Cosmological Thermal Decoupling and Primordial Molecules†

By Denis Puy

Institute of Theoretical Physics, University of Zurich, 8057 Zurich (Switzerland)
and
Paul Scherrer Institute, Laboratory for Astrophysics, 5232 Villigen (Switzerland)
puy@physik.unizh.ch

Primordial chemistry began, at 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.

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 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 photons process. Nevertheless the Universe expanded and cooled faster than recombination could completed, and small fraction of free electrons and protons remained.
The principles of calculations of the primordial recombination have been mentionned initially by Shklovskii (1967), Novikov & 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 & 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. Temperature of matter and radiation as well as the density are not so high and we have possible collisional reactions between the species. However, in this cosmological context we have metal-free gas which does not allow the efficient reaction of adsorption on the surface of grains.
The literature on the chemistry in the post-recombination epoch has grown considerably in the recent years. Many authors have developped studies of primordial chemistry in different contexts. For example Lepp & Shull (1984), Latter & Black (1991), Puy et al. (1993), Stancil et al. (1996), Galli & Palla (1998) for the chemical network; Palla, Galli & Silk (1995), Puy & Signore (1996, 1997, 1998a, 1998b), Abel et al. (1997) and Galli & Palla (1998) in the context of the formation of the first objects.
Chemistry of the early Universe 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.

† Talk given at the JENAM, May 29th-June 3rd 2000, Moscow (Russia)

The complete chemical network consists of 90 reactions (see Puy et al. 1993 and more recently Galli & Palla 1998 and references therein).
Molecules could lead to radiative processes through the excitation of the rotational levels, and contribute to the thermal evolution of the medium. Puy et al. (1993) examined the thermal balance in the early Universe and showed that the molecular cooling and heating functions have a slight influence on the decrease of the temperature of the matter. Nevertheless molecules could play a more decisive role in the collapse of protoclouds, since molecular cooling can trigger thermal instability prior the gravitational instability, as mentionned Puy & Signore (1996, 1998a, 1998b). Protocloud evolute in three phases:

- linear evolution which approximatively follows expansion.
- *turn-around* epoch when the protocloud reaches its maximum value.
- non-linear evolution of the collapse.

At the turn-around point it is crucial to know the initial condition and particularly the temperature of the pre-collapse. In this contribution, I will recall the thermal function generated by the primordial molecules (Sect. 2), then I will show the influence on the thermal decoupling (Sect. 3). In Sect. 4, the role of the molecules on the turn-around point will be discussed and a brief outlook will be presented in Sect. 5.

2. Molecular thermal function

The disappearance of free charged particles reduces the scattering cross-section (Thomson scattering). The photons decouple from the rest of the matter; this happens at $T = T_{dec} \sim 0.26$ eV where T_{dec} is the temperature of the matter corresponding to the redshift $z_{dec} \sim 1100$. After the recombination, although the density-decrease acts against molecular formation, it turns out that the temperature is small enough for this formation occur.
The chemical composition of the primordial gas consists of electrons, protons, hydrogen (H, H^-, H_3^+, H_2^+, H_2), deuterium (D, D^+, HD, HD^+, H_2D^+), helium (H_e, He^+, He^{++}, HeH^+) and lithium (Li, Li^+, Li^-, LiH, LiH^+). Thus from the abundances of primordial atoms, given by the standard model of nucleosynthesis (see Table 1), we integrate the network of coupled chemical equations which is an initial value problem for stiff differential equations. Lepp & Shull (1984), Puy et al. (1993) and more recently Galli & Palla (1998) calculated, as function of redshift, the fractional abundances starting at the redshift $z \sim 10^4$ where He, H, D and Li are fully ionized.

Helium: He/H	Deuterium: D/H	Lithium Li/H
$\sim 8 \times 10^{-2}$	$\sim 4.3 \times 10^{-5}$	$\sim 2.4 \times 10^{-10}$

TABLE 1. Initial abundances given by the standard of the nucleosynthesis (see Sarkar 1996).

The reaction rates depend on the temperature, thus the temperature and density evolution equation must be solved simultaneously, which needs in turn the simultaneous determination of molecular cooling and heating rates (see Puy et al. 1993, Galli & Palla 1998). The abundances of the main molecules are obtained in Table 2.

The finite amount of primordial molecules, such as H_2, HD and LiH formed immediately after the recombination of cosmological hydrogen can induce a thermal response of molecules on the medium through the interaction with the radiation. The presence of non-zero permanent electric dipole moment makes HD and LiH a potentially more important coolant than H_2 at modest temperatures, although HD and LiH are much less abundant than H_2. Below 3000

e^-/H	H_2/H	HD/H	LiH/H
$\sim 3 \times 10^{-4}$	$\sim 10^{-6}$	1.2×10^{-9}	$\sim 7 \times 10^{-20}$

TABLE 2. abundances of primordial molecules at $z = 5$.

K, only the rotational levels of the molecules can be excited. The population of the rotational levels is mainly due to collisional excitation and de-excitation with H, H_2 and He on one hand and to radiative processes (absorption from cosmic background radiation and spontaneous or induced emission) on the other hand. Molecular cooling corresponds to collisional excitation followed by radiative transition, provided that no further absorption occurs. Molecular heating is due to the radiative excitation from cosmic microwave background followed by collisional de-excitation. Notice that, although the radiative de-excitation is faster than collisional one (because the excitation have the opposite ordering), the full cooling and heating processes must be evaluated. Molecular thermal function Ψ_{molec}, characterized by the two processes (molecular heating and cooling), is defined by:

$$\Psi_{molec} = \sum_k \Big[\Psi_k\Big] \tag{2.1}$$

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

$$\Psi_k = \sum_j n_j \sum_i n_i \Big(B_{ij} u^{ij} P^c_{ij} - n_x C^x_{ij} P^r_{ij}\Big)\epsilon_{ij} \quad \text{in erg cm}^{-3}\ \text{s}^{-1} \tag{2.2}$$

where n_j and n_i is respectively the population of the rotational level j and i. C^x_{ij} is the rate of collision with the species x (with the density n_x), B_{ij} the second Einstein coefficient, u^{ij} the radiative density of cosmic microwave background radiation at the energy ϵ_{ij}, which corresponds to the transition between the levels i and j; P^c_{ij} and P^r_{ij} 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. (2.2) corresponds to molecular heating when the second term corresponds to molecular cooling.

3. Cosmological thermal decoupling

The evolution of the energy density u_{gas} of a homogeneous gas is described by the equation:

$$du_{gas} = d\Big(\frac{3}{2} n k T_m\Big) = \mathcal{Q} dt \tag{3.3}$$

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

$$\mathcal{Q} = \Psi_{molec} + \Gamma_{compt}, \tag{3.4}$$

where (see Peebles 1968):

$$\Gamma_{compt} = \frac{4\sigma_T a_{bb} T_r^4}{m_e c} n_e \big(T_r - T_m\big). \tag{3.5}$$

σ_T is the Thomson cross-section, a_{bb} is the black body constant, c the speed light, m_e the mass of electron and n_e the electronic density. T_r is the temperature of the radiation. Thus Eq. (3.3) leads to the evolution of matter temperature T_m:

$$\frac{3}{2}nk\,\frac{dT_m}{dt} \;=\; -\Lambda_{ad} + \Gamma_{compt} + \Psi_{molec}, \tag{3.6}$$

where Λ_{ad} defines the adiabatic cooling due to the expansion of the Universe:

$$\Lambda_{ad} \;=\; 3nkT_m\,H_o(1+z)^{3/2}, \tag{3.7}$$

H_o is the Hubble constant (hereafter $H_o = 67$ Km s^{-1} 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 Fig 1 Compton heating and thermal molecular function (in unit 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.

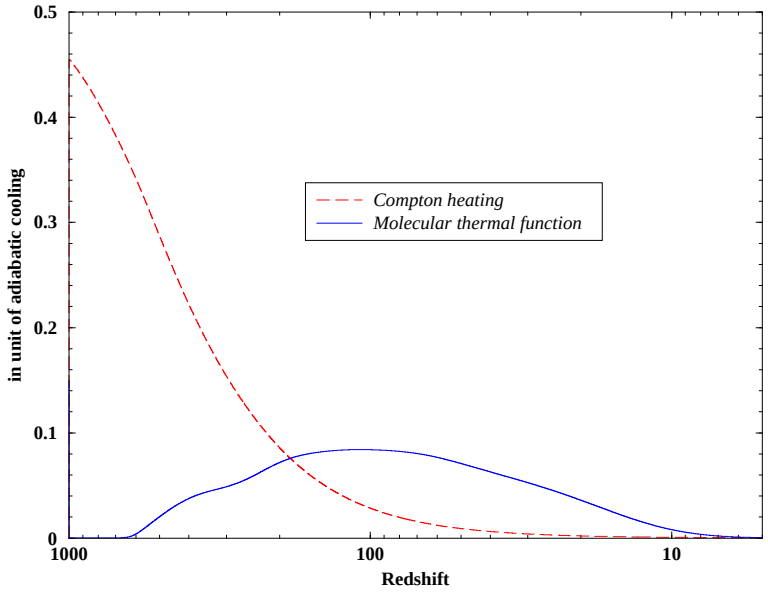

FIGURE 1. Evolution of the thermal function, i.e. Compton heating Γ_{compt} and molecular Ψ_{molec} in unit of adiabatic cooling Λ_{ad}.

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 can 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 turn-around temperature) is given by

$$T_{turn} \sim \left(\frac{3\pi}{4}\right)^{4/3} T_m(z_{ta}) \tag{4.8}$$

where $T_m(z_{ta})$ is the temperature of the matter at the redshift of the turn-around z_{ta}. Generally it is assumed an isothermal perturbation described by the initial mass spectrum:

$$\frac{\delta\rho}{\rho} = \left[\frac{M}{M_\star}\right]^\alpha (1+z)^{-1}, \tag{4.9}$$

where M is the mass of an overdense region (i.e. the mass of a cloud) and $M_\star = 10^{15}$ $M_\odot$ is a typical mass of a supercluster. Gott & Rees (1975) take $\alpha \sim -1/3$. Thus the redshift of the turn-around is given by:

$$z_{ta} = \left(\frac{3\pi}{4}\right)^{-2/3} \left[\frac{M}{M_\star}\right]^\alpha. \tag{4.10}$$

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 & Signore (1996) which correspond to turn-around redshift in the range: $10 < z_{ta} < 150$, which is the typical period of the formation of the first objects.
The evolution of turn-around temperature is shown in Fig. 2 without and with the molecular contributions, the evolution of radiation temperature is also plotted. We see two regimes for the two turn-around temperatures: one corresponds to a temperature higher than the radiation temperature T_r, the second is relative to temperature below T_r. It is important to estimate the redshift z_i where the turn-around temperature is equal to T_r, this point govern the initial behaviour of the gas: if the turn-around temperature is below the radiation temperature the gas heats, when the gas cools when the radiative temperature is below the turn-around temperature. Thus this condition is located at the redshift $z_i \sim 130$ in the case without molecules and $z_i \sim 105$ in the case with molecules. Another interesting point is the point which corresponds to the turn-around redshift $z = 55$. This redshift corresponds to a typical value 10^9 $M_\odot$ of a collapsing mass (see Puy & Signore 1997). We find (see Fig 2) that the turn-around temperature $T_{turn} \sim 70$ K without molecules and $T_{turn} \sim 100$ K for the turn-around temperature with molecules. The consequences could be important if we notice that the lower excitation temperature for HD (main thermal molecular function) is 112 K (close to 100 K) .

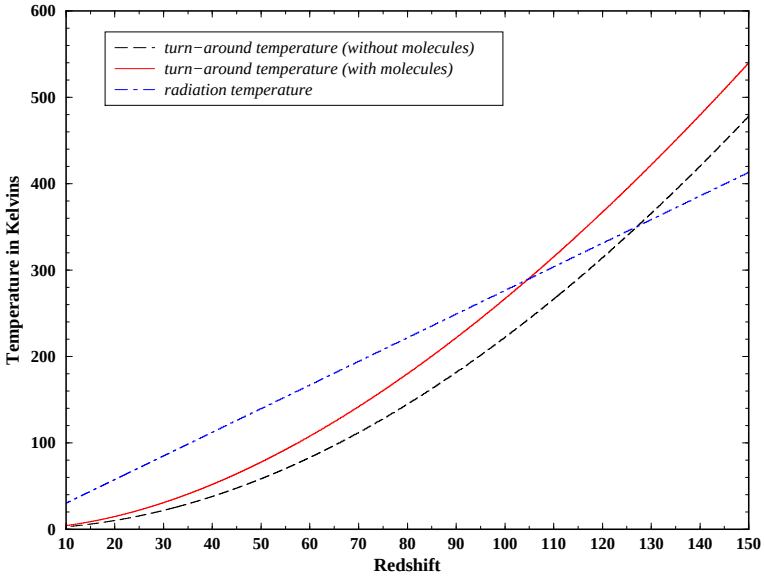

FIGURE 2. Evolution of the turn-around temperature (with and without molecules) and of the radiation temperature.

5. Outlook

This work shows a possible thermal modification, due to the primordial molecules, at the beginning of the collapse. This thermal mechanism could modify the initial conditions of a gravitational collapse. The following analysis could reveal processes of fragmentation trigerred by the thermal molecular function (see Puy & 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 times, the primordial molecules abundance and the reaction rate of the chemical reaction are both quite uncertain.

The author gratefully acknowledge the JENAM organizers for organizing such a pleasant conference. I would like to thank Andrei Doroshkevich and Victor Dubrovich for valuable and fruitful comments and discussions. Part of this work has been supported by the *Dr Tomalla Foundation* and by the Swiss National Science Foundation.

REFERENCES

ABEL T., ANNINOS P., ZHANG Y., NORMAN M., 1997 *New Astr.* **2**, 181.
DUBROVICH V., 1977 *Sov. Astr. Lett.* **3**, 128.
DUBROVICH V., 1993 *Astron. Lett.* **19**, 53.
GOTT III R., REES M., 1975 *A& A* **45**, 265.
GALLI D., PALLA F., 1998 *A & A* **335**, 403
LAHAV O., 1986 *MNRAS* **220**, 259.
LATTER W., BLACK J., 1991 *ApJ* **371**, 161.
LEPP S., SHULL M., 1984 *ApJ.* **280**, 465.

Novikov I., Zel'dovich Ya., 1967 *Ann. Rev. Astr. Ap.* **5**, 627.
Palla F., Galli D., Silk J., 1995 *ApJ* **451**, 44.
Peebles P.J.E., 1968 *ApJ* **153**, 1.
Peebles P.J.E., 1980 in: *The large scale structure of the Universe* (Princeton University Press)
Puy D., Alecian G., Lebourlot J., Leorat J., Pineau des Forets, 1993 *A& A* **267**, 337.
Puy D., Signore M., 1996 *A& A* **305**, 371.
Puy D., Signore M., 1997 *New Astr.,* **27**, 622.
Puy D., Signore M., 1998a *New Astr.,* **3** , 27.
Puy D., Signore M., 1998b *New Astr.,* **3** , 247.
Puy D., Signore M., 2000 *New Astr. Rev.,* accepted
Sarkar S., 1996 *Rep. Prog. Phys-* **59**, 1493.
Shklovskii I., 1967 in Proceedings *4th Texas Conf. on Relativistic Ap.* **5**, 627.
Stancil P., Lepp S., Dalgarno A., 1996 *ApJ* **458**, 401.