Cosmological thermal decoupling and primordial molecules

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COSMOLOGICAL THERMAL DECOUPLING AND PRIMORDIAL MOLECULES

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Primordial chemistry began, in the recombination epoch, when the adiabatic expansion caused the temperature of the radiation to fall below 4000K. The chemistry of the early Universe involves the elements hydrogen, its isotope deuterium, helium with its isotopic forms and lithium. In this contribution I will discuss the influence of the primordial molecules on the cosmological decoupling.

In the framework of the gravitational instability theory, each protostructure started as a tiny local overdensity. As long as these inhomogeneities are small, their evolution can be studied by the classical linear perturbation theory. Once the deviations become large, the linear theory is no more valid. We present the role played by these molecules on the transition between the linear regime and the non-linear regime, and show that the molecules can lead to a thermal change at the turn-around point between these two regimes.

KEY WORDS Cosmology, cosmological decoupling, primordial molecules

1 INTRODUCTION

At early times the Universe was filled with an extremely dense and hot gas. Due to the expansion it cooled below the binding energies of hydrogen, deuterium, helium, lithium which led to the formation of these nuclei (Sarkar, 1996). After this nucleosynthesis period the recombination process is not instantaneous because the electrons, captured into different atomic energy levels, could not cascade instantaneously down to the ground state. Atoms reached the ground state either through the cosmological redshifting of the Lyman α line photons or by the 2s–1s two photon process. Nevertheless the Universe expanded and cooled faster than the recombination could be completed, and small fraction of free electrons and protons remained.

The principles of calculations of the primordial recombination were mentioned initially by Shklovskii (1967), Novikov and Zel’dovich (1967). Peebles (1968) was the first to present a theory in which the very complicated recombination process is
reduced to simpler terms (see Puy and Signore, 2000 for the historical description and references therein).

At the end of the recombination period, it is plausible to imagine that molecules could be formed. The temperature of matter and radiation as well as the density were not so high and we have possible collisional reactions between the species. However, in this cosmological context we have a metal-free gas which does not allow the efficient reaction of adsorption onto the surface of grains.

The literature on the chemistry in the post-recombination epoch has grown considerably in recent years. Many authors have developed studies of primordial chemistry in different contexts. For example Lepp and Shull (1984), Latter and Black (1991), Puy et al. (1993), Stancil et al. (1996), Galli and Palla (1998) for the chemical network; Palla, Galli and Silk (1995), Puy and Signore (1996, 1997, 1998a, 1998b), Abel et al. (1997) and Galli and Palla (1998) in the context of the...
Table 1. Initial abundances given by the standard nucleosynthesis (see Sarkar 1996).

<table>
<thead>
<tr>
<th>Helium: He/H</th>
<th>Deuterium: D/H</th>
<th>Lithium Li/H</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sim 8 \times 10^{-2}$</td>
<td>$\sim 4.3 \times 10^{-5}$</td>
<td>$\sim 2.4 \times 10^{-10}$</td>
</tr>
</tbody>
</table>

Table 2. Abundances of primordial molecules at $z = 5$.

<table>
<thead>
<tr>
<th>$e^-/H$</th>
<th>$H_2/H$</th>
<th>$HD/H$</th>
<th>$LiH/H$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sim 3 \times 10^{-4}$</td>
<td>$\sim 10^{-6}$</td>
<td>$1.2 \times 10^{-9}$</td>
<td>$\sim 7 \times 10^{-20}$</td>
</tr>
</tbody>
</table>

happens at $T = T_{\text{dec}} \sim 0.26$ eV where $T_{\text{dec}}$ is the temperature of the matter corresponding to the redshift $z_{\text{dec}} \sim 1100$. After the recombination, although the density-decrease acts against molecular formation, it turns out that the temperature is small enough for this formation to occur.

The primordial gas consists of electrons, protons, hydrogen ($H, H^-, H^+_3, H^+_2, H_2^-$), deuterium ($D, D^+, HD, HD^+, D^+_2$), helium ($He, He^+, He^{++}, He^+_2$), and...
the radiative de-excitation is faster than collisional (because the excitations have the opposite ordering), the full cooling and heating processes must be evaluated. The molecular thermal function $\Psi_{\text{molec}}$, characterized by the two processes (molecular heating and cooling), is defined by:

$$\Psi_{\text{molec}} = \sum_k [\Psi_k],$$  \hspace{1cm} (1)

where the index $k$ is defined for each molecule ($H_2$, HD or LiH) and $\Psi_k$ is the molecular thermal function for the molecule $k$ defined by:

$$\Psi_k = \sum_j n_j \sum_i n_i (B_{ij} u_{ij} P_{ij}^c - n_x C_{ij}^\pi P_{ij}^r) \epsilon_{ij} \text{ in erg cm}^{-3} \text{ s}^{-1},$$  \hspace{1cm} (2)

where $n_j$ and $n_i$ are respectively the population of the rotational level $j$ and $i$. $C_{ij}^\pi$ is the rate of collision with the species $z$ (with density $n_x$), $B_{ij}$ the second Einstein coefficient, $u_{ij}$ the radiative density of cosmic microwave background radiation at the energy $\epsilon_{ij}$, which corresponds to the transition between the levels $i$ and $j$; $P_{ij}^c$ and $P_{ij}^r$ define respectively the probability of collisional de-excitation and the probability of radiative de-excitation (here we consider 10 rotational levels for each molecule). The first term of Eq. (2) corresponds to molecular heating when the second term corresponds to molecular cooling.

### COSMOLOGICAL THERMAL DECOUPLING

The evolution of the energy density $\rho_{\text{gas}}$ of a homogeneous gas is described by the equation:

$$\frac{d\rho_{\text{gas}}}{dt} = -nkT, \hspace{1cm} (3)$$

where $k$ is the Boltzmann constant, $n$ the matter density, $T_m$ the temperature of matter and $Q$ the external energy density which depends on the molecular thermal function $\Psi_{\text{molec}}$ and on the net transfer of energy $r_{\text{compt}}$ from the cosmic background radiation to the gas via Compton scattering of cosmic background photons on electrons. Thus we have:

$$r_{\text{compt}} = 4\pi a T^4 n_e (T, T_m),$$  \hspace{1cm} (5)
\[ \sigma_T \] is the Thomson cross-section, \( a_{bb} \) is the black body constant, \( c \) the speed of light, \( m_e \) the mass of an electron and \( n_e \) the electronic density. \( T_r \) is the temperature of the radiation. Thus Eq. (3) leads to the evolution of matter temperature \( T_m \):

\[
\frac{3}{2} n k \frac{dT_m}{dt} = -\Lambda_{ad} + \Gamma_{\text{compt}} + \Psi_{\text{molec}},
\]

(6)

where \( \Lambda_{ad} \) defines the adiabatic cooling due to the expansion of the Universe:

\[
\Lambda_{ad} = 3nkT_mH_0(1+z)^{3/2},
\]

(7)

\( H_o \) is the Hubble constant (hereafter \( H_o = 67 \text{ km s}^{-1} \text{ Mpc}^{-1} \)) and \( z \) the redshift. We have neglected the chemical heating and cooling due to the enthalpy of reactions (see Puy et al., 1993).

We adopt the standard cosmological model with zero cosmological constant (Einstein–De Sitter Universe). Thus the matter temperature \( T_m \) and the radiation temperature \( T_r \) remained the same until a redshift of about 1100, the beginning of the recombination era, after which Compton scattering was no longer able to overcome the cooling by expansion and \( T_m \) fell below \( T_r \). In this context the adiabatic cooling becomes dominant.

In Figure 1 Compton heating and the thermal molecular function (in units of adiabatic cooling) are compared. The thermal molecular function, which is mainly a molecular heating, dominates the Compton heating when \( z < 180 \). This fact should be important for the evolution of the matter after this redshift, particularly for the collapse of the first objects.
4 TURN-AROUND PERIOD AND PROTO-COLLAPSE

We assume that, at some time in the past, there were small deviations from homogeneity in our Universe. These deviations could grow due to gravitational instability. As long as these inhomogeneities are small, their evolution can be studied by the classical linear perturbation theory. Once the deviations from the homogeneous Universe become large, the linear theory is no more valid. It is reasonable to expect that regions which are significantly overdense will collapse and eventually form gravitationally bound objects. In these overdense regions, the self-gravity of the local mass concentration will work against the expansion of the Universe; i.e. this region expands at a progressively slower rate compared to the background Universe. Such a slowing down will increase the density contrast between the overdense region and the background Universe and, consequently, make the gravitational potential of the local mass concentration more and more dominant. Eventually, such a region will collapse under its own self-gravity and will form a bound system. The details of the above process will depend on the initial density profile. The simplest model which one can study analytically is based on the assumption that the overdense region is spherically symmetric.

Peebles (1980) described the transition between the linear regime (where the expansion of the perturbation is maximum) and the non-linear regime (where the perturbation begins to collapse) by introducing the turn-around point. In an Einstein-De Sitter Universe, the temperature at the turn-around point (hereafter the turn-around temperature) is given by

\[ T_{m}(z_{ta}) \]

where \( T_{m}(z_{ta}) \) is the temperature of the matter at the redshift of the turn-around \( z_{ta} \).

Generally an isothermal perturbation described by the initial mass spectrum is assumed:

\[ M = M^* \]

Thus the redshift of the turn-around is given by:

\[ \%a = \frac{F}{g} \]

It is crucial to know the temperature of the matter at the turn-around redshift in order to evaluate the thermal initial condition of the collapse. We consider the same order of magnitude for the mass of the fluctuations given by Lahav (1986) and Puy and Signore (1996) which correspond to a turn-around redshift in the range: \( 10 < z_{te} < 150 \), which is the typical period of formation of the first objects.
The evolution of turn-around temperature is shown in Figure 2 with and without molecular contributions. The turn-around temperature is equal to the radiation temperature at a redshift of $z_i \approx 130$ without molecules and $z_i \approx 105$ with molecules. Another interesting point is the turn-around redshift $z = 55$. This redshift corresponds to a typical value of the collapsing mass (see Puy and Signore 1997). We find (see Figure 2) that the turn-around temperature $T_{\text{turn}}$ is 70 K without molecules and 100 K with molecules. The consequences could be important if we notice that the lower excitation temperature for HD (the main thermal molecular function) is 112 K (close to 100 K).
conditions of a gravitational collapse. The following analysis could reveal processes of fragmentation triggered by the thermal molecular function (see Puy and Signore 1997, 1998b). This last point is crucial for the estimation of the amplitude of secondary cosmic microwave background anisotropies. Dubrovich (1977, 1993) showed that resonant elastic scattering must be considered as the most efficient process in coupling matter and radiation at high redshift. He noted that the cross section for resonant scattering between the cosmic microwave background and molecules is several orders of magnitude larger than Thomson scattering, even with a modest abundance of primordial molecules. Let us only emphasize that, again at present, the primordial molecule abundance and the reaction rate of the chemical reactions are both quite uncertain.

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References