Astrophysics with the Computer: Propagation of Ionization Fronts in Interstellar Gas

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1 Astrophysics

A hot star is born in an interstellar gas cloud. At first all the gas (hydrogen and helium) is neutral and therefore oprically thick to the ultraviolet ($\lambda < 91$ nm) radiation of the star. Where the radiation hits the gas, a layer will be ionised and hence become optically thin. Thus the stellar photons can penetrate even deeper into the gas. The boundary between neutral and ionised gas (the ionization front) will thus propagate away from the star in to the gas cloud, as long as there is an excess of stellar ionising photons over those which get absorbed by the gas. After about one recombination time scale ($\tau_{\rm rek} = 1/n_e\alpha$, see below) an equilibrium state is reached and the front stops moving. Then we have reached the phase of a stationary Strömgren sphere. Very similar phenomena occur when the central star of a planetary nebula on its evolution from a red giant to a white dwarf turns into a phase of very high temperatures (10^5 K).

We shall consider the following model: A hot star (radius R_*, blackbody spectrum with temperature T_*) is embedded in a very large cloud of gas of hydrogen and helium. The gas density $n = n(\mathrm{H}) + n(\mathrm{He})$ shall be constant everywhere, and the gas shall be at a constant temperature (electron temperature T_e). Therefore the ionization front will be a spherical shell, and the problem can be treated in one dimension, the radial distance from the star. For every instant of time, we shall step radially outward, starting at the stellar surface, and compute the ionization in the gas. The ionization is calculated from the stellar radiation field, whose flux decreases with increasing distance from the star, but which is also attenuated by the remaining fraction of neutral gas. Hereby we have to take into account that the ionization fronts $\mathrm{H}^0/\mathrm{H}^+$, $\mathrm{He}^0/\mathrm{He}^+$, and $\mathrm{He}^+/\mathrm{He}^{++}$ are relatively thin in comparison to the size of the ionized region, and that this will necessitate that the radial step width has to be decreased accordingly. Once the ionization stratification is computed for the entire structure, the procedure is repeated for the next time step ....

With this program we can compute the time evolution of HII regions and planetary nebulae. We can study how the equilibrium configuration of the Strömgren sphere is reached. If we include also helium, we can study the interaction of the ionization fronts.

Please note that this program computes the time evolution of an object by calculating a series of models. Therefore it is quite important that all parts of the program should be built with computational speed in mind.

2 The equations

It is recommendable to start with a version for hydrogen only. The time-dependent ionisation is described by the rate equation for the ionized species:

$$\frac{dn(\mathrm{H}^+)}{dt} = n(\mathrm{H}^0)\Gamma(\mathrm{H}^0) - n(\mathrm{H}^+)n_e\alpha(\mathrm{H}^+) \tag{1}$$

and the conservation of number of hydrogen species

$$n(\mathrm{H}^0) + n(\mathrm{H}^+) = nA(\mathrm{H}) \tag{2}$$

With these quantities

$n(\mathrm{H}^0)$	particle density of neutral atoms
$n(\mathrm{H}^+)$	particle density of protons
n	particle density of the gas
n_e	particle density of electron
$\alpha(\mathrm{H}^+)$	recombination coefficient
$A(\mathrm{H})$	abundance of hydrogen

The rate of photoionizations

$$\Gamma(\mathrm{H}^0) = \int_{\nu(\mathrm{H}^0)}^{\infty} \frac{4\pi J_\nu}{h\nu} a(\mathrm{H}^0) d\nu \tag{3}$$

contains the frequency-dependent photoionization cross section $a(\mathrm{H}^0)$ of the hydrogen atom and the mean intensity of the radiation field at the position under consideration:

$$J_\nu(r) = B_\nu(\nu, T_*)(\frac{R_*}{2r})^2 \exp(-\tau(\nu, r)) \tag{4}$$

at a distance r from the star. The Planck function $B_\nu(\nu, T_*)$ depends on the stellar temperature. The factor $(R_*/2r)^2$ – valid for $r \gg R_*$ – describes the attenuation of the stellar radiation by the geometrical dilution. The third term is the frequency-dependent attenuation of the stellar radiation by the absorption by the gas between the stellar surface and the considered position. The optical depth

$$\tau(\nu, r) = \int_{R_1}^{r} \kappa(\nu, r') dr' \tag{5}$$

is the sum of the absorption between the inner boundary of the nebula (e.g. $R_1 = R_*$) and the distance r. The absorption coefficient

$$\kappa(\nu, r) = \begin{cases} 0 & \text{for } \nu < \nu(\mathrm{H}^0) \\ n(\mathrm{H}^0, r)a(\mathrm{H}^0) & \text{for } \nu \geq \nu(\mathrm{H}^0) \end{cases} \tag{6}$$

Here we consider atomic hydrogen as the only absorber, which absorbs only above the frequency $\nu(\mathrm{H}^0)$ of its ionisation energy of 13.56 eV.

Finally we demand charge neutrality, i.e. all electrons come from the ionization of hydrogen:

$$n_e = n(\mathrm{H}^+) \tag{7}$$

3 How to solve them

3.1 Compute ionization at given position

In principle one could use directly the rate equation to compute the changes of the particle densities during a small time interval Δt:

$$\Delta n(\mathrm{H}^+) = \frac{dn(\mathrm{H}^+)}{dt}\Delta t \tag{8}$$

and

$$\Delta n(\mathrm{H}^0) = -\Delta n(\mathrm{H}^+) \tag{9}$$

The stability of the calculation depends on whether the derivative $dn(\mathrm{H}^+)/dt$ is evaluated at the old or the new time instant.

However, we shall use a different method: If we assume that Γ and $n_e\alpha$ do not change during the time step Δt, we can solve the rate equation analytically: Let us define:

$$x = \frac{n(\mathrm{H}^+)}{n(\mathrm{H}^0)+n(\mathrm{H}^+)} \tag{10}$$

$$y = \frac{n(\mathrm{H}^0)}{n(\mathrm{H}^0)+n(\mathrm{H}^+)} \tag{11}$$

$$\delta = \Gamma(\mathrm{H}^0) + n_e\alpha(\mathrm{H}^+) \tag{12}$$

then you can show (please do this!) that the result is:

$$x(t+\Delta t) = (x(t)-x_0)e^{\delta\Delta t} + x_0 \tag{13}$$

with $x_0 = \Gamma(\mathrm{H}^0)/\delta$ and

$$y(t+\Delta t) = (y(t)-y_0)e^{\delta\Delta t} + y_0 \tag{14}$$

with $y_0 = n_e\alpha(\mathrm{H}^+)/\delta$. This method has the advantage that even at large time step width it will lead towards the equilibrium solution.

Close to the central star the gas is highly ionized, hence $x \approx 1$ and $y \ll 1$; here is is better to compute $y(t+\Delta t)$ from the above formula and then compute $x = 1-y$. When $x \approx 0.1$ one can first compute $x(t+\Delta t)$ and then $y = 1-x$. In this way one uses only one formula and ensures the conservation of particles ($x+y=1$) with machine precision.

For the actual computation one takes $x(t+\Delta t)$ and $y(t+\Delta t)$ as guess values, which are improved by the iteration for charge neutrality:

1. set $n_e = n$
2. solve the ionisation equations
3. get ionic density xn

4. as long as $|xn - n_e|$ is larger than some tolerance (0.00001*n) compute $n_e^{new} = \sqrt{n_e * xn}$ and go back to solve ionisation equations

5. otherwise: done!

The integration over the frequencies for the photoionization rate Γ will be evaluated as the sum over a discrete frequency grid:

$$\int_a^b f(x)dx = \sum_{i=n}^{m} f(x_i)w_i \tag{15}$$

The frequency grid is best a logarithmically equi-spaced grid starting from the ionization frequency $\nu(\mathrm{H}^0)$ to about $10 \times \nu(\mathrm{H}^0)$. Depending on the stellar temperature it may be necessary to use a higher upper frequency limit. The integration weights w_i are computed from the trapezoidal role or Simpson's rule or any suitable method, depending on the required accuracy. Try out! But about 100 frequency points and trapezoidal rule should be sufficient.

For testing and for instruction it is useful at this point to study the evolution of the ionization in a single gas element at some distance r from the star, and to watch the change from the initial neutral state into the equilibrium ionized state. Also, it is interesting to follow the evolution from a fully ionized state when suddenly the stellar radiation is set to zero. What happens? What is the time scale?

3.2 Improving the ionization

When the ionization is known at one position, i.e. at one point of the radial grid, all the other quantities, such as absorption coefficient can be computed.

As we shall see later, it was necessary for the computation of the ionization to estimate the increment of the optical depths (at all frequencies) between the previous radial grid point r_{i-1} and the current one r_i. With the knowledge of the conditions at r_i we can improve this estimation. We compute the optical depths until r_i

$$\tau^{new}(\nu, r_i) = \tau(\nu, r_{i-1}) + \frac{\kappa(\nu, r_i) + \kappa(\nu, r_{i-1})}{2}(r_i - r_{i-1}) \tag{16}$$

where the $\kappa(\nu, r_i)$ are the newly computed opacities.

With these new estimates of the optical depths, we obtain a new estimate for the radiation field, and thus we have to recompute the ionization balance at radius r_i. This iteration will proceed until the values $x(t+\Delta t)$ and $y(t+\Delta t)$ have stabilized enough. It is useful to check the progress and accuracy of this iteration by observing the ratio $\xi = x/y$, and to demand a tolerance of about $10^{-3}..10^{-5}$.

3.3 Proceeding to the next radial point

When the ionization at radius r_i has been found, we now have to prepare for the computation of the ionization at the next grid point r_{i+1}: For this purpose we shall make use of the fact that from the stellar surface outwards the optical depth τ at the ionization threshold $\nu(\mathrm{H}^0)$ steadily increases. Within the ionization front it increases rapidly from small values (0.01) to very large ones (> 100). We determine the next radius by demanding that the increment in optical depth shall remain sufficiently small, so that we achieve a sufficient accuracy for the overall model. It is recommended that the criterion for the acceptable growth in optical depth is linked to the optical depth, for example

$\tau < 0.01$	$\delta = \tau_{i+1}/\tau_i = 4$
$0.01 < \tau < 1$	$\delta = 1.5$
$1 < \tau < 100$	$\delta = 1.1$
$100 < \tau$	stop computation because neutral zone reached

The ranges for τ and the increment factors δ are best found by experimentation.

The radius of the next grid point is obtained by linear extrapolation:

$$(r_{i+1} - r_i) = (r_i - r_{i-1}) \frac{\log(\delta)}{\log(\tau_i/\tau_{i-1})} \tag{17}$$

Next, the opacities for the next radius are estimated:

$$\kappa^{est}(\nu, r_{i+1}) = \kappa(\nu, r_i) + \frac{\kappa(\nu, r_i) - \kappa(\nu, r_{i-1})}{r_i - r_{i-1}} (r_{i+1} - r_i) \tag{18}$$

as well as the optical depths

$$\tau^{est}(\nu, r_{i+1}) = \tau(\nu, r_i) + \frac{\kappa(\nu, r_i) + \kappa^{est}(\nu, r_{i+1})}{2} (r_{i+1} - r_i) \tag{19}$$

With these estimates the expected radiation field at the next radius is computed, and the afore described iteration for the ionization is executed.

3.4 Overall procedure

In this manner the ionization stratification is computed beginning at the stellar surface (or the inner boundary of the nebula) until the optical depth becomes large (e.g. 100) at the ionization threshold.

For the next time instant, an entirely new model is computed. It is important to keep in mind that at every time the radial grid is completely reconstructed. This means that the degrees of ionization at the previous time step are on a different radial grid, and must be interpolated onto the current radial grid. For simplicity this is done by linear interpolation.

3.5 The first radial point

For the first grid point we have to use special treatments:

- the distance to the next radial point is best chosen as the mean free path of the photons in neutral gas: $r_2 - r_1 = 1/(n * a(\mathrm{H}^0, \nu(\mathrm{H}^0)))$
- since there is no gas between the stellar surface and the inner boundary of the nebula, we do not need to improve the optical depths and the ionization at the first radius
- the estimate for the opacity is $\kappa^{est}(\nu, r_2) = \kappa(\nu, r_1)$
- the estimate for the optical depth: $\tau^{est}(\nu, r_2) = \tau(\nu, r_1) + \kappa(\nu, r_1)(r_2 - r_1)$

4 Further comments

- at every time step the run through the ionized portion is computed up to the radius where the ionization has dropped to about $x = 10^{-4}$ or the optical depth exceeds a large value, e.g. 100
- since we have to compute a series of models, with each running through a radial grid, it is best to store for each time step the model in a separate file. The data can be displayed by reading the models for various instants of time. Also, it is then possible to read a model and continue its evolution, for instance with a different time step ... or simply to split a long evolution in several parts
- to make the program run faster, it is recommended
  - do not recompute quantities that you use several times. Store them in a variable!
  - quantities that do not change in a loop, should be taken outside
  - multiplication may be faster than division – depends on the compiler
  - depending on the compiler, it may be faster to compute A+A than 2*A, A*A instead of A**2, A**2 instead of A**2.0, SQRT(A*A*A) instead of A**(3/2) ...
  - functions like exp, log, sin, cos, ... take time
  - loops can be time-eaters
  - try to accelerate iterations by careful testing and using appropriate improving measures
  - avoid unnecessary operations: A=B+C costs time, even when B=C=0 for a part of the loop. Run the loop only over parts which contribute to the result.
  - iterations have the nasty habit of disappearing into an endless loop. Observe carefully the convergence behaviour (monotonic, oscillating, divergence, ...) before you trust the routine to do any work. When running, break off if the required tolerance is not reached after a certain number of iteration steps ...

4.1 The time step

The choice of the time step will be a compromise between accuracy (better with smaller time step) and computing time (shorter with larger time step). The method of solution of the ionization equation will be stable also at larger step widths. The evolution of an HII region reaches the equilibrium within the recombination time scale ($t_{\rm rek} \approx 1/(n_e \alpha(\mathrm{H}^+)$. With $\Delta t = 0.01 t_{\rm rek}$ one reaches this state with some 100 time steps. If the program took 1 s per model, the entire evolution would be done in a few minutes. Thus, one could decrease the time step in the hope to get more accurate results by running the program a couple of hours or overnight!

As mentioned above, storage of models from different times as files allows to use a file as a start model for a subsequent evolution. This makes it also possible to use different time steps for different phases of the evolution.

4.2 Atomic Data

- Frequency of ionization threshold [Hz]
  $\nu(\mathrm{H}^0) = 3.2879\,10^{15}$
- Photoionization cross section[m^2]
  $a(\mathrm{H}^0, \nu) = 6.3\,10^{-22}(\nu(\mathrm{H}^0)/\nu)^3$ for $\nu \geq \nu(\mathrm{H}^0)$
- Recombination coefficient [$\mathrm{m}^3\mathrm{s}^{-1}$]
  $\alpha(\mathrm{H}^+) = 5.197\,10^{-20}\sqrt{x}(0.4288 + 0.5\ln x + 0.469 x^{-1/3})$ with $x = h\nu(\mathrm{H}^0)/kT_e$
- Electron temperature $T_e = 10000$ K is a good approximation

4.3 Global Tests

The convenient analytical method of solution for the ionisation equation makes it possible to use rather large time steps. Therefore one should expect that for a time step larger than the recombination time scale one would obtain the stationary Strömgren sphere. In this configuration the number of ionizing photons emitted per second by the central star is equal to the total rate of recombinations in the ionized region:

$$4\pi R_*^2 \int_{\nu(\mathrm{H}^0)}^{\infty} \frac{\pi B(\nu, T_*)}{h\nu} d\nu = \int n(\mathrm{H}^+) n_e \alpha(\mathrm{H}^+) dVol \tag{20}$$

The outer radius of the ionized region is called the Strömgren radius R_S.

The time evolution of an HII region can roughly be represented by the volume $V(t)$ taken up by the ionized gas approaching the volume of the Strömgren sphere $4\pi R_S^3/3$ like

$$V(t) = \frac{4\pi}{3} R_S^3 (1 - \exp(-n\alpha t)) \tag{21}$$

This means that after one recombination time scale ($1/n\alpha$) about 62 percent of the final volume is reached. As one can show by differentiation, the speed of the ionization front

is of the order of

$$v \approx \frac{1}{n}(\frac{R_*}{r})^2 \int_{\nu(\mathrm{H}^0)}^{\infty} \frac{\pi B_\nu(\nu, T_*)}{h\nu} d\nu \tag{22}$$

hence it decreases with distance from the central star.

5 Extension: Helium

Once the program works for a nebula of pure hydrogen gas, it is not too difficult to add helium. The following needs to be done:

The frequency grid has to be modified to account for the ionization thresholds $\nu(\mathrm{He}^0)$ and $\nu(\mathrm{He}^+)$. In order that the integration takes care of the threshold structure, the frequency points closest to the helium frequencies are shifted to these values. Also, the point just below these points are shifted to a value close to the threshold, e.g. $0.999 * \nu(\mathrm{He}^0)$. It is best to keep the indices for the threshold frequencies, so that the integration routine can start at these indices.

Since helium has three stages of ionization, there are two ionization equations. The analytical approach is similar: With the photoionization integrals

$$\Gamma(\mathrm{He}^0) = \int_{\nu(\mathrm{He}^0)}^{\infty} \frac{4\pi J_\nu}{h\nu} a(\mathrm{He}^0) d\nu \tag{23}$$

$$\Gamma(\mathrm{He}^+) = \int_{\nu(\mathrm{He}^+)}^{\infty} \frac{4\pi J_\nu}{h\nu} a(\mathrm{He}^+) d\nu \tag{24}$$

the definitions

$$x(\mathrm{He}^+) = \frac{n(\mathrm{He}^+)}{n(\mathrm{He}^0) + n(\mathrm{He}^+) + n(\mathrm{He}^{++})} \tag{25}$$

$$x(\mathrm{He}^{++}) = \frac{n(\mathrm{He}^{++})}{n(\mathrm{He}^0) + n(\mathrm{He}^+) + n(\mathrm{He}^{++})} \tag{26}$$

and the abbreviations

$$\delta_{\mathrm{He}} = \frac{1}{2}(\delta_0 + \delta_1) + \sqrt{(\delta_0 - \delta_1)^2 + n_e \alpha(\mathrm{He}^{++}) \Gamma(\mathrm{He}^+)} \tag{27}$$

$$\delta_0 = \Gamma(\mathrm{He}^0) + n_e \alpha(\mathrm{He}^+) \tag{28}$$

$$\delta_1 = \Gamma(\mathrm{He}^+) + n_e \alpha(\mathrm{He}^{++}) \tag{29}$$

$$\omega = (\Gamma(\mathrm{He}^0) + \Gamma(\mathrm{He}^+))/(n_e \alpha(\mathrm{He}^{++})) \tag{30}$$

$$x_0 = \Gamma(\mathrm{He}^0)/(\delta_0 + \omega) \tag{31}$$

$$y_0 = \omega/(\delta_0 + \omega) \tag{32}$$

one gets

$$x(\mathrm{He}^+, t + \Delta t) = (x(\mathrm{He}^+, t) - x_0) e^{\delta_{\mathrm{He}} \Delta t} + x_0 \tag{33}$$

$$x(\mathrm{He}^{++}, t + \Delta t) = (x(\mathrm{He}^{++}, t) - y_0) e^{\delta_{\mathrm{He}} \Delta t} + y_0 \tag{34}$$

For the iteration to find the electron density one now has to include the contributions from helium:

$$n_{\rm ion} = n({\rm H}^+) + n({\rm He}^+) + 2n({\rm He}^{++}) \tag{35}$$

The local absorption coefficient also includes contributions from helium:

$$\kappa(\nu) = \begin{cases} 0 & \text{for } \nu < \nu({\rm H}^0) \\ n({\rm H}^0)a({\rm H}^0) & \text{for } \nu({\rm H}^0 \geq \nu < \nu({\rm He}^0) \\ n({\rm H}^0)a({\rm H}^0) + n({\rm He}^0)a({\rm He}^0) & \text{for } \nu({\rm He}^0 \geq \nu < \nu({\rm He}^+) \\ n({\rm H}^0)a({\rm H}^0) + n({\rm He}^0)a({\rm He}^0) + n({\rm He}^+)a({\rm He}^+) & \text{for } \nu({\rm He}^+ \geq \nu \end{cases} \tag{36}$$

In the automatic control of the radial step width one has to deal with the ionizations fronts $\rm He^0/He^+$ and $\rm He^+/He^{++}$ in a similar way as with $\rm H^0/H^+$. We can use the fact that the ionization decreases outwards: at radii which the $\rm He^0/He^+$ has not reached yet ($\tau(\nu({\rm He}^0)) > 100$), the $\rm He^+/He^{++}$ front need not to be considered!

5.1 Atomic Data

- Frequency of ionization thresholds [Hz]
  $\nu({\rm He}^0) = 5.9451\,10^{15}$
  $\nu({\rm He}^+) = 1.3158\,10^{16}$

- Photoionization cross sections [$\rm m^2$]
  $a({\rm He}^0, \nu) = 7.83\,10^{-22}(\frac{\nu({\rm He}^0)}{\nu})^2(1.66 - 0.66\frac{\nu({\rm He}^0)}{\nu})$ for $\nu \geq \nu({\rm H}^0)$
  $a({\rm He}^+, \nu) = 1.5\,10^{-22}(\frac{\nu({\rm He}^0)}{\nu})^3$ for $\nu \geq \nu({\rm H}^0)$

- Recombination coefficients [$\rm m^3 s^{-1}$]
  $\alpha({\rm He}^+) = 4.3\,10^{-19}(T_e/10^4{\rm K})^{-0.672}$
  $\alpha({\rm He}^{++}) = 1.04\,10^{-19}\sqrt{x}(0.4288 + 0.5\ln x + 0.469x^{-1/3})$ with $x = h\nu({\rm He}^+)/kT_e$

6 Literature

- D.E.Osterbrock, *Astrophysics of Gaseous Nebulae*, Freeman, 1974