/1\text{pc}}\right)^2 \times \left(\frac{R_\odot}{4\text{pc}}\right)^2$$

where the last term is but a constant factor. Likewise, in the integral over the frequencies, one may scale the frequencies  $\nu$  to the threshold frequency  $\nu_0$  and thus handling numbers in the order of unity rather than numbers of order  $10^{15}$ . Looking a bit more closely at the expressions, we can identify similar possibilities to scale the terms under the integration to reasonable numbers.

## 3.2 Displaying the Results

The results will usually be plots of any variable, such as the degree of ionization or the ionization ratio  $\xi$ , as a function of time. Make sure that you have the proper time resolution to observe accurately the behaviour, in particular when the lifetime of the ionizing source is much larger than the recombination time!

Also, it is convenient to compare the results with the quantities expected from ionization equilibrium (Equation 9). Sometimes, it is more useful to plot instead of a variable itself the ratio or the difference of the quantity with its equilibrium value.

## 4. Suggested problems

1. Let's first do a few completely theoretical studies: switch on suddenly a star of given ionization numbers in a gas of various densities, how does the ionization evolve and how closely does it follow the instantaneous equilibrium value? Change all parameters over a wide range! The ionization shows an initial delay with respect to the equilibrium value. Which parameter determines this?
2. Consider now what happens after a source is switched off! First, of course, you ionize the gas to its equilibrium value. How much time does it take for the ionization to disappear? Which parameter is responsible?
3. What happens when the star makes a short sharp eruption in ionizing flux, that is when the duration of the radiation is comparable or shorter than the recombination time-scale? How long after this flash does the gas remain ionized? Can you imagine situations where this could be occurring?
4. Since the recombination time is not the time-constant of an exponential behaviour, this time-scale depends on the state of ionization! How long does the remnant ionization last when you consider configurations with partial ionization ( $x \approx 0.5$ )?
5. Compute models for HII regions. Place the test volume at about one half of the Strömgren radius. The lifetime of a massive star is a few million years. In which environments (gas density) would the recombination time be comparable to the life-time of the star, i.e. to the duration of the flash of ionizing radiation?
6. Do models for planetary nebulae. Again, assume a fixed lifetime, and also a fixed density.
7. During its evolution, a planetary nebula expands away from the star — typical expansion speed is 30 km/s — and thus the density in the expanding nebula will decrease, if the total mass of the nebula shell remains constant! Make a simple model: a constant expansion speed gives the nebula radius  $R = v_{exp}t$  and the density of a spherical shell drops so that  $M = (4\pi R^3 mn)/3$  remains constant (with  $m$  the mass of the hydrogen atom). Add this density variation to the differential equation and solve the new problem in a similar way.

8. Use the published evolutionary track of the central star of a planetary nebula (T.Bloecker (1995) A&A 299, 755; on-line catalog available from Vizier, bibliographic code 1995yCat..32990755B, download Table 3 of hydrogen burning models, explanations of the data are in that file; this file contains the tracks of three models with different mass of the central star. 0.605 solar masses would be representative for the average nebula) to get the evolution of temperature and luminosity (hence radius) and compute the number of ionizations (Equation 5) as a function of time, and use this in your code. One could read the published data into a table, and compute for every time the integral of the number of ionizations. These tabulated data are then used to get by linear interpolation the value of  $\mathcal{N}$  for every time the ionization module needs this quantity.
9. There are also giant HII regions, composed of many O stars – have a look at the literature!
10. Novae have outburst and go through a nebular phase ...
11. X-ray sources may also have outbursts ... one may approximate the ionizing spectrum by a power law of the flux  $F_\nu(\nu)$ . What do you expect?
12. Hydrogen is a special case, having only two stages of ionization. If we added also helium to the gas, there are three effects. Firstly, helium has three stages of ionization, so we must consider two more equations: the evolution of neutral helium, and the evolution of singly ionized helium. In the latter

$$\frac{dn_{He+}}{dt} = n_{He0} \frac{\pi R_*^2}{4\pi r^2} \mathcal{N}_0 - n_{He+} \frac{\pi R_*^2}{4\pi r^2} \mathcal{N}_+ - n_e n_{He++} \alpha_{B+}$$

the second term are the ionizations into the doubly ionized state, whose density we denote by  $n_{He++}$ . Moreover, our trick with introducing the variable  $\xi$  would have to be modified ... Secondly, the number of electrons now is determined by hydrogen as well as the two helium ions:

$$n_e = n_{H+} + n_{He+} + 2 * n_{He++}$$

In this way, all ionization equations are coupled, so we have to invent some good method of solution to solve them consistently. And thirdly, the atomic data for helium and ionized helium is different from the one for hydrogen. Thereby the recombination times differ, and hence the intensity ratios of helium and hydrogen lines would behave differently. (ask me for the formulae of those atomic data).

The table below gives the basic parameters of hot main sequence stars which form HII regions, and central stars of planetary nebulae. For each star and density, the Strömgren radius is given, which represents the greatest distance up to which a star can ionize gas. The lifetimes of hot main sequence stars are several million years, while the phase of a planetary nebula is about 30000 years.



Object	Stellar Temperature	Stellar Luminosity	No.Ionizations [1/s]	Density [cm <sup>-3</sup> ]	Strömgren radius [pc]
O5V star	40000	10 <sup>6</sup>	9 10 <sup>7</sup>	1	115
				10	25
				100	5
				1000	1
B0V star	25000	10 <sup>4</sup>	6 10 <sup>6</sup>	1	17
				10	4
				100	0.8
				1000	0.2
young PN	30000	10 <sup>4</sup>	2 10 <sup>7</sup>	10 <sup>4</sup>	0.05
				1000	0.2
old PN	100000	10 <sup>4</sup>	5 10 <sup>9</sup>	1000	0.3
				100	1

## 5. General Remarks, Hints, and Kinks (I know you won't read this!!!)

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.
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 time integration is contained in a separate 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. When adapting the program to a different problem, one merely re-arranges the modules. The main program may then be just a control program to call the subprograms in the particular order, and gets and supplies data from and to each part.
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. Do 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 may formulate, must be reproduced accurately.
4. **Provide Error Messages and Tracing:** Especially during testing, you will print out everything that is useful to judge on what the program does and what decisions it makes. For example, have a print out of the energies and angular momentum of the system. It is recommendable to define one or more variables that can be used to switch on these print-outs. In this way, one can always check every part of the program, even after it has been considered finished. If you later want to try out some modification, and the results are either complete rubbish (because you made some error) or you just want to understand how the solution behaves, this option is very useful. Provide written messages if something goes not normal, e.g. if the automatic stepwidth goes below or above specified values. This become more important as the program grows in size and complexity.
5. **Take Time For Comments:** Don't be lazy with putting comments into the program. Not only for the general description what each subprogram does, what data it needs, and what variables it changes. But also if you change just a line for a test. Often one forgets after a few days about it, and is quite surprised about the results. Save yourself the panic! Plenty of comments are vital, if you find some time later that you might use it for something, but you can't remember about its inner workings. Don't wait for them after "the program is finished". It never happens, or you won't have the time.
6. **Be highly skeptic of anything that the program produces.**

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”.

## 6. Simulations for Comparison

At <http://astro.u-strasbg.fr/~koppen/tioni/> you will find a Java applet which solves this problem for any time dependence of the number of ionizations  $\mathcal{N}$ , whose input is done graphically, as well as for any density and distance from the source. All the variables of the results can be inspected. There are two other applets that might be helpful here:

<http://astro.u-strasbg.fr/~koppen/stroemgren/StroemgrenTwo.html>

computes the basic Strömngren sphere in a uniform medium, and with

<http://astro.u-strasbg.fr/~koppen/stroemgren/Stroemgren.html> one can interpret observational data of HII regions and planetary nebulae.