Primordial Star Forming Regions in a CDM Universe

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Abstract.
We developed a three-dimensional 2-level hierarchical cosmological code with a realistic and robust treatment of multi-species non-equilibrium ionization and radiative cooling processes, and use it to investigate primordial star forming regions that originate from high-$\sigma$ perturbations in a standard CDM dominated cosmology. We find it is possible to produce gravitationally bound and cooled structures at very high redshift ($z \sim 40$) with baryonic masses as small as $\sim 10^3 M_\odot$. The molecular hydrogen formation in these small scale structures follows very well the analytical predictions of Abel (1995) and Tegmark et al. (1996). We also discuss the minimum mass that cosmological structures must have in order to be able to cool and collapse.

I INTRODUCTION

Models for structure formation are based on the growth of small primordial density fluctuations by gravitational instability on a homogeneously expanding background universe. Depending on the nature of the dark matter and whether the primordial fluctuations were adiabatic or isothermal, the first mass scale to collapse could be as small as one solar mass (very heavy cold dark matter particles) or as high as $\sim 10^{12} M_\odot$ (hot dark matter scenarios). In CDM cosmogonies the fluctuation spectrum at small wavelengths has only a logarithmic dependence for mass scales smaller than $\sim 10^8 M_\odot$, which indicates that the small scale fluctuations in this model collapse nearly simultaneously in time. This leads to very complex dynamics during the formation of these structures, that can be studied accurately only by using realistic numerical computations to model the fluid motion and micro-physical processes as well as the dark matter component.

We have recently been able to develop methods that allow us to study the problem in three dimensions [5]. We describe this code briefly in section III but...
first review the process of $\text{H}_2$ formation during small scale structure collapse in the following section. A more extensive discussion of our results is given in a separate publication [3].

II MOLECULAR CHEMISTRY AND COOLING

The cooling in small scale fluctuations is dominated by the rotational/vibrational modes of hydrogen molecules. In primordial gas at low temperatures ($\lesssim 6000\text{K}$) molecular hydrogen can not be destroyed efficiently unless there is a radiation flux higher than $\sim 3 \times 10^{-26} \text{erg cm}^{-2} \text{s}^{-1}$ in the Lyman Werner Bands. Once self-shielding is important, even higher fluxes would be needed. The dominating $\text{H}_2$ producing gas phase reaction is the dissociative attachment reaction: $\text{H}^- + \text{H} \rightarrow \text{H}_2 + e^-$. In the absence of an external UV background one can integrate the rate equations to find the molecular hydrogen fraction formed during the collapse of primordial gas clouds with neutral hydrogen number density $n_\text{H}$, temperature $T$, and initial free electron fraction $x_0$ to be [1,10]:

$$f_{\text{H}_2}(t) - f_{\text{H}_2}(0) = \frac{k_{PA}}{k_r} \ln(x_0 n_\text{H} k_r t + 1) = 10^{-8} T^{1.53} \ln(t/t_\text{r}^0 + 1), \quad (1)$$

where $k_{PA}$ and $k_r$ denote the rates for photo-attachment to $\text{H}^-$ and recombination of hydrogen, respectively. The production of $\text{H}_2$ only depends logarithmically on time with a typical time scale of one initial recombination time. The temperature dependence is due to the ratio of recombination and $\text{H}^-$ formation time scales, which is a measure of the number of electrons available to produce $\text{H}^-$. A typical $\text{H}_2$ fraction of $\sim 10^{-3}$ is produced during the collapse of structures with virial temperatures greater than $10^3 \text{K}$. For initial (virial) temperatures higher than 6000 K the charge exchange with protons will efficiently destroy $\text{H}_2$, and equation (1) will not be applicable. However, during the collapse of clouds with such high virial temperatures the final $\text{H}_2$ fraction will, nevertheless, be $f_{\text{H}_2}(T \sim 6000 \text{K}) \sim \text{few} \times 10^{-3}$ [2].

III NUMERICAL RESULTS AND DISCUSSION

We achieve high spatial and mass resolution with the two-level hierarchical three-dimensional code (HERCULES) that we have developed for cosmology [4,5]. This code is designed to simulate structure formation in an expanding dark matter dominated universe with Newtonian gravity, multi-fluid hydrodynamics, radiative cooling, non-equilibrium chemistry and external radiation fields. Furthermore, the code independently evolves the following nine species: neutral hydrogen $H$, ionized hydrogen $H^+$, negatively-charged hydrogen $H^-$, hydrogen molecules $H_2$, ionized hydrogen molecules $H_2^+$, neutral helium $He$,
singly–ionized helium \( He^+ \), doubly–ionized helium \( He^{++} \) and free electrons \( e^- \). The 28 most important chemical rate equations (including radiation processes) are solved in non–equilibrium for the abundances of each of the nine species. The reaction rates and an extensive discussion of the chemistry model are provided in [2]. We have also implemented a comprehensive model for the radiative cooling of the gas that includes atomic line excitation, recombination, collisional ionization, free–free transitions, molecular line excitations, and Compton scattering of the cosmic background radiation (CBR) by electrons.

We apply our code to high redshift pre–galactic structure formation and evolution, investigating specifically the collapse of the first high–\( \sigma \) bound objects with total masses in the range \( 10^5 - 10^9 M_\odot \). Our model background spacetime is a flat (\( \Omega_0 = 1 \)) cold dark matter dominated universe with Hubble constant \( H_0 = 50 \) km s\(^{-1} \) Mpc\(^{-1} \), baryonic fraction \( \Omega_B = 0.06 \), and a hydrogen mass fraction of 76%. The baryonic matter is composed of hydrogen and helium in cosmic abundance with a hydrogen mass fraction of 76% and ratio of specific heats \( \gamma = 5/3 \). The initial data for the baryonic and dark matter perturbations is the Harrison–Zel’dovich power spectrum modulated with a CDM transfer function and normalized to the cluster scale \( \sigma_{8h} = 0.7 \).

The data is initialized at redshift \( z = 100 \) using Bertschinger’s [6] constrained realization procedure to construct 3 and 4\( \sigma \) fluctuations in cubes of comoving length 1024kpc, 512kpc, and 128kpc, with total masses of \( 7.5 \times 10^{10} M_\odot \), \( 9.3 \times 10^9 M_\odot \), and \( 1.5 \times 10^8 M_\odot \), respectively.

We reproduced the work of Tegmark et al. 1996 with the same cooling function [9] we have used in our cosmological hydrodynamics code so that we can compare their findings directly to our 3D numerical results. (We note that Tegmark et al. used a modified form of the Hollenbach and McKee (1979) \( H_2 \) cooling function.) Figure 1a is analogous to Fig. 6 of Tegmark et al. 1996 but includes the mass evolution in our numerical results for the 4\( \sigma \) perturbations. The dotted lines are found by adding up the total mass \( M_{200} \) found in cells with dark matter overdensities exceeding 200. It is obvious that the use of a different cooling function has a very strong influence on the predicted mass that can collapse. Although, the quantitative results are very different, the shape for these two different \( M_c(z) \) curves is rather similar at redshifts \( 30 < z < 100 \). The slopes are consistent with \( M_c \propto (1+z)^{-3/2} \) indicating a constant virial temperature since \( T_{\text{vir}} \propto M^{2/3}(1+z) \). A constant virial temperature in turn implies a roughly constant final \( H_2 \) fraction given by equation (1). For the case in Tegmark et al., the virial temperature in that regime is \( \sim 1000 \) K which yields \( f_{H_2} \sim 4 \times 10^{-4} \) which they argued to be roughly a constant universal value which, if exceeded, allows the cloud to collapse at its free fall rate. Using the Lepp and Shull \( H_2 \) cooling function we find that the virial temperature needed to fulfill the Tegmark et al. requirement for collapse is \( \approx 200 \) K for redshifts \( > 30 \). This translates to a molecular fraction of only \( \sim 3 \times 10^{-5} \). Our simulations, however, show that, although we used the Lepp and Shull cooling function, the \( H_2 \) fraction at the time when the baryons are
collapsing into the DM potential wells is also about $\sim 5 \times 10^{-4}$. Hence, we find roughly the same critical $H_2$ fraction as derived by Tegmark et al. (1996) even with a very different cooling function.

In Figure 1b we test equation (1) against results from the $4\sigma_{128}$ kpc (open circles) and the $4\sigma_{512}$ kpc simulations. The fit is astonishingly good, although the initial temperature (or redshift) is somewhat difficult to pick out in this case since the heating due to adiabatic compression is slow and the initial (virial) temperature is not as well defined as in the case of collapse on larger mass scales. Analyzing the time derivative of equation (1) one finds for large times that $\dot{f}_{H_2} \propto T^{1.53}/t$ which, for the spherical collapse model, translates to $\dot{f}_{H_2} \propto H_0 M (1 + z_{vir})^{1.53}$ when we compare the slopes for different mass scales at the present time. This explains that the divergence of the two graphs in Figure 1b for low redshifts is due to differences in collapse mass and redshift.

It has been stressed by various authors that early small scale structure might influence the entire pregalactic medium and subsequently play an important role for structure formation on larger mass scales (e.g. [7]). They are in prin-
ciple capable of ionizing a large fraction of the pregalactic medium as well as to enrich it with metals. We hope to achieve the required dynamical range in future work to estimate the IMF using adaptive mesh refinement techniques and so be able to quantify the feedback of collapsing small scale structure.

We happily acknowledge discussions with M.J. Rees and Max Tegmark. This work is done under the auspices of the Grand Challenge Cosmology Consortium (GC3) and supported in part by NSF grant ASC-9318185. The simulations were performed on the CRAY-C90 at the PSC, and the CONVEX-3880 at the NCSA.

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