Evolution of primordial $H_2$ for different cosmological models †

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Primordial chemistry began in the recombination epoch when the adiabatic expansion caused the temperature of the radiation to fall below 4000 K. The chemistry of the early Universe involves the elements hydrogen, its isotope deuterium, helium with its isotopic forms and lithium. In this talk I will present results on the evolution of the primordial $H_2$ abundance for different cosmological models and the influence on the thermal decoupling.

1. Introduction

At early times the Universe was filled up with an extremely dense and hot gas. Due to the expansion it cooled below the binding energies of hydrogen, deuterium, helium, lithium, and thus one can expect the formation of these nuclei. As soon as neutrons and protons leave the equilibrium, the formation of deuterium followed by fast reactions lead finally to the formation of tritium and helium. Thus deuterium is the first stone of the nucleosynthesis but also the passage obligé for heavier elements such as lithium, beryllium and boron. The basic conclusions of the big bang nucleosynthesis on the baryon density $\Omega_\rho$ are

$$0.01 < \Omega_\rho h^2 < 0.025$$

(1.1)

See Sarkar (1996), Olive (1999) and references in Signore & Puy (1999).

2. Post-recombination chemistry

The study of chemistry in the post recombination epoch has grown considerably in recent years. From the pioneer works of Šaslaw & Zipoy (1967), Shechkinov & Enté (1983), Lepp & Shull (1987), Dalgarno & Lepp (1987) and Black (1988), many authors have developed studies of primordial chemistry in different contexts. Latter & Black (1991), Puy et al. (1993), Stancil et al. (1996) for the chemical network and the thermal balance, Palla, Galli & Silk (1995), Puy & Signore (1996, 1997, 1998a, 1998b), Abel et al. (1997) and Galli & Palla (1998) for the study of the initial conditions of the formation of the first objects.

2.1. History

From the recombination phase, the electron density decreases which leads to the decoupling between temperature of the matter and temperature of radiation. Chemistry of the early Universe (i.e. $z < 2000$) is the gaseous chemistry of the hydrogen, helium, lithium and electrons species. The efficiencies of the molecular formation processes is controlled by collisions, matter temperature and temperature of the cosmic microwave background radiation (CMBR). In the cosmological context we have metal-free gas, and thus the formation of $H_2$ is not similar to the formation in the interstellar medium by adsorption on the surface of the interstellar grains.

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The chemical composition of the primordial gas consists of a mixture of: $H$, $H^+$, $H^-$, $D$, $D^+$, $He$, $He^+$, $He^{e2+}$, $Li$, $Li^+$, $Li^-$, $H_2$, $H_2^+$, $HD$, $HD^+$, $HeH^+$, $LiH$, $LiH^+$, $H_3^+$, $H_2D^+$, $e^-$, and $\gamma$ which leads to 90 reactions in the chemical network.

It is more convenient to reduce the reactions to only those that are essential to accurately model the chemistry and to reduce computer times. We adopt the concept of minimal model developed by Abel et al. (1997), and focus on the formation of molecular hydrogen. This way we can reduce the chemical network to 20 reactions.

From Saslaw & Zipoy (1967), and Shchekinov & Entéł (1983) we know that the formation of primordial molecular hydrogen is due to the two main reactions:

\[
H^- + H \rightarrow H_2 + e^-
\]  
\[
H_2^+ + H \rightarrow H_2 + H^+.
\]

These reactions are coupled with the photo-reactions, the associative, recombination and charge exchange reactions (Puy et al. 1993, and Galli & Palla 1998).

### 2.2. Equations of evolution

We consider here the chemical and thermal evolution in the framework of the Friedmann cosmological models. The relation between the time $t$ and the redshift $z$ is given by:

\[
\frac{dz}{dt} = -H_o(1+z) \sqrt{1+\Omega_o z}
\]  

where $H_o$ is the Hubble constant and $\Omega_o$ the parameter of density of the Universe (open Universe $\Omega_o < 1$, flat Universe $\Omega_o = 1$ and closed Universe for $\Omega_o > 1$). The expansion is characterized by the adiabatic cooling:

\[
\Lambda_{ad} = 3nkT_m H_o(1+z) \sqrt{1+\Omega_o z},
\]

with the density of matter $n$ and the temperature of matter $T_m$. The evolution of the matter density is given by:

\[
\frac{dn}{dt} = -3nH_o(1+z) \sqrt{1+\Omega_o z}.
\]

and for temperature of radiation:

\[
\frac{dT_m}{dt} = \frac{2}{3nk} \left[ -\Lambda_{ad} + \Gamma_{compt} + \Psi_{molec} \right],
\]

where $\Gamma_{compt}$ is the Compton scattering of CMBR photons on electrons. Below 4000 K only the rotational levels of $H_2$ can be excited (quadrupolar transitions). In the cosmological context Puy et al. (1993) have shown that the molecules heat the medium (due to the interactions between primordial molecules and the CMBR photons). The thermal molecular function $\Psi_{molec}$ (heating minus cooling) is positive in this context.

All these equations are coupled with the set of chemical equations in order to calculate the evolution of the abundance of $H_2$.

### 2.3. Evolution of molecular hydrogen

We consider three sets of parameter for $\Omega_o$ which characterize the three particular Universe (open with $\Omega = 0.1$, flat with $\Omega_o = 1$ and closed with $\Omega_o = 2$). Moreover we consider two values for the baryonic fraction, the lower value obtained with the primordial nucleosynthesis $\Omega_\rho = 0.02$, and the other which characterizes a full baryonic Universe $\Omega_\rho = 1$.

In Fig. 1, we have plotted the different curves for the evolution of $H_2$. We see the classical two steps of $H_2$ formation (the first step correspond to the $H_2^+$ channel and
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Primordial Molecular Hydrogen

Figure 1. Evolution of the post-recombination abundance of primordial hydrogen for different cosmological models ($\Omega_\text{b}$ is the parameter of geometry and $\Omega_\rho$ the baryonic fraction. The upper curves correspond to the lower baryonic fraction ($\Omega_\rho = 0.02$), and vice versa, the lower curves correspond to the higher baryonic fraction ($\Omega_\rho = 1$).

the second one to the $H^-$ channel). After this transient growth $H_2$ abundance becomes constant.

3. Cosmological thermal decoupling

In Fig. 2, we have plotted the ratio between $T_{\text{molec}}$, which is the temperature of matter with primordial molecules and $T_{\text{compt}}$, the temperature of matter without molecules (we consider in this context only the Compton heating). The ratio is close to unity for the lower value of baryonic fraction and close to 2.5 for the higher value. For $\Omega_b > 0.02$, we can expected that $T_{\text{molec}} \sim 1.25 \times T_{\text{compt}}$.

4. Outlook

The change of temperature, due to $H_2$, on the thermal decoupling could play a role during the transition between the linear regime and the non-linear regime (the turn-around point of gravitation collapse), (Puy & Signore 1996, Signore & Puy 1999). The temperature at the turn-around point is given by

$$T_{\text{turn}} \sim \left(\frac{3\pi}{4}\right)^{4/3} T_{\text{compt}}$$

where $T_{\text{compt}}$ is the temperature of matter without the influence of molecules (Padmanabhan 1993). Taking into account the influence of the molecules, the temperature is 25 per cent more important than $T_{\text{compt}}$. Thus molecules could give other initial conditions for the dynamics of the gravitational collapse than ones predicted by the classical theory.

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**Figure 2.** Evolution of the thermal decoupling for different cosmological models (\( \Omega_\text{\scriptsize o} \) is the parameter of geometry and \( \Omega_\text{\scriptsize \rho} \) the baryonic fraction).

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