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Solution of the Saha equation from ionization fraction and temperature histories for astrophysical reionization models

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SUMMARY – The accurate understanding of the ionization history of the universe plays a fundamental role in the modern cosmology. A significant complication in the physical treatment of this process comes out when from a simplistic approximation of a plasma of pure protons and electrons one has to model the complexity of the mixture of elements produced by cosmological nucleosynthesis. On the other hand, for many cosmological applications, considering a mixture of hydrogen, H, and helium, He, represents an accurate enough approximation, since before stellar nucleosynthesis the fraction of the other elements is very small. We provide here explicit formulas to derive, on the basis of the Saha equation and given the evolution of the free electron fraction, χ_e, and of the electron temperature, T, the evolution of the repartition of H and He in their ionization states.

1 Introduction

The accurate understanding of the ionization history of the universe plays a fundamental role in the modern cosmology. The classical theory of hydrogen recombination for pure baryonic cosmological models [2, 8] has been subsequently extended to non-baryonic dark matter models [7, 1, 5] and recently accurately updated to include also helium recombination in the current cosmological scenario (see [6] and references therein). Various models of the subsequent universe ionization history have been considered to take into account additional sources of photon and energy production, possibly associated to the early stages of structure and star formation, able to significantly increase the free electron fraction, χ_e, above the residual fraction ($\sim 10^{-3}$) after the standard recombination epoch at the redshift $z_{\rm rec} \simeq 10^3$.

A significant complication in the physical treatment of this process comes out when from a simplistic approximation of a plasma of pure protons and electrons one has to model the complexity of the mixture of elements produce by cosmological nucleosynthesis. On the other hand, for many cosmological applications, considering a mixture of hydrogen, H, and helium, He, represents an accurate enough approximation, since before stellar nucleosynthesis the fraction of the other elements is very small.

Many reionization models published in the literature provide only the evolution of the free electron fraction, χ_e, and, optionally, of the electron temperature, T, but not the repartition of these elements in their possible ionization states. For many applications, e.g. the computation of cosmic microwave background (CMB) anisotropy angular power spectrum, the knowledge of the evolution of χ_e is what one needs. On the other hand, for other applications, e.g. the computation of CMB spectral distortions, one needs to know the evolution of T and also of he repartition of H and He in their ionization states, since, for instance, the bremsstrahlung process [4] depends on them and not only on the free electron density and matter temperature.

The goal of this report is to provide explicit formulas to derive, on the basis of the Saha equation and given the evolution of χ_e and T, the evolution of the repartition of H and He in their ionization states jointly considering these elements, since their overall contribution to χ_e.

2 Ionization history and Saha equation

The electron ionization fraction, χ_e, describes the time variation of the number of free electrons compared to the total ones. We assume here the following definition

$$\chi_e = \frac{n_e^{free}}{n_e^{tot}} \,. \tag{1}$$

Note that in the literature it is common to find also χ_e normalized to the H number density. Obviously, it is simple to switch between these two conventions (by definition, in the convention adopted here $\chi_e \leq 1$, while in the other one full ionization is characterized by a χ_e value slightly larger than 1).

For a mixture of H and He, if we denote with f_H the mass fraction of primordial H, we can derive the total number density of electrons, such as

$$n_e^{tot} = \frac{1+f_H}{2}\frac{\rho_b}{m_b} \,, \tag{2}$$

where ρ_b is the baryon density and m_b the baryon mean mass. Given χ_e from a specified reionization history, the number density of free electrons is a known quantity at each redshift.

For an accurate analysis of an ionization history is important to take into account the ionization fraction of both H and He.

The process of reionization can be studied on the basis of the Saha equation that describes the ratio between two different ionization states of an element. Known the free electron number density and the temperature, we can write

$$\frac{n_{i+1}n_e}{n_i} = \frac{2}{\Lambda^3}\frac{g_{i+1}}{g_i}e^{-\frac{\epsilon_{i+1}-\epsilon_i}{k_B T}}\,, \tag{3}$$

where n_i is the density of atoms in the $i-th$ state of ionization, n_e the electron density, g_i the degeneracy of states for the $i-$ions, ϵ_i the energy required to remove i electrons from a neutral atom, and Λ the thermal de Broglie wavelength of an electron, defined by

$$\Lambda = \sqrt{\frac{h^2}{2\pi m_e k_B T}}\,. \tag{4}$$

The unknowns $\chi_H, \chi_{H^+}, \chi_{He}, \chi_{He^+}, \chi_{He^{++}}$, defined as the relative abundances of the different ionization states of each element with respect to the global number density of the element, can now be computed from this set of equation, separately for all species.

From the nuclei conservation law for H and He we also know that

$$n_H^{tot} = \frac{\rho_b}{m_b}\left[f_H\left(\chi_H + \chi_{H^+}\right)\right] \tag{5}$$

$$n_{He}^{tot} = \frac{\rho_b}{m_b}\left[\frac{1-f_H}{4}\left(\chi_{He} + \chi_{He^+} + \chi_{He^{++}}\right)\right]\,, \tag{6}$$

where the sum of the ionization fraction of each specie is equal to unity.

In the next section, the fundamental steps to provide these quantities will be provided.

3 Solutions

3.1 Hydrogen Ionization fraction

In the case of H, taking into account the Saha equation and the charge conservation law, the system to be solved is

$$\begin{cases} \chi_H + \chi_{H^+} = 1 \\ \\ \chi_{H^+} = \frac{2}{1+f_H}\frac{m_b}{\rho_b}\frac{\chi_H}{\chi_e}\frac{1}{\Lambda^3}e^{-\frac{\epsilon_{H^+}-\epsilon_H}{k_B T}}\,, \end{cases} \tag{7}$$

since, for this specie

$$2\frac{g_{H^+}}{g_H} = 1\,. \tag{8}$$

Defining

$$\begin{cases} \Delta\epsilon_H = \epsilon_{H^+} - \epsilon_H \\ \\ C_1 = \frac{2}{1+f_H}\frac{m_b}{\rho_b}\frac{1}{\chi_e\Lambda^3}e^{-\frac{\Delta\epsilon_H}{k_B T}}\,, \end{cases} \tag{9}$$

we can derive the simple solution

$$\begin{cases} \chi_H = \frac{1}{1+C_1} \\ \\ \chi_{H^+} = \frac{C_1}{1+C_1} \, . \end{cases} \tag{10}$$

3.2 Helium Ionization fraction

When counting for He, we have to consider its double ionization. Thus, the system has one more equation

$$\begin{cases} \chi_{He} + \chi_{He^+} + \chi_{He^{++}} = 1 \\ \\ \chi_{He^+} = \frac{8}{1+f_H} \frac{m_b}{\rho_b} \frac{\chi_{He}}{\chi_e} \frac{1}{\Lambda^3} e^{-\frac{\epsilon_{He^+} - \epsilon_{He}}{k_B T}} \\ \\ \chi_{He^{++}} = \frac{2}{1+f_H} \frac{m_b}{\rho_b} \frac{\chi_{He^+}}{\chi_e} \frac{1}{\Lambda^3} e^{-\frac{\epsilon_{He^{++}} - \epsilon_{He^+}}{k_B T}} \, , \end{cases} \tag{11}$$

since, for this specie

$$\begin{cases} 2 \frac{g_{He^+}}{g_{He}} = 4 \\ \\ 2 \frac{g_{He^{++}}}{g_{He^+}} = 1 \, . \end{cases} \tag{12}$$

Defining

$$\begin{cases} \Delta\epsilon_{He} = \epsilon_{He^+} - \epsilon_{He} \\ \\ \Delta\epsilon_{He^+} = \epsilon_{He^{++}} - \epsilon_{He^+} \\ \\ C_2 = \frac{8}{1+f_H} \frac{m_b}{\rho_b} \frac{1}{\chi_e \Lambda^3} e^{-\frac{\Delta\epsilon_{He^+}}{k_B T}} \\ \\ C_3 = \frac{2}{1+f_H} \frac{m_b}{\rho_b} \frac{1}{\chi_e \Lambda^3} e^{-\frac{\Delta\epsilon_{He}}{k_B T}} \, , \end{cases} \tag{13}$$

we derive the solution for the Helium

$$\begin{cases} \chi_{He} = \frac{1}{1+C_2+C_2C_3} \\ \\ \chi_{He^+} = \frac{C_2}{1+C_2+C_2C_3} \\ \\ \chi_{He^{++}} = \frac{C_2C_3}{1+C_2+C_2C_3} \, . \end{cases} \tag{14}$$

4 Conclusion

We have presented simple, explicit formulas to derive, on the basis of the Saha equation and given the evolution of χ_e and T, the evolution of the repartition of H and He in their ionization states jointly considering these elements, since their overall contribution to χ_e.

This is useful for several cosmological applications, such as the computation of CMB spectral distortions through accurate numerical codes able to solve the complete Kompaneets equation in cosmological context (Procopio & Burigana 2009). In particular, we plan to apply this formalism to the precise computation of late CMB spectral distortions associated to the cosmological reionization process.

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