1. Preamble

Hydrogen in the universe recombined about half a million years after the Big Bang, and cooled down to a temperature of a few kelvins until the first non-linearities developed, and evolved into stars, galaxies, and black holes that lit up the universe again. In currently popular cold dark matter flat cosmologies ($\Lambda$CDM), some time beyond a redshift of 10 the gas within halos with virial temperatures $T_{\text{vir}} \gtrsim 10^4$ K − or, equivalently, with masses $M \gtrsim 10^8 [(1+z)/10]^{-3/2} M_\odot$ − cooled rapidly due to the excitation of hydrogen Ly$\alpha$ and fragmented. Massive stars formed with some initial mass function (IMF), synthesized heavy elements, and exploded as Type II supernovae after a few $\times 10^7$ yr, enriching the surrounding medium: these subgalactic stellar systems, aided perhaps by an early population of accreting black holes in their nuclei, generated the ultraviolet radiation and mechanical energy that contributed to the reheating and reionization of the cosmos. It is widely believed that collisional excitation of molecular hydrogen may have allowed gas in even smaller systems − virial temperatures of a thousand K, corresponding to masses around $5 \times 10^5 [(1+z)/10]^{-3/2} M_\odot$ − to cool and form stars at even earlier times (Couchman & Rees 1986; Haiman et al. 1996; Tegmark et al. 1997; Abel et al. 2000, 2002; Fuller & Couchman 2000; Bromm et al. 2002; Reed et al. 2005; Kuhlen & Madau 2005). Throughout the epoch of structure formation, the all-pervading intergalactic medium (IGM), which contains most of the ordinary baryonic material left over from the Big Bang, becomes clumpy under the influence of gravity, and acts as a source for the gas that gets accreted, cools, and forms stars within subgalactic fragments, and as a sink for the metal enriched material, energy, and radiation which they eject. The well-established existence of heavy elements like carbon and silicon in the Ly$\alpha$ forest clouds at $z = 2 − 6$ (Songaila 2001; Pettini et al. 2003; Ryan-Weber et al. 2006) may be indirect evidence for such an early episode of pregalactic star formation. The recently released Wilkinson Microwave Anisotropy Probe (WMAP) 3-year data require the universe to be fully reionized by redshift $z_r = 11 \pm 2.5$ (Spergel et al. 2006), another indication that significant star-formation activity started at very early cosmic times.

The last decade has witnessed great advances in our understanding of the high redshift universe, thanks to breakthroughs achieved with satellites, 8-10m class telescopes, and cosmic microwave background (CMB) experiments. Large surveys such as the Sloan Digital Sky Survey (SDSS), together with the use of novel instruments and observational techniques have led to the discovery of galaxies and quasars at redshifts in excess of 6. At the time of writing, 9 quasars have already been found with $z > 6$ (Fan 2006), and one actively star-forming has been spectroscopically confirmed at $z = 6.96$ (Iye et al. 2006). These sources probe an epoch when the universe was $< 7\%$ of its current age. Keck and VLT observations of redshifted H I Ly$\alpha$ (`forest’) absorption have been shown to be sensitive probe of the distribution of gaseous matter in the universe (see Rauch 1998 for a review). Gamma-ray bursts have recently displayed their potential to replace quasars as the preferred probe of early star formation and chemical enrichment: GRB050904, the most distant event known to date, is at $z = 6.39$ (Haislip et al. 2006). The underlying goal of all these efforts is to understand the growth of cosmic structures, the properties
of galaxies and their evolution, and ultimately to map the transition from the cosmic “dark age” to a ionized universe populated with luminous sources.

Progress has been equally significant on the theoretical side. The key idea of currently popular cosmological scenarios, that primordial density fluctuations grow by gravitational instability driven by collisionless CDM, has been elaborated upon and explored in detail through large-scale numerical simulations on supercomputers, leading to a hierarchical (‘bottom-up’) scenario of structure formation. In this model, the first objects to form are on subgalactic scales, and merge to make progressively bigger structures (‘hierarchical clustering’). Ordinary matter in the universe follows the dynamics dictated by the dark matter until radiative, hydrodynamic, and star formation processes take over. According to these calculations, a truely inter- and proto-galactic medium (the main repository of baryons at high redshift) collapses under the influence of dark matter gravity into flattened and filamentary structures, which are seen in absorption against background QSOs. Gas condensation in the first baryonic objects is possible through the formation of H$_2$ molecules, which cool via roto-vibrational transitions down to temperatures of a few hundred kelvins. In the absence of a UV photodissociating flux and of ionizing X-ray radiation, three-dimensional simulations of early structure formation show that the fraction of cold, dense gas available for accretion onto seed black holes or star formation exceeds 20% for halos more massive than $10^6$ M$_\odot$ already at redshifts 20 (Machacek et al. 2003; Yoshida et al. 2003).

In spite of some significant achievements in our understanding of the formation of cosmic structures, there are still many challenges facing hierarchical clustering theories. While quite successful in matching the observed large-scale density distribution (like, e.g., the properties of galaxy clusters, galaxy clustering, and the statistics of the Ly$\alpha$ forest), CDM simulations appear to produce halos that are too centrally concentrated compared to the mass distribution inferred from the rotation curves of (dark matter-dominated) dwarf galaxies, and to predict too many dark matter subhalos compared to the number of dwarf satellites observed within the Local Group (Moore et al. 1999; Klypin et al. 1999). Another perceived difficulty (arguably connected with the “missing satellites problem”, e.g. Bullock et al. 2000) is our inability to predict when and how the universe was reheated and reionized, i.e. to understand the initial conditions of the galaxy formation process and the basic building blocks of today’s massive baryonic structures. We know that at least some galaxies and quasars had already formed when the universe was less than $10^9$ yr old. But when did the first luminous clumps form, was star formation efficient in baryonic objects below the atomic cooling mass, and what was the impact of these early systems on the surrounding intergalactic gas? The crucial processes of star formation and “feedback” (e.g. the effect of the energy input from the earliest generations of sources on later ones) in the nuclei of galaxies are still poorly understood. Accreting black holes can release large amounts of energy to their surroundings, and may play a role in regulating the thermodynamics of the interstellar, intracluster, and intergalactic medium. The detailed astrophysics of these processes is, however, unclear. Although we may have a sketchy history of the production of the chemical elements in the universe, we know little about how and where exactly they were produced and how they are distributed in the IGM and in the intracluster medium. Finally, where are the first stars and their remnants now, and why are the hundreds of massive satellites predicted to survive today in the Milky Way halo dark?

In these lectures I will describe some of the basic tools that have been developed to study the dawn of galaxies, the lessons learned, and summarize our current understanding of the birth of the earliest astrophysical objects.
2. The Dark Ages

2.1. Cosmological preliminaries

Recent CMB experiments, in conjunction with new measurements of the large-scale structure in the present-day universe, the SNIa Hubble diagram, and other observations, have lead to a substantial reduction in the uncertainties in the parameters describing the ΛCDM concordance cosmology. We appear to be living in a flat ($Ω_m + Ω_Λ = 1$) universe dominated by a cosmological constant and seeded with an approximately scale-invariant primordial spectrum of Gaussian density fluctuations. A ΛCDM cosmology with $Ω_m = 0.24$, $Ω_Λ = 0.76$, $Ω_b = 0.042$, $h = H_0/100$ km s$^{-1}$ Mpc$^{-1} = 0.73$, $n = 0.95$, and $σ_8 = 0.75$ is consistent with the best-fit parameters from the WMAP 3-year data release (Spergel et al. 2006). Here $Ω_m = ρ_m^0/ρ_0^0\dagger$ is the present-day matter density (including cold dark matter as well as a contribution $Ω_b$ from baryons) relative to the critical density $ρ_c^0 = 3H_0^2/8πG$, $Ω_Λ$ is the vacuum energy contribution, $H_0$ is the Hubble constant today, $n$ is the spectral index of the matter power spectrum at inflation, and $σ_8$ normalizes the power spectrum: it is the root-mean-square amplitude of mass fluctuations in a sphere of radius $8h^{-1}$ Mpc. The lower values of $σ_8$ and $n$ compared to WMAP 1-year results (Spergel et al. 2003) have the effect of delaying structure formation and reducing small-scale power. In this cosmology, and at the epochs of interest here, the expansion rate $H$ evolves according to the Friedmann equation

$$H = \frac{1}{a} \frac{da}{dt} = H_0[Ω_m(1+z)^3 + Ω_Λ]^{1/2},$$

(2.1)

where $z$ is the redshift. Light emitted by a source at time $t$ is observed today (at time $t_0$) with a redshift $z ≡ 1/a(t) − 1$, where $a$ is the cosmic scale factor [$a(t_0) ≡ 1$]. The age of the (flat) universe today is

$$t_0 = \int_0^∞ \frac{dz'}{(1+z')H(z')} = \frac{2}{3H_0\sqrt{Ω_m}} \ln \left[ \frac{√Ω_Λ + 1}{√Ω_m} \right] = 1.025 H_0^{-1} = 13.7 \text{ Gyr}$$

(2.2)

(Ryden 2003). At high redshift, the universe approaches the Einstein-de Sitter behaviour, $a \propto t^{2/3}$, and its age is given by

$$t(z) ≈ \frac{2}{3H_0\sqrt{Ω_m}} (1+z)^{-3/2}.$$

(2.3)

The average baryon density today is $n_b^0 = 2.5 \times 10^{-7}$ cm$^{-3}$, and the hydrogen density is $n_H = (1 - Y_p)n_b = 0.75 n_b$, where $Y_p$ is the primordial mass fraction of helium. The photon density is $n_e^0 = (2.4/π^2)(k_B T_0/hc)^3 = 400$ cm$^{-3}$, where $T_0 = 2.728 \pm 0.004$ K (Fixsen et al. 1996), and the cosmic baryon-to-photon ratio is then $η = n_b/n_γ = 6.5 \times 10^{-10}$. The electron scattering optical depth to redshift $z_r$ is given by

$$τ_e(z_r) = \int_0^{z_r} dz' n_e σ_T e dz = \int_0^{z_r} dz' \frac{n_e(z)σ_T e}{(1+z)H(z)}$$

(2.4)

where $n_e$ is the electron density at redshift $z$ and $σ_T$ the Thomson cross-section. Assuming a constant electron fraction $x_e ≡ n_e/n_H$ with redshift, and neglecting the vacuum energy contribution in $H(z)$, this can be rewritten as

$$τ_e(z_r) = \frac{x_e n_e^0 σ_T e}{H_0\sqrt{Ω_m}} \int_0^{z_r} dz' \frac{1}{√1+z'} = 0.0022 [(1+z_r)^{3/2} - 1].$$

(2.5)

\dagger Hereafter densities measured at the present epoch will be indicated either by the superscript or the subscript ‘0’. 

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**Piero Madau: Early Galaxy Formation**
Ignoring helium, the 3-year WMAP polarization data requiring \( \tau_e = 0.09 \pm 0.03 \) are consistent with a universe in which \( x_e \) changes from essentially close to zero to unity at \( z_r = 11 \pm 2.5 \), and \( x_e \approx 1 \) thereafter.

Given a population of objects with proper number density \( n(z) \) and geometric cross-section sigma \( \Sigma(z) \), the incremental probability \( dP \) that a line of sight will intersect one of the objects in the redshift interval \( dz \) at redshift \( z \) is

\[
dP = n(z)\Sigma(z)c\frac{dt}{dz} = n(z)\Sigma(z)c\frac{dz}{(1+z)H(z)}. \tag{2.6}
\]

### 2.2. Physics of recombination

Recombination marks the end of the plasma era, and the beginning of the era of neutral matter. Atomic hydrogen has an ionization potential of \( I = 13.6 \) eV; it takes 10.2 eV to raise an electron from the ground state to the first excited state, from which a further 3.4 eV will free it,

\[
\gamma + H \leftrightarrow p + e^-.
\tag{2.7}
\]

According to Boltzmann statistics, the number density distribution of non-relativistic particles of mass \( m_i \) in thermal equilibrium is given by

\[
n_i = g_i \left( \frac{m_i k_B T}{2\pi \hbar^2} \right)^{3/2} \exp \left( \frac{\mu_i - m_i c^2}{k_B T} \right),
\tag{2.8}
\]

where \( g_i \) and \( \mu_i \) are the statistical weight and chemical potential of the species. When photoionization equilibrium also holds, then \( \mu_e + \mu_p = \mu_H \). Recalling that \( g_e = g_p = 0.5 \) and \( g_H = 2 \), one then obtains the Saha equation:

\[
\frac{n_e n_p}{n_H n_{HI}} = \frac{x_e^2}{1-x_e} = \frac{(2\pi m_e k_B T)^{3/2}}{n_H (2\pi \hbar^2)^3} \exp \left( -\frac{I}{k_B T} \right),
\tag{2.9}
\]

which can be rewritten as

\[
\ln \left( \frac{x_e^2}{1-x_e} \right) = 52.4 - 1.5 \ln(1+z) - 58,000 (1+z)^{-1}.
\tag{2.10}
\]

The ionization fraction goes from 0.91 to 0.005 as the redshift decreases from 1500 to 1100, and the temperature drops from 4100 K to 3000 K. The elapsed time is less than 200,000 yr.

Although the Saha equation describes reasonably well the initial phases of the departure from complete ionization, the assumption of equilibrium rapidly ceases to be valid in an expanding universe, and recombination freezes out. The residual electron fraction can be estimated as follows. The rate at which electrons recombine with protons is

\[
\frac{dn_e}{dt} = -\alpha_B n_e n_p \equiv -\frac{n_p}{t_{rec}},
\tag{2.11}
\]

where \( t_{rec} \) is the characteristic time for recombination and \( \alpha_B \) is the radiative recombination coefficient. This is the product of the electron capture cross-section \( \sigma_n \) and the electron velocity \( v_e \), averaged over a thermal distribution and summed over all excited states \( n \geq 2 \) of the hydrogen atom, \( \alpha_B = \sum \langle \sigma_n v_e \rangle \). The radiative recombination coefficient is well approximated by the fitting formula

\[
\alpha_B = 6.8 \times 10^{-13} T_3^{-0.8} \text{ cm}^3 \text{ s}^{-1} = 1.85 \times 10^{-10} (1+z)^{-0.8} \text{ cm}^3 \text{ s}^{-1},
\tag{2.12}
\]

where \( T_3 \equiv T/3000 \text{ K} \) and in the second equality I used \( T = T_0(1+z) \). When the recombination rate falls below the expansion rate, i.e. when \( t_{rec} > 1/H, \) the formation of neutral atoms ceases and the remaining electrons and protons have negligible probability
Figure 1. Helium and hydrogen recombination for a WMAP 3-year cosmology. The step at earlier times in the left panel is due to the recombination of He $\text{III}$ into He $\text{II}$. We used the code RECFAST (Seager et al. 1999) to compute the electron fraction $x_e$. Note that the residual electron fraction (determined by the condition $t_{\text{rec}} H = 1$) scales with cosmological parameters as $x_e \propto \sqrt{\Omega_m/\Omega_b h}$.

for combining with each other:

$$t_{\text{rec}} H = H_0 \sqrt{\Omega_m} \frac{x_e n_{\text{H}}^0 \alpha_B}{x_e n_{\text{H}}^0 (1 + z)^{-3/2}} = 0.0335 (1 + z)^{-0.7} = 2.5 \times 10^{-4} x_e,$$

(2.13)

where I assumed $z = 1100$ in the third equality. The recombination of hydrogen in an expanding universe is actually delayed by a number of subtle effects that are not taken into account in the above formulation. An $e^-$ captured to the ground state of atomic hydrogen produces a photon that immediately ionizes another atom, leaving no net change. When an $e^-$ is captured instead to an excited state, the allowed decay to the ground state produces a resonant Lyman series photon. These photons have large capture cross-sections and put atoms in a high energy state that is easily photoionized again, thereby annihilating the effect. That leaves two main routes to the production of atomic hydrogen: 1) two-photon decay from the $2s$ level to the ground state; and (2) loss of Ly$\alpha$ resonance photons by the cosmological redshift. The resulting recombination history was derived by Peebles (1968) and Zel’dovich et al. (1969).

In the redshift range $800 < z < 1200$, the fractional ionization varies rapidly and is given approximately by the fitting formula

$$x_e = 0.042 \left( \frac{z}{1000} \right)^{11.25}.$$

(2.14)

This is a fit to a numerical output from the code RECFAST – an improved calculation of the recombination of H $\text{I}$, He $\text{I}$, and He $\text{II}$ in the early universe involving a line-by-line treatment of each atomic level (Seager et al. 1999). Using this expression, we can again compute the optical depth of the universe for Thomson scattering by free electrons:

$$\tau_e(z) = \int_0^z \frac{d\tau}{d\sigma} \frac{x_e n_{\text{H}} \sigma T}{(1 + z) H(z)} \approx 0.3 \left( \frac{z}{1000} \right)^{12.75}.$$

(2.15)

This optical depth is unity at $z_{\text{dec}} = 1100$. From the optical depth we can compute the visibility function $P(\tau)$, the probability that a photon was last scattered in the interval
(z, z + dz). This is given by
\[ P(\tau) = e^{-\tau} \frac{d\tau}{dz} = 0.0038 \left( \frac{z}{1000} \right)^{11.75} e^{-0.3(z/1000)^{12.75}}, \] (2.16)
and has a sharp maximum at \( z = z_{\text{dec}} \) and a width of \( \Delta z \approx 100 \). The finite thickness of the last scattering surface has important observational consequences for CMB temperature fluctuations on small scales.

### 2.3. Coupling of gas and radiation

The CMB plays a key role in the early evolution of structures. First, it sets the epoch of decoupling, when baryonic matter becomes free to move through the radiation field to form the first generation of gravitationally bound systems. Second, it fixes the matter temperature that in turns determines the Jeans scale of the minimum size of the first bound objects.

Following Peebles (1993), consider an electron \( e^- \) moving at non-relativistic speed \( v \ll c \) through the CMB. In the \( e^- \) rest-frame, the CMB temperature measured at angle \( \theta \) from the direction of motion is
\[ T(\theta) = T \left( 1 + \frac{v}{c} \cos \theta \right). \] (2.17)
The radiation energy density per unit volume per unit solid angle \( d\Omega = d\phi d\cos \theta \) around \( \theta \) is
\[ du = [a_B T^4(\theta)] \frac{d\Omega}{4\pi} \] (2.18)
(here \( a_B \) is the radiation constant), and the net drag force (i.e. the component of the momentum transfer along the direction of motion, integrated over all directions of the radiation) felt by the electron is
\[ F = \int_{4\pi} \sigma_T du \cos \theta = 4 \sigma_T (a_B T^4) \left( 1 + \frac{v}{c} \cos \theta \right)^4 \cos \theta \frac{d\Omega}{4\pi} \]
\[ = \frac{4}{3} \frac{\sigma_T a_B T^4}{c} v. \] (2.19)
This force will be communicated to the protons through electrostatic coupling. The formation of the first gravitationally bound systems is limited by radiation drag, as the drag force per baryon is \( x_e F \), where \( x_e \) is the fractional ionization. The mean force divided by the mass \( m_p \) of a hydrogen atom gives the deceleration time of the streaming motion:

\[
\tau_s^{-1} = \frac{1}{v} \frac{dv}{dt} = \frac{4}{3} \frac{\sigma_T a_B T_0^4 (1 + z)^4}{m_p c x_e}.
\]  

(2.20)

The product of the expansion rate \( H \) and the velocity dissipation time \( \tau_s \) is

\[
t_s H = 7.6 \times 10^5 h x_e^{-1} (1 + z)^{-5/2}.
\]

(2.21)

Prior to decoupling \( t_s H \ll 1 \). Since the characteristic time for the gravitational growth of mass density fluctuations is of the order of the expansion timescale, baryonic density fluctuations become free to grow only after decoupling.

We can use the above results to find the rate of relaxation of the matter temperature \( T_e \) to that of the radiation. The mean energy per electron in the plasma is \( E = 3k_B T_e / 2 = m_e \langle v^2 \rangle \). The rate at which an electron is doing work against the radiation drag force if \( F v \), so the plasma transfers energy to the radiation at the mean rate, per electron:

\[
\frac{dE}{dt} = (Fv) = \frac{4}{3} \frac{\sigma_T a_B T_e^4}{c \langle v^2 \rangle} \times T_e.
\]

(2.22)

At thermal equilibrium \( T_e = T \), and this rate must be balanced by the rate at which photons scattering off electrons increase the matter energy:

\[
\frac{dE}{dt} = \frac{4}{3} \frac{\sigma_T a_B T_e^4}{c} \frac{3k_B}{m_e} (T - T_e).
\]

(2.23)

Thus the rate of change of the matter temperature is

\[
\frac{dT_e}{dt} = \frac{2}{3k_B} \frac{dE}{dt} = \frac{4x_e}{(1 + x_e)} \frac{8\sigma_T a_B T_e^4}{3m_e c} (T - T_e),
\]

(2.24)

The factor \( x_e / (1 + x_e) \) accounts for the fact that the plasma energy loss rate per unit volume is \( -n_e dE/dt = -x_e n_H dE/dt \), while the total plasma energy density is \( (n_e + n_p + n_{HI}) 3k_B T_e / 2 = n_H (1 + x_e) 3k_B T_e / 2 \). The expression above can be rewritten as

\[
\frac{dT_e}{dt} = \frac{T - T_e}{t_c},
\]

(2.25)

where the “Compton cooling timescale” is

\[
t_c = \frac{3m_e c}{4\sigma_T a_B T_e^4} \frac{1 + x_e}{2x_e} = \frac{7.4 \times 10^{19} \text{s}}{(1 + z)^4} \left( \frac{1 + x_e}{2x_e} \right).
\]

(2.26)

The characteristic condition for thermal coupling is then

\[
t_c H = \frac{240h \sqrt{\Omega_m}}{(1 + z)^{5/2}} \frac{1 + x_e}{2x_e} \left( \frac{T}{T_e} - 1 \right)^{-1} < 1.
\]

(2.27)

For fully ionized gas \( x_e = 1 \) and the Compton cooling timescale is shorter than the expansion time at all redshifts \( z > z_c = 5 \). With increasing redshift above 5, it becomes increasingly difficult to keep optically thin ionized plasma hotter than the CMB. At redshift \( z > 100 \), well before the first energy sources (stars, accreting black holes) turn on, hydrogen will have the residual ionization \( x_e = 2.5 \times 10^{-4} \). With this ionization, the characteristic relation for the relaxation of the matter temperature is

\[
t_c H = \frac{1.7 \times 10^5}{(1 + z)^{5/2}} \left( \frac{T}{T_e} - 1 \right)^{-1}.
\]

(2.28)
Figure 3. Evolution of the radiation (dashed line, labeled CMB) and matter (solid line, labeled GAS) temperatures after recombination, in the absence of any reheating mechanism.

The coefficient of the fractional temperature difference reaches unity at the “thermalization redshift” \( z_{th} \approx 130 \). That is, the residual ionization is enough to keep the matter in temperature equilibrium with the CMB well after decoupling. At redshift lower than \( z_{th} \), the temperature of intergalactic gas falls adiabatically faster than that of the radiation, \( T_e \propto a^{-2} \). From the analysis above, the rate of change of the radiation energy density due to Compton scattering can be written as

\[
\frac{du}{dt} = \frac{4}{3} \frac{\sigma_T A_B T^4}{c} \frac{3 k_B n_e}{m_e} (T_e - T),
\]  

(2.29)

or

\[
\frac{du}{u} = 4dy, \quad dy = (n_e \sigma_T c dt) \frac{k_B(T_e - T)}{m_e c^2} = d\tau_e \frac{k_B(T_e - T)}{m_e c^2}.
\]  

(2.30)

Compton scattering causes a distortion of the CMB spectrum, depopulating the Rayleigh-Jeans regime in favor of photons in the Wien tail. The “Compton-parameter”

\[
y = \int_0^\tau \frac{k_B T_e}{m_e c^2} \frac{d\tau_e}{dz} dz
\]  

(2.31)

is a dimensionless measure of this distortion, and is proportional to the pressure of the electron gas \( n_e k_B T_e \). The COBE satellite has shown the CMB to be thermal to high accuracy, setting a limit \( y \leq 1.5 \times 10^{-5} \) (Fixsen et al. 1996). This can be shown to imply

\[
\langle x_e T_e \rangle [(1 + z)^{3/2} - 1] < 4 \times 10^7 \text{K}.
\]  

(2.32)

A universe that was reionized and reheated at \( z = 20 \) to \( (x_e, T_e) = (1, > 4 \times 10^5 \text{K}) \), for example, would violate the COBE \( y \)-limit.
and electrons and ions, through the reactions that controls the formation of the first stars in subgalactic systems. It is the ability of dust-free gas to cool down to low temperatures in the recombination era. The presence of even a trace abundance of $\mathrm{H}_2$ is of direct relevance for the cooling properties of primordial gas. In the absence of heavy metals or dust grains, the processes of radiative cooling, cloud collapse, and star formation in the earliest astrophysical objects were undoubtedly quite different from those today. Saslaw & Zipoy (1967) and Peebles & Dicke (1968) were the first to realize the importance of gas phase reactions for the formation of the simplest molecule, $\mathrm{H}_2$, in the post-recombination epoch. The presence of even a trace abundance of $\mathrm{H}_2$ is of direct relevance for the cooling properties of primordial gas. In the absence of molecules this would be an extremely poor radiator: cooling by Lyα photons is ineffective at temperatures $\lesssim 8000$ K, well above the matter and radiation temperature in the post-recombination era. It is the ability of dust-free gas to cool down to low temperatures that controls the formation of the first stars in subgalactic systems.  

The formation of $\mathrm{H}_2$ in the intergalactic medium is catalyzed by the residual free electrons and ions, through the reactions

\[
\begin{align*}
\mathrm{H} + e^- &\rightarrow \mathrm{H}^- + \gamma, \\
\mathrm{H}^- + \mathrm{H} &\rightarrow \mathrm{H}_2 + e^-,
\end{align*}
\]

and

\[
\begin{align*}
\mathrm{H}^+ + \mathrm{H} &\rightarrow \mathrm{H}_2^+ + \gamma, \\
\mathrm{H}_2^+ + \mathrm{H} &\rightarrow \mathrm{H}_2 + \mathrm{H}^+.
\end{align*}
\]

2.4. Hydrogen molecules in the early universe

Table 1. Reaction network for primordial $\text{H}_2$ chemistry

| reaction | rate (cm$^3$ s$^{-1}$ or s$^{-1}$) | notes |
|----------|----------------------------------|-------|
| $\text{H}^+ + e \rightarrow \text{H} + \gamma$ | $R_{e2} = 8.76 \times 10^{-11} (1+z)^{-0.58}$ | |
| $\text{H} + e \rightarrow \text{H}^+ + e$ | $R_{2e} = 2.41 \times 10^{15} T^{1.5} \exp \left(-\frac{29172}{T}\right) \times R_{e2}$ | |
| $\text{H} + e \rightarrow \text{H}^- + \gamma$ | $1.4 \times 10^{-18} T^{0.928} \exp \left(-\frac{13800}{T}\right)$ | |
| $\text{H}^- + \gamma \rightarrow \text{H} + e$ | $1.1 \times 10^{-1} T^{2.13} \exp \left(-\frac{8835}{T}\right)$ | |
| $\text{H}^- + \text{H} \rightarrow \text{H}_2 + e$ | $1.5 \times 10^{-9}$ | $T_e \leq 300$
| | $4.0 \times 10^{-9} T^{-0.17}$ | $T_e > 300$
| $\text{H}^- + \text{H}^+ \rightarrow 2\text{H}$ | $5.7 \times 10^{-5} T_e^{0.5} + 6.3 \times 10^{-8}$ | |
| $\text{H} + \text{H}^+ \rightarrow \text{H}_2 + \gamma$ | $\text{dex} \left[-19.38 - 1.523 \log T_e\right] + 1.118(\log T_e)^2 - 0.1269(\log T_e)^3$ | $T_e \leq 10^{1.5}$
| $\text{H}_2^+ + \gamma \rightarrow \text{H} + \text{H}^+$ | $2.0 \times 10^1 T^{1.59} \exp \left(-\frac{32400}{T}\right)$ | $v = 0$
| | $1.63 \times 10^7 \exp \left(-\frac{32400}{T}\right)$ | LTE
| $\text{H}_2^+ + \text{H} \rightarrow \text{H}_2 + \text{H}^+$ | $6.4 \times 10^{-10}$ | |
| $\text{H}_2 + \text{H}^+ \rightarrow \text{H}_2^+ + \text{H}$ | $3.0 \times 10^{-10} \exp \left(-\frac{21050}{T_e}\right)$ | $T_e \leq 10^4$
| | $1.5 \times 10^{-10} \exp \left(-\frac{14000}{T_e}\right)$ | $T_e > 10^4$
| $\text{He} + \text{H}^+ \rightarrow \text{HeH}^+ + \gamma$ | $7.6 \times 10^{-18} T_e^{-0.5}$ | $T_e \leq 10^3$
| | $3.45 \times 10^{-16} T_e^{-1.06}$ | $T_e > 10^3$
| $\text{HeH}^+ + \gamma \rightarrow \text{He} + \text{H}_2^+$ | $9.1 \times 10^{-10}$ | |
| $\text{HeH}^+ + \gamma \rightarrow \text{He} + \text{H}_2^+$ | $6.8 \times 10^{-1} T^{1.5} \exp \left(-\frac{22750}{T}\right)$ | |

In the absence of heavy metals or dust grains, the processes of radiative cooling, cloud collapse, and star formation in the earliest astrophysical objects were undoubtedly quite different from those today. Saslaw & Zipoy (1967) and Peebles & Dicke (1968) were the first to realize the importance of gas phase reactions for the formation of the simplest molecule, $\mathrm{H}_2$, in the post-recombination epoch. The presence of even a trace abundance of $\mathrm{H}_2$ is of direct relevance for the cooling properties of primordial gas. In the absence of molecules this would be an extremely poor radiator: cooling by Lyα photons is ineffective at temperatures $\lesssim 8000$ K, well above the matter and radiation temperature in the post-recombination era. It is the ability of dust-free gas to cool down to low temperatures that controls the formation of the first stars in subgalactic systems.
The second sequence produces molecular hydrogen at a higher redshift than the first, as the dissociation energy thresholds of the intermediaries species $\text{H}_2^+$ and $\text{H}^-$ are 2.64 and 0.75 eV, respectively. The direct radiative association of $\text{H} + \text{H} \rightarrow \text{H}_2 + \gamma$ is highly forbidden, owing to the negligible dipole moment of the homonuclear $\text{H}_2$ molecule. The amount of $\text{H}_2$ that forms depends on the evolution of the gas density. Galli & Palla (1998) have analyzed in detail the case where the hydrogen follows the general expansion of the universe. Table 1 shows the reaction rates for hydrogen and helium species that enter in what they call the minimal model, i.e. the reduced set of processes that reproduces with excellent accuracy the full chemistry of $\text{H}_2$ molecules. Column 1 gives the reaction, column 2 the rate coefficient (in $\text{cm}^3$ $\text{s}^{-1}$ for collisional processes, in $\text{s}^{-1}$ for photon-processes), and column 3 the temperature range of validity of the rate coefficients and remarks on the rate (see Galli & Palla 1998). The gas and radiation temperatures are indicated by $T_e$ and $T$, respectively.

The evolution of the abundance of $\text{H}_2$ follows the well known behaviour (e.g. Lepp & Shull 1984) where an initial steep rise at $z \sim 400$ is determined by the $\text{H}_2^+$ channel, followed by a small contribution from $\text{H}^-$ at $z \sim 100$. The freeze-out primordial fraction of $\text{H}_2$ is $[\text{H}_2/\text{H}] \sim 10^{-6}$. This is too small to trigger runaway collapse, fragmentation, and star formation. The fate of a subgalactic system at high redshifts depends therefore on its ability to rapidly increase its $\text{H}_2$ content following virialization. In the low-density limit ($n_\text{H} < 0.1$ cm$^{-3}$), the $\text{H}_2$ cooling function $\Lambda_{\text{H}_2}$ (in erg cm$^3$ s$^{-1}$) is well approximated by the expression

$$\log \Lambda_{\text{H}_2}[n_\text{H} \rightarrow 0] = -103.0 + 97.59 \log T_e - 48.05(\log T_e)^2 + 10.80(\log T_e)^3 - 0.9032(\log T_e)^4,$$

over the range $10$ K $\leq T_e \leq 10^4$ K (Galli & Palla 1998).

3. The Emergence of Cosmic Structure

3.1. Linear theory

As shown above, it is only after hydrogen recombination that baryons can start falling into the already growing dark matter perturbations. Gas pressure can resist the force of gravity, and small-scale perturbations in the baryonic fluid will not grow in amplitude. However, at sufficiently large scales, gravity can overpower pressure gradients, thereby allowing the perturbation to grow.

The linear evolution of sub-horizon density perturbations in the dark matter-baryon fluid is governed in the matter-dominated era by two second-order differential equations:

$$\ddot{\delta}_{\text{dm}} + 2H\dot{\delta}_{\text{dm}} = \frac{3}{2}H^2\Omega_m^z (f_{\text{dm}}\delta_{\text{dm}} + f_b\delta_b)$$

(3.38)

for the dark matter, and

$$\ddot{\delta}_b + 2H\dot{\delta}_b = \frac{3}{2}H^2\Omega_m^z (f_{\text{dm}}\delta_{\text{dm}} + f_b\delta_b) - \frac{c_s^2}{a^2}k^2\delta_b$$

(3.39)

for the baryons, where $\delta_{\text{dm}}(k)$ and $\delta_b(k)$ are the Fourier components of the density fluctuations in the dark matter and baryons, $f_{\text{dm}}$ and $f_b$ are the corresponding mass fractions, $c_s$ is the gas sound speed, $k$ the (comoving) wavenumber, and the derivates are taken with respect to cosmic time. Here $\Omega_m^z = 8\pi G \rho(t)/3H^2 = \Omega_m(1+z)^3/\Omega_m(1+z)^3 +$

† For each fluid component ($i = \text{dm, b}$) the real space fluctuation in the density field, $\delta_i(x) \equiv \delta \rho_i(x)/\rho_i$, can be written as a sum over Fourier modes, $\delta_i(x) = \int d^3k (2\pi)^{-3} \delta_i(k) \exp i k \cdot x$. 

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In the case where $f_b \simeq 0$ and the universe is static ($H = 0$), equation (3.38) becomes

$$
\dot{\delta}_{\text{dm}} = 4\pi G \rho \delta_{\text{dm}} \equiv \frac{\delta_{\text{dm}}}{t_{\text{dyn}}^2},
$$

where $t_{\text{dyn}}$ denotes the dynamical timescale. This equation admits solution $\delta_{\text{dm}} = A_1 \exp(t/t_{\text{dyn}}) + A_2 \exp(-t/t_{\text{dyn}})$. After a few dynamical times, only the exponentially growing term is significant: gravity tends to make small density fluctuations in a static pressureless medium grow exponentially with time. The additional term $\propto H \dot{\delta}_{\text{dm}}$ present in an expanding universe can be thought as a “Hubble friction” term that acts to slow down the growth of density perturbations. Equation (3.38) admits the general solution for the growing mode:

$$
\delta_{\text{dm}}(a) = \frac{5\Omega_m}{2} \frac{H_0^2}{H} \int_0^a \frac{da'}{(a')^2},
$$

where the constant have been chosen so that an Einstein-de Sitter universe ($\Omega_m = 1, \Omega \Lambda = 0$) gives the familiar scaling $\delta_{\text{dm}}(a) = a$ with coefficient unity. The right-hand side of equation (3.41) is called the linear growth factor $D(a)$. Different values of $\Omega_m, \Omega \Lambda$ lead to different linear growth factors: growing modes actually decrease in density, but not as fast as the average universe. Note how, in contrast to the exponential growth found in the static case, the growth of perturbations even in the case of an Einstein-de Sitter universe is just algebraic. A remarkable approximation formula to the growth factor in a flat universe follows from Lahav et al. (1991),

$$
\delta_{\text{dm}}(a) = D(a) \simeq \frac{5\Omega_m}{2(1+z)} \left[ (\Omega_m^z) \frac{4}{7} - \frac{(\Omega_m^z)^2}{140} + \frac{209}{140} \Omega_m + \frac{1}{70} \right]^{-1}.
$$

This is good to a few percent in regions of plausible $\Omega_m, \Omega \Lambda$.

Equation (3.39) shows that, on large scales (i.e. small $k$), pressure forces can be neglected and baryons simply track the dark matter fluctuations. On the contrary, on small scales (i.e. large $k$), pressure dominates and baryon fluctuations will be suppressed relative to the dark matter. Gravity and pressure are equal at the characteristic Jeans scale:

$$
k_J = \frac{a}{c_s} \sqrt{4\pi G \rho}.
$$

Corresponding to this critical wavenumber $k_J$ there is a critical cosmological Jeans mass $M_J$, defined as the total (gas + dark matter) mass enclosed within the sphere of physical radius equal to $\pi a/k_J$,

$$
M_J = \frac{4\pi}{3} \rho \left( \frac{\pi a}{k_J} \right)^3 = \frac{4\pi}{3} \rho \left( \frac{5\pi k_B T_e}{12 G p m_p \mu} \right)^3 \approx 8.8 \times 10^4 M_\odot \left( \frac{a T_e}{\mu} \right)^{3/2},
$$

where $\mu$ is the mean molecular weight. The evolution of $M_J$ is shown in Figure 4. In the post-recombination universe, the baryon-electron gas is thermally coupled to the CMB, $T_e \propto a^{-1}$, and the Jeans mass is independent of redshift and comparable to the mass of globular clusters, $M_J \approx 10^5 M_\odot$. For $z < z_{\text{th}}$, the gas temperature drops as $T_e \propto a^{-2}$, and the Jeans mass decreases with time, $M_J \propto a^{-3/2}$. This trend is reversed by the reheating of the IGM. The energy released by the first collapsed objects drives the Jeans mass up to galaxy scales (Figure 4): baryonic density perturbations stop growing as their mass drops below the new Jeans mass. In particular, photo-ionization by the ultraviolet radiation from the first stars and quasars would heat the IGM to temperatures of $\approx 10^4 K$
(corresponding to a Jeans mass $M_J \sim 10^{10} M_\odot$ at $z_r = 11$), suppressing gas infall into low mass systems and preventing new (dwarf) galaxies from forming.$\dagger$

3.2. **Statistics of density fields**

The observed uniformity of the CMB guarantees that density fluctuations must have been quite small at decoupling, implying that the evolution of the density contrast can be studied at $z \lesssim z_{\text{dec}}$ using linear theory, and each mode $\delta(k)$ evolves independently. The inflationary model predicts a scale-invariant primordial power spectrum of density fluctuations $P(k) \equiv \langle |\delta(k)|^2 \rangle \propto k^n$, with $n = 1$ (the so-called Harrison-Zel’dovich spectrum). It is the index $n$ that governs the balance between large and small-scale power. In the case of a Gaussian random field with zero mean, the power spectrum contains the complete statistical information about the density inhomogeneity. It is often more convenient to use the dimensionless quantity $\Delta^2_k \equiv [k^3P(k)/2\pi^2]$, which is the power per logarithmic interval in wavenumber $k$. In the matter-dominated epoch, this quantity retains its initial primordial shape ($\Delta^2_k \propto k^{n+3}$) only on very large scales. Small wavelength modes enter the horizon earlier on and their growth is suppressed more severely during the radiation-dominated epoch: on small scales the amplitude of $\Delta^2_k$ is essentially suppressed by four powers of $k$ (from $k^{n+3}$ to $k^{n-1}$). If $n = 1$, then small scales will have nearly the same power except for a weak, logarithmic dependence. Departures from the initially scale-free form are described by the transfer function $T(k)$, defined such that $T(0) = 1$:

$$P(k, z) = A k^n \left[ \frac{D(z)}{D(0)} \right]^2 T^2(k), \quad (3.45)$$

where $A$ is the normalization. An accurate fitting function for $T(k)$ in a $\Lambda$CDM universe is

$$T_k = \ln(1 + 2.34q) \left[ 1 + 3.89q + (16.1q)^2 + (5.46q)^3 + (6.71q)^4 \right]^{-1/4}, \quad (3.46)$$

$\dagger$ When the Jeans mass itself varies with time, linear gas fluctuations tend to be smoothed on a (filtering) scale that depends on the full thermal history of the gas instead of the instantaneous value of the sound speed (Gnedin & Hui 1998).
where
\[ q \equiv \frac{k/{\text{Mpc}^{-1}}}{\Omega_m h^2 \exp(-\Omega_b - \Omega_b/\Omega_m)}. \]  
(3.47)

This is the fit given by Bardeen et al. (1986) modified to account for the effects of baryon density following Sugiyama (1995).

Another useful measurement of inhomogeneity is the quantity
\[ \sigma^2(M) = \frac{1}{2\pi^2} \int_0^\infty dk k^2 P(k)|W(kR)|^2. \]  
(3.48)

This is the mass variance of the density field smoothed by a window function \( W(kR) \) over a spherical volume of comoving radius \( R \) and average mass \( M = H_0^2 \Omega_m R^3/(2G) \). If the window is a top-hat in real space, then its Fourier transform is \( W(kR) = 3(kR)^{-3}(\sin kR - kR \cos kR) \). The significance of the window function is the following: the dominant contribution to \( \sigma(M) \) comes from perturbation components with wavelengths \( \lambda = 2\pi/k > R \), because those with higher frequencies tend to be averaged out within the window volume. As the fluctuation spectrum is falling with decreasing \( k \), waves with much larger \( \lambda \) contribute only a small amount. Hence, in terms of a mass \( M \propto \lambda^3 \propto k^{-3} \), we have
\[ \sigma(M) \propto M^{-(3+n)/n}. \]  
(3.49)

Since \( P(k) \) is not a strict power law, \( n \) should be thought of as an approximate local value \( d\ln P/d\ln k \) in the relevant range. For \( n > -3 \), the variance \( \sigma_M \) decreases with increasing \( M \); this implies that, on the average, smaller masses condense out earlier than larger masses. Structures grow by the gradual separation and collapse of progressively larger units. Each parent unit will in general be made up of a number of smaller progenitor clumps that had collapsed earlier. This leads to a hierarchical pattern of clustering. In CDM, \( n \geq -3 \) at small \( M \), increases with increasing \( M \) and reaches the asymptotic value \( n = 1 \) for \( M \gtrsim 10^{15} \, M_\odot \). The power spectrum on galactic scales can be approximated by \( n \approx -2 \).

3.3. Spherical collapse

At late times the density contrast at a given wavelength becomes comparable to unity, linear perturbation theory fails at this wavelength, and a different model must be used to follow the collapse of bound dark matter systems (“halos”). Small scales are the first to become non-linear. Consider, at some initial time \( t_i \), a spherical region of size \( r_i \) and mass \( M \) that has a slight constant overdensity \( \delta_i \) relative to the background \( \rho_b \),
\[ \rho(t_i) = \rho_b(t_i)(1 + \delta_i). \]  
(3.50)

As the universe expands, the overdense region will expand more slowly compared to the background, will reach a maximum radius, and eventually collapse under its own gravity to form a bound virialized system. Such a simple model is called a spherical top-hat. As long as radial shells do not cross each other during the evolution, the motion of a test particle at (physical) radius \( r \) is governed by the equation (ignoring the vacuum energy component)
\[ \frac{d^2r}{dt^2} = \frac{-GM}{r^2}. \]  
(3.51)

where \( M = (4\pi/3) r_i^3 \rho_b(t_i)(1 + \delta_i) \) = const. Integrating we obtain
\[ \frac{1}{2} \left( \frac{dr}{dt} \right)^2 - \frac{GM}{r} = E, \]  
(3.52)
where $E$ is a constant of integration. If $E > 0$ then $\dot{r}^2$ will never become zero and the shell will expand forever. If $E < 0$ instead, then as $r$ increases $\dot{r}$ will eventually become zero and later negative, implying a contraction and a collapse. Let’s choose $t_i$ to be the time at which $\delta_i$ is so small that the overdense region is expanding along with the Hubble flow. Then $\dot{r}_i = (\dot{a}/a)r_i = H(t_i)r_i \equiv H_i r_i$ at time $t_i$, and the initial kinetic energy will be

$$K_i \equiv \left(\frac{\dot{r}^2}{2}\right)_{t=t_i} = \frac{H_i^2 r_i^2}{2}. \quad (3.53)$$

The potential energy at $t = t_i$ is

$$|U| = \left(\frac{GM}{r}\right)_{t=t_i} = \frac{G4\pi}{3} \rho_b(t_i)(1 + \delta_i)r_i^2 = \frac{1}{2} H_i^2 r_i^2 \Omega_i(1 + \delta_i) = K_i \Omega_i(1 + \delta_i), \quad (3.54)$$

with $\Omega_i$ denoting the initial value of the matter density parameter of the smooth background universe. The total energy of the shell is therefore

$$E = K_i - K_i \Omega_i(1 + \delta_i) = K_i \Omega_i(\Omega_i^{-1} - 1 - \delta_i). \quad (3.55)$$

The condition $E < 0$ for the shell to eventually collapse becomes $(1 + \delta_i) > \Omega_i^{-1}$, or

$$\delta_i > \Omega_i^{-1} - 1. \quad (3.56)$$

In a Einstein-de Sitter universe at early times ($\Omega_i = 1$), this condition is satisfied by any overdense region with $\delta_i > 0$. In this case the patch will always collapse.

Consider now a shell with $E < 0$ in a background Einstein-de Sitter universe that expands to a maximum radius $r_{\text{max}}$ (‘turnaround’, $\dot{r} = 0$) and then collapses. The solution to the equation of motion can be written as the parametric equation for a cycloid

$$r = \frac{r_{\text{max}}}{2}(1 - \cos \theta), \quad t = t_{\text{max}} \frac{\theta - \sin \theta}{\pi}. \quad (3.57)$$

The background density evolves as $\rho_b(t) = (6\pi G t^2)^{-1}$, and the density contrast becomes

$$\delta = \frac{\rho(t)}{\rho_b(t)} - 1 = \frac{9}{2} \left(\frac{\theta - \sin \theta}{1 - \cos \theta}\right)^2 - 1. \quad (3.58)$$

For comparison, linear theory (in the limit of small $t$) gives

$$\delta_L = \frac{3}{20} \left(\frac{6\pi t}{t_{\text{max}}}\right)^{2/3} = \frac{3}{20} \left[6(\theta - \sin \theta)\right]^{2/3}. \quad (3.59)$$

This all agrees with what we knew already: at early times the sphere expands with the $a \propto t^{2/3}$ Hubble flow and density perturbations grow proportional to $a$. We can now see how linear theory breaks down as the perturbation evolves. There are three interesting epochs in the final stage of its development, which we can read directly from the above solutions.

**Turnaround.** The sphere breaks away from the Hubble expansion and reaches a maximum radius at $\theta = \pi$, $t = t_{\text{max}}$. At this point the true density enhancement with respect to the background is

$$\delta = \frac{9}{2} \pi^2 - 1 = \frac{9}{16} \pi^2 - 1 = 4.55, \quad (3.60)$$

which is definitely in the non-linear regime. By comparison, linear theory predicts

$$\delta_L = \frac{3}{20} (6\pi)^{2/3} = 1.062. \quad (3.61)$$
Collapse. If only gravity operates, then the sphere will collapse to a singularity at $\theta = 2\pi$, $t = 2t_{\text{max}}$. This occurs when

$$\delta_L = \frac{3}{20}(12\pi)^{2/3} = 1.686.$$  \hfill (3.62)

Thus from equation (3.42) we see that a top-hat collapses at redshift $z$ if its linear overdensity *extrapolated to the present day* is

$$\delta_c(z) = \frac{\delta_L}{D(z)} = 1.686(1 + z),$$  \hfill (3.63)

where the second equality holds in a flat Einstein-de Sitter universe. This is termed the critical overdensity for collapse. An object of mass $M$ collapsing at redshift $z$ has an overdensity that is $\nu_c$ times the linearly extrapolated density contrast today, $\sigma_0(M)$, on that scale,

$$\nu_c = \frac{\delta_c(z)}{\sigma_0(M)}. \hfill (3.64)$$

The mass scale associated with typical $\nu_c = 1-\sigma$ non-linear fluctuations in the density field decreases from $10^{13} \, M_\odot$ today to about $10^7 \, M_\odot$ at redshift 5. At $z = 10$, halos of $10^{10} \, M_\odot$ collapse from much rarer $\nu_c = 3-\sigma$ fluctuations.

Virialization. Collapse to a point at $\theta = 2\pi$ ($t = 2t_{\text{max}} \equiv t_{\text{vir}}$) will never occur in practice as, before this happens, the approximation that matter is distributed in spherical shells and that the random velocities of the particles are small will break down. The dark matter will reach virial equilibrium by a process known as ‘violent relaxation’: since the gravitational potential is changing with time, individual particles do not follow orbits that conserve energy, and the net effect is to widen the range of energies available to them. Thus a time-varying potential can provide a relaxation mechanism that operates on the dynamical timescale rather than on the much longer two-body relaxation time. This process will convert the kinetic energy of collapse into random motions.

At $t = t_{\text{max}}$ all the energy is in the form of gravitational potential energy, and $E = U = -GM/r_{\text{max}}$. At virialization $U = -2K$ (virial theorem) and $E = U + K = U/2 = -GM/(2r_{\text{vir}})$. Hence $r_{\text{vir}} = r_{\text{max}}/2$. The mean density of the virialized object is then $\rho_{\text{vir}} = 2^3\rho_{\text{max}}$, where $\rho_{\text{max}}$ is the density of the shell at turnaround. From equation (3.60) we have $\rho_{\text{max}} = (9/16)\pi^2\rho_b(t_{\text{max}})$, and $\rho_b(t_{\text{max}}) = \rho_b(t_{\text{vir}})/(t_{\text{vir}}/t_{\text{max}})^2 = 4\rho_b(t_{\text{vir}})$. Combining these relations we get:

$$\rho_{\text{vir}} = 2^3\rho_{\text{max}} = 2^4(9/16)\pi^2\rho_b(t_{\text{max}}) = 2^4(9/16)\pi^24\rho_b(t_{\text{vir}}) = 18\pi^2\rho_b(t_{\text{vir}}).$$  \hfill (3.65)

Therefore the density contrast at virialization in an Einstein-de Sitter universe is

$$\Delta_c = 178. \hfill (3.66)$$

In a universe with a cosmological constant, the collapse of a top-hat spherical perturbation is described by

$$\frac{d^2r}{dt^2} = -\frac{GM}{r^2} + \frac{\Lambda}{3} r^3.$$  \hfill (3.67)

In a flat $\Omega_m + \Omega_\Lambda = 1$ cosmology, the final overdensity relative to the critical density gets modified according to the fitting formula (Bryan & Norman 1998)

$$\Delta_c = 18\pi^2 + 82d - 39d^2, \hfill (3.68)$$

where $d \equiv \Omega_m^z - 1$ is evaluated at the collapse redshift. A spherical top-hat collapsing today in a universe with $\Omega_m = 0.24$ has a density contrast at virialization of $\Delta_c = 93$. This corresponds to an overdensity relative to the background matter density (=$
\( \Omega_m \rho_c^0 \) of \( \Delta_c/\Omega_m = 388 \): the faster expansion of a low-density universe means that the perturbation turns around and collapses when a larger density contrast has been produced. For practical reason a density contrast of 200 relative to the background is often used to define the radius, \( r_{200} \), that marks the boundary of a virialized region.

A halo of mass \( M \) collapsing at redshift \( z \) can be described in terms of its virial radius \( r_{\text{vir}} \), circular velocity \( V_c \) and virial temperature \( T_{\text{vir}} \) (Barkana & Loeb 2001):

\[
\begin{align*}
  r_{\text{vir}} &= \left[ \frac{2GM}{\Delta_c H^2} \right]^{1/3} = 1.23 \, \text{kpc} \left( \frac{M}{10^8 \, M_\odot} \right)^{1/3} f^{-1/3} \left( \frac{1+z}{10} \right)^{-1}, \\
  V_c &= \left( \frac{GM}{r_{\text{vir}}} \right)^{1/2} = 21.1 \, \text{km s}^{-1} \left( \frac{M}{10^8 \, M_\odot} \right)^{1/3} f^{1/6} \left( \frac{1+z}{10} \right)^{1/2}, \\
  T_{\text{vir}} &= \frac{\mu m_p V_c^2}{2 k_B} = 1.6 \times 10^4 \, \text{K} \left( \frac{M}{10^8 \, M_\odot} \right)^{2/3} f^{1/3} \left( \frac{1+z}{10} \right),
\end{align*}
\]

where \( f \equiv (\Omega_m/\Omega_m^0)(\Delta_c/18\pi^2) \) and \( \mu = 0.59 \) is the mean molecular weight for fully ionized primordial gas (\( \mu = 1.23 \) for neutral primordial gas). The binding energy of the halo is approximately

\[
E_b = \frac{1}{2} \frac{GM^2}{r_{\text{vir}}} = 4.42 \times 10^{53} \, \text{erg} \left( \frac{M}{10^8 \, M_\odot} \right)^{5/3} f^{1/3} \left( \frac{1+z}{10} \right),
\]

where the coefficient of 1/2 is exact for a singular isothermal sphere. The binding energy of the baryons is smaller by a factor \( \Omega_m/\Omega_b \simeq 5.7 \). The energy deposition by supernovae in the shallow potential wells of subgalactic systems may then lift out metal-enriched material from the host (dwarf) halos, causing the pollution of the IGM at early times (Madau et al. 2001).

### 3.4. Dark halo mergers

The assumption that virialized objects form from smooth spherical collapse, while providing a useful framework for thinking about the formation histories of gravitationally bound dark matter halos, does not capture the real nature of structure formation in CDM theories. In these models galaxies are assembled hierarchically through the merging of many smaller subunits that formed in a similar manner at higher redshift (see Fig. 5). Galaxy halos experience multiple mergers during their lifetime, with those between comparable-mass systems (“major mergers”) expected to result in the formation of elliptical galaxies (see, e.g., Barnes 1988; Hernquist 1992). Figure 6 shows the number of major mergers (defined as mergers where the mass ratio of the progenitors is \( > 0.3 \)) per unit redshift bin experienced by halos of different masses. For galaxy-sized halo this quantity happens to peak in the redshift range 2-4, the epoch when the observed space density of optically-selected quasar also reaches a maximum.

The merger between a large parent halo and a smaller satellite system will evolve under two dynamical processes: dynamical friction, that causes the orbit of the satellite to decay toward the central regions, and tidal stripping, that removes material from the satellite and adds it to the diffuse mass of the parent. Since clustering is hierarchical, the satellite will typically form at earlier times and have a higher characteristic density and a smaller characteristic radius. The study of the assembly history of dark matter halos by repeated mergers is particularly well suited to the N-body methods that have been developed in the past two decades. Numerical simulations of structure formation by dissipationless hierarchical clustering from Gaussian initial conditions indicate a roughly
universal spherically-averaged density profile for the resulting halos (Navarro et al. 1997, hereafter NFW):

$$\rho_{\text{NFW}}(r) = \frac{\rho_s}{cx(1+cx)^2},$$

where $x \equiv r/r_{\text{vir}}$, and the characteristic density $\rho_s$ is related to the concentration parameter $c$ by

$$\rho_s = \frac{3H^2}{8\pi G} \frac{\Delta_c}{3} \frac{c^3}{\ln(1+c) - c/(1+c)}.$$

This function fits the numerical data presented by NFW over a radius range of about two orders of magnitude. Equally good fits are obtained for high-mass (rich galaxy cluster) and low-mass (dwarf) halos. Power-law fits to this profile over a restricted radial range have slopes that steepen from $-1$ near the halo center to $-3$ at large $cr/r_{\text{vir}}$. Bullock et al. (2001) found that the concentration parameter follows a log-normal distribution where the median depends on the halo mass and redshift,

$$c_{\text{med}}(M, z) = \frac{c_*}{1+z} \left( \frac{M}{M_*} \right)^{\alpha},$$

where $M_*$ is the mass of a typical halo collapsing today. The halos in the simulations by
Figure 6. Mean number of major mergers experienced per unit redshift by halos with masses $> 10^{10} \, M_\odot$. Solid line: progenitors of a $M_0 = 2 \times 10^{13} \, M_\odot$ halo at $z = 0$. Dashed line: same for $M_0 = 3 \times 10^{12} \, M_\odot$. Dotted line: same for $M_0 = 10^{11} \, M_\odot$. (From Volonteri et al. 2003.)

Bullock et al. were best described by $\alpha = -0.13$ and $c_* = 9.0$, with a scatter around the median of $\sigma_{\log c} = 0.14$ dex.

“Via Lactea”, the highest resolution N-body simulation to date of the formation of a Milky Way-sized halo (Diemand et al. 2007a,b), shows that the fitting formula proposed by NFW with concentration $c = 12$ provides a reasonable approximation to the density profile down a convergence radius of $r_{\text{conv}} = 1.3$ kpc. Within the region of convergence, deviations from the best-fit NFW matter density are typically less than 10%. From 10 kpc down to $r_{\text{conv}}$ Via Lactea is actually denser than predicted by the NFW formula. Near $r_{\text{conv}}$ the density approaches the NFW value again while the logarithmic slope is shallower ($-1.0$ at $r_{\text{conv}}$) than predicted by the NFW fit.

3.5. Assembly history of a Milky Way halo

The simple spherical top-hat collapse ignores shell crossing and mixing, accretion of self-bound clumps, triaxiality, angular momentum, random velocities, and large scale tidal forces. It is interesting at this stage to use “Via Lactea” and study in more details, starting from realistic initial conditions, the formation history of a Milky Way-sized halo in a $\Lambda$CDM cosmology. The Via Lactea simulation was performed with the PKDGRAV tree-code (Stadel 2001) using the best-fit cosmological parameters from the WMAP 3-year data release. The galaxy-forming region was sampled with 234 million particles of mass $2.1 \times 10^4 \, M_\odot$, evolved from redshift 49 to the present with a force resolution of 90 pc and adaptive time-steps as short as 68,500 yr, and centered on an isolated halo that had no major merger after $z = 1.7$, making it a suitable host for a Milky Way-like disk galaxy (see Fig. 8). The number of particles is an order of magnitude larger than used in previous simulations. The run was completed in 320,000 CPU hours on NASA’s Project Columbia supercomputer, currently one of the fastest machines available. (More details about the Via Lactea run are given in Diemand et al. 2007a,b. Movies, images, and data
Figure 7. Top: logarithmic slope of the density profile of the “Via Lactea” halo, as a function of radius. Densities were computed in 50 radial logarithmic bins, and the local slope was determined by a finite difference approximation using one neighboring bin on each side. The thin line shows the slope of the best-fit NFW profile with concentration $c = 12$. The vertical dotted line indicates the estimated convergence radius: local densities (but not necessarily the logarithmic slopes) should be correct to within 10% outside of this radius. Bottom: the residuals in percent between the density profile and the best-fit NFW profile, as a function of radius. Here $r_{200}$ is the radius within which the enclosed average density is 200 times the background value, $r_{200} = 1.35 r_{\text{vir}}$ in the adopted cosmology. (From Diemand et al. 2007a.)

are available at http://www.ucolick.org/~diemand/vl.) The host halo mass at $z = 0$ is $M_{200} = 1.8 \times 10^{12} \, M_\odot$ within a radius of $r_{200} = 389 \, \text{kpc}$.

Following the spherical top-hat model, the common procedure used to describe the assembly of a dark matter halo is to define at each epoch a virial radius $r_{\text{vir}}$ (or, equivalently, $r_{200}$), which depends on the cosmic background density at the time. As the latter decreases with the Hubble expansion, formal virial radii and masses grow with cosmic time even for stationary halos. Studying the transformation of halo properties within $r_{\text{vir}}$ (or some fraction of it) mixes real physical change with apparent evolutionary effects caused by the growing radial window, and makes it hard to disentangle between the two. Figure 9 shows the formation of Via Lactea where radial shells enclosing a fixed mass, $r_M$, have been used instead. Unlike $r_{\text{vir}}$, $r_M$ stops growing as soon as the mass distribution of the host halo becomes stationary on the corresponding scale. Note that mass and substructure are constantly exchanged between these shells, as $r_M$ is not a Lagrangian radius enclosing the same material at all times, just the same amount of it. The fraction of material belonging to a given shell in the past that still remains within the same shell today is shown in Figure 10. The mixing is larger before stabilization, presumably because of shell crossing during collapse, and smaller near the center, where
most of the mass is in a dynamically cold, concentrated old component (Diemand et al. 2005b). Outer shells number 9 and 10, for example, retain today less than 25% of the particles that originally belonged to them at $a < 0.4$. Note that the collapse times also appear to differ from the expectations of spherical top-hat. Shell number five, for example, encloses a mean density of about $100 \rho_0$ today, a virial mass of $1.5 \times 10^{12} M_\odot$ and should have virialized just now according to spherical top-hat. It did so instead much earlier, at $a = 0.6$. Even the next larger shell with $1.8 \times 10^{12} M_\odot$ stabilized before
Figure 9. Evolution of radii $r_M$ enclosing a fixed mass versus cosmic time or scale factor $a$. The enclosed mass grows in constant amounts of $0.3 \times 10^{12} M_\odot$ from bottom to top. Initially all spheres are growing in the physical (non comoving) units used here. Inner shells turn around, collapse and stabilize, while the outermost shells are still expanding today. Solid circles: points of maximum expansion at the turnaround time $t_{max}$. Open squares: time after turnaround where $r_M$ first contracts within 20% of the final value. These mark the approximate epoch of “stabilization”.

$a = 0.8$. It appears that spherical top-hat provides only a crude approximation to the virialized regions of simulated galaxy halos.

To understand the mass accretion history of the Via Lactea halo it is useful to analyze the evolution of mass within fixed physical radii. Figure 11 shows that the mass within all radii from the resolution limit of $\approx 1$ kpc up to 100 kpc grows during a series of major mergers before $a = 0.4$. After this phase of active merging and growth by accretion the halo mass distribution remains almost perfectly stationary at all radii. Only the outer regions ($\sim 400$ kpc) experience a small amount of net mass accretion after the last major merger. The mass within 400 kpc increases only mildly, by a factor of 1.2 from $z = 1$ to the present. During the same time the mass within radii of 100 kpc and smaller, the peak circular velocity and the radius where this is reached, all remain constant to within 10%. The fact that mass definitions inspired by spherical top-hat fail to accurately describe the real assembly of galaxy halos is clearly seen in Figure 11, where $M_{200}$ is shown to increase at late times even when the halo physical mass remains the same. This is just an artificial effect caused by the growing radial windows $r_{\text{vir}}$ and $r_{200}$ as the background density decreases. For Via Lactea $M_{200}$ increases by a factor of 1.8 from $z = 1$ to the present, while the real physical mass within a 400 kpc sphere grows by only a factor of 1.2 during the same time interval, and by an even smaller factor at smaller radii.

3.6. Smallest SUSY-CDM microhalos

As already mentioned above, the key idea of the standard cosmological paradigm for the formation of structure in the universe, that primordial density fluctuations grow by gravitational instability driven by cold, collisionless dark matter, is constantly being
elaborated upon and explored in detail through supercomputer simulations, and tested against a variety of astrophysical observations. The leading candidate for dark matter is the neutralino, a weakly interacting massive particle predicted by the supersymmetry (SUSY) theory of particle physics. While in a SUSY-CDM scenario the mass of bound dark matter halos may span about twenty order of magnitudes, from the most massive galaxy clusters down to Earth-mass clumps (Green et al. 2004), it is the smallest microhalos that collapse first, and only these smallest scales are affected by the nature of the relic dark matter candidate.

Recent numerical simulations of the collapse of the earliest and smallest gravitationally bound CDM clumps (Diemand et al. 2005a; Gao et al. 2005) have shown that tiny virialized microhalos form at redshifts above 50 with internal density profiles that are quite similar to those of present-day galaxy clusters. At these epochs a significant fraction of neutralinos has already been assembled into non-linear Earth-mass overdensities. If this first generation of dark objects were to survive gravitational disruption during the early hierarchical merger and accretion process – as well as late tidal disruption from stellar encounters (Zhao et al. 2007) – then over $10^{15}$ such clumps may populate the halo of the Milky Way. The nearest microhalos may be among the brightest sources of $\gamma$-rays from neutralino annihilation. As the annihilation rate increases quadratically with the matter density, small-scale clumpiness may enhance the total $\gamma$-ray flux from nearby extragalactic systems (like M31), making them detectable by the forthcoming GLAST satellite or the next-generation of air Cerenkov telescopes.

The possibility of observing the fingerprints of the smallest-scale structure of CDM in direct and indirect dark matter searches hinges on the ability of microhalos to survive the hierarchical clustering process as substructure within the larger halos that form at later times. In recent years high-resolution N-body simulations have enabled the study
Figure 11. Mass accretion history of Via Lactea. Masses within spheres of fixed physical radii centered on the main progenitor are plotted against the cosmological expansion factor $a$. The thick solid lines correspond to spheres with radii given by the labels on the left. The thin solid lines correspond to nine spheres of intermediate radii that are $1.3, 1.6, 2.0, 2.5, 3.2, 4.0, 5.0, 6.3$ and $7.9$ times larger than the next smaller labeled radius. Dashed line: $M_{200}$. The halo is assembled during a phase of active merging before $a \approx 0.37$ ($z \approx 1.7$) and its net mass content remains practically stationary at later times.

of gravitationally-bound subhalos with $M_{\text{sub}}/M \gtrsim 10^{-6}$ on galaxy (and galaxy cluster) scales (e.g. Moore et al. 1999; Klypin et al. 1999; Stoehr et al. 2003). The main differences between these subhalos – the surviving cores of objects which fell together during the hierarchical assembly of galaxy-size systems – and the tiny sub-microhalos discussed here is that on the smallest CDM scale the effective index of the linear power spectrum of mass density fluctuations is close to $-3$. In this regime typical halo formation times depend only weakly on halo mass, the capture of small clumps by larger ones is very rapid, and sub-microhalos may be more easily disrupted.

In Diemand et al. (2006) we presented a large N-body simulation of early substructure in a SUSY-CDM scenario characterized by an exponential cutoff in the power spectrum at $10^{-6} M_{\odot}$. The simulation resolves a $0.014 M_{\odot}$ parent “SUSY” halo at $z = 75$ with 14 million particles. Compared to a $z = 0$ galaxy cluster substructure within the SUSY host is less evident both in phase-space and in physical space (see Figs. 12 and 13), and it is less resistant against tidal disruption. As the universe expands by a factor of 1.3, between 20 and 40 percent of well-resolved SUSY substructure is destroyed, compared to only $\sim 1$ percent in the low-redshift cluster. Nevertheless SUSY substructure is just as abundant as in $z = 0$ galaxy clusters, i.e. the normalized mass and circular velocity functions are very similar.
Figure 12. Local dark matter density maps. The left panels illustrate the almost simultaneous structure formation in the SUSY run at different epochs, within a sphere of physical radius \( r \) including a mass of \( 0.014 \, M_\odot \). A galaxy cluster halo (right panels) forms in the standard hierarchical fashion: the dark matter distribution is shown within a sphere of radius \( r \) including a mass of \( 5.9 \times 10^{14} \, M_\odot \). The SUSY and cluster halos have concentration parameter for a NFW profile of \( c = 3.7 \) and \( c = 3.5 \), respectively. In each image the logarithmic color scale ranges from 10 to \( 10^6 \rho_c(z) \).

4. The Dawn of Galaxies

4.1. Uncertainties in the power spectrum

As mentioned in the Introduction, some shortcomings on galactic and sub-galactic scales of the currently favored model of hierarchical galaxy formation in a universe dominated by CDM have recently appeared. The significance of these discrepancies is still debated, and ‘gastrophysical’ solutions involving feedback mechanisms may offer a possible way
Figure 13. Phase-space density \((\rho/\sigma^3)\), where \(\sigma\) is the one-dimensional velocity dispersion) map for a \(z = 75\) SUSY halo (left) and a \(z = 0\) galaxy cluster (right). Note the different color scales: relative to the average phase-space density, the logarithmic color scale ranges from \(10\) to \(10^5\) in the SUSY halo and from \(10\) to \(10^7\) in the cluster halo.

Other models have attempted to solve the apparent small-scale problems of CDM at a more fundamental level, i.e. by reducing small-scale power. Although the ‘standard’ ΛCDM model for structure formation assumes a scale-invariant initial power spectrum of density fluctuations with index \(n = 1\), the recent WMAP data find strong evidence for a departure from scale invariance, with a best fit value \(n = 0.951^{+0.015}_{-0.019}\). Furthermore the 1-year WMAP results favored a slowly varying spectral index, \(dn/d\ln k = -0.031^{+0.016}_{-0.018}\), i.e. a model in which the spectral index varies as a function of wavenumber \(k\) (Spergel et al. 2003). In the 3-year WMAP data such a ‘running spectral index’ leads to a marginal improvement in the fit. Models with either \(n < 1\) or \(dn/d\ln k < 0\) predict a significantly lower amplitude of fluctuations on small scales than standard ΛCDM. The suppression of small-scale power has the advantage of reducing the amount of substructure in galactic halos and makes small halos form later (when the universe was less dense) hence less concentrated (Zentner & Bullock 2002).

Figure 14 shows the linearly extrapolated (to \(z = 0\)) variance of the mass-density field for a range of cosmological parameters. Note that the new WMAP results prefer a low value for \(\sigma_8\), the rms mass fluctuation in a \(8\ h^{-1}\)Mpc sphere. This is consistent with a normalization by the \(z = 0\) X-ray cluster abundance (Reiprich & Böringer 2002). For comparison we have also included a model with a higher normalization, \(\sigma_8 = 0.9\), from the best-fit model to 1-year WMAP data. As in the CDM paradigm structure formation proceeds bottom-up, it then follows that the loss of small-scale power modifies structure formation most severely at the highest redshifts, significantly reducing the number of self-gravitating objects then. This, of course, will make it more difficult to reionize the universe early enough.

It has been argued, for example, that one popular modification of the CDM paradigm, warm dark matter (WDM), has so little structure at high redshift that it is unable to explain the WMAP observations of an early epoch of reionization (Barkana et al. 2001). And yet the WMAP running-index model may suffer from a similar problem. A look
Figure 14. The variance of the matter-density field vs. mass $M$, for several different cosmologies, all based on WMAP results. Solid curve: 3-year WMAP-only best-fit model. Dotted curve: WDM with a particle mass $m_X = 2$ keV, otherwise same as before. Dashed curve: 3-year year WMAP best-fit running spectral index model. Dash-dotted curve: 1-year WMAP-only best-fit tilted model. Here $n$ refers to the spectral index at $k = 0.05 \text{Mpc}^{-1}$. The horizontal line at the top of the figure shows the value of the extrapolated critical collapse overdensity $\delta_c(z)$ at the reionization redshift $z = 11$.

at Figure 14 shows that $10^6 M_\odot$ halos will collapse at $z = 11$ from $2.4 \sigma$ fluctuations in a tilted $\Lambda$CDM model with $n = 0.951$ and $\sigma_8 = 0.74$ (best-fit 3-year WMAP model), but from much rarer $3.7$ and $3.6 \sigma$ fluctuations in the WDM and running-index model, respectively. The problem is that scenarios with increasingly rarer halos at early times require even more extreme assumptions (i.e. higher star formation efficiencies and UV photon production rates) in order to be able to reionize the universe suitably early (e.g. Somerville et al. 2003; Wyithe & Loeb 2003; Ciardi et al. 2003; Cen 2003). Figure 15 depicts the mass fraction in all collapsed halos with masses above the cosmological filtering mass for a case without reionization and one with reionization occurring at $z \approx 11$. At early epochs this quantity appears to vary by orders of magnitude in different models.

4.2. First baryonic objects

The study of the non-linear regime for the baryons is far more complicated than that of the dark matter because of the need to take into account pressure gradients and radiative processes. As a dark matter halo grows and virializes above the cosmological Jeans mass through merging and accretion, baryonic material will be shock heated to the effective virial temperature of the host and compressed to the same fractional overdensity as the dark matter. The subsequent behavior of gas in a dark matter halo depends on the efficiency with which it can cool. It is useful here to identify two mass scales for the host halos: (1) a molecular cooling mass $M_{H_2}$ above which gas can cool via roto-vibrational levels of $H_2$ and contract, $M_{H_2} \approx 10^5 [(1 + z)/10]^{-3/2} M_\odot$ (virial temperature above 200 K); and (2) an atomic cooling mass $M_H$ above which gas can cool efficiently and fragment via excitation of hydrogen Ly$\alpha$, $M_H \approx 10^8 [(1 + z)/10]^{-3/2} M_\odot$ (virial temperature above $10^4$ K). Figure 16 shows the cooling mechanisms at various temperatures for
Figure 15. Mass fraction in all collapsed halos above the cosmological filtering (Jeans) mass as a function of redshift, for different power spectra. Curves are the same as in Figure 14. Left panel: filtering mass computed in the absence of reionization. Right panel: filtering mass computed assuming the universe is reionized and reheated to $T_e = 10^4$ K by ultraviolet radiation at $z \simeq 11$.

Figure 16. Cooling rates for Bremsstrahlung (dotted line), H (dashed line) and He (dash-dotted line) line cooling, and H$_2$ (circles) cooling. The $e^-$, H II, He II, and He III abundances were computed assuming collisional equilibrium, and the H$_2$ fractional abundance was fixed at $3 \times 10^{-4}$, which is typical for early objects. At temperatures between 100 and 10,000 K, the H$_2$ molecule is the most effective coolant (From Fuller & Couchman 2000).

primordial gas, while Figure 17 shows the fraction of the total mass in the universe that is in collapsed dark matter halos with masses greater than $M_{H_2}$ and $M_H$ at different epochs.

High-resolution hydrodynamics simulations of early structure formation are a powerful tool to track in detail the thermal and ionization history of a clumpy IGM and guide studies of primordial star formation and reheating. Such simulations performed in the context of ΛCDM cosmologies have shown that the first stars (the so-called 'Population III') in the universe formed out of metal-free gas in dark matter minihalos of mass above a few $\times 10^5$ $M_\odot$ (Abel et al. 2000; Fuller & Couchman 2000; Yoshida et al. 2003; Reed
et al. 2005) condensing from the rare high-$\nu_c$ peaks of the primordial density fluctuation field at $z > 20$, and were likely very massive (e.g. Abel et al. 2002; Bromm et al. 2002; see Bromm & Larson 2004 and Ciardi & Ferrara 2005 for recent reviews). In Kuhlen \\& Madau (2005) we used a modified version of enzo, an adaptive mesh refinement (AMR), grid-based hybrid (hydro+N-body) code developed by Bryan \\& Norman (see http://cosmos.ucsd.edu/enzo/) to solve the cosmological hydrodynamics equations and study the cooling and collapse of primordial gas in the first baryonic structures. The simulation samples the dark matter density field in a 0.5 Mpc box with a mass resolution of 2000 M$_\odot$ to ensure that halos above the cosmological Jeans mass are well resolved at all redshifts $z < 20$. The AMR technique allows us to home in, with progressively finer resolution, on the densest parts of the “cosmic web”. During the evolution from $z = 99$ to $z = 15$, refined (child) grids are introduced with twice the spatial resolution of the coarser (parent) grid when a cell reaches a dark matter overdensity (baryonic overdensity) of 2.0 (4.0). Dense regions are allowed to dynamically refine to a maximum resolution of 30 pc (comoving). The code evolves the non-equilibrium rate equations for nine species (H, H$^+$, H$^-$, e, He, He$^+$, He$^{++}$, H$_2$, and H$_2^+$) in primordial self-gravitating gas, including radiative losses from atomic and molecular line cooling, and Compton cooling by the cosmic background radiation.

The clustered structure around the most massive peaks of the density field is clearly seen in Figure 18, a 3D volume rendering of the simulated volume at redshifts 21 and 15.5. The figure shows gas at $4 < \delta_b < 10$, with the locations of dark matter minihalos marked by spheres colored and sized according to their mass (the spheres are only markers, the actual shape of the halos is typically non-spherical). Several interleaving filaments are visible, at the intersections of which minihalos are typically found. At $z = 21$, 55 bound halos are identified in the simulated volume: by $z = 17.5$ this number has grown to 149, and by $z = 15.5$ to 262 halos. At this epoch, only four halos have reached the critical virial temperature for atomic cooling, $T_{\text{vir}} = 10^4$ K.
Figure 18. A 3D volume rendering of the IGM in the inner 0.5 Mpc simulated box at $z = 21$ (left panel) and $z = 15.5$ (right panel). Only gas with overdensity $4 < \delta_b < 10$ is shown; the locations of dark matter minihalos are marked by spheres with sizes proportional to halo mass. At these epochs, the halo finder algorithm identifies 55 ($z = 21$) and 262 ($z = 15.5$) bound clumps within the simulated volume. (From Kuhlen & Madau 2005.)

Figure 19. Left: Fraction of cold and cold+dense gas within the virial radius of all halos identified at $z = 17.5$ with $T_{\text{vir}} > 400$ K, as a function of halo mass. Triangles: $f_c$, fraction of halo gas with $T < 0.5 T_{\text{vir}}$ and overdensity $\delta_b > 1000$ that cooled via roto-vibrational transitions of H$_2$. Diamonds: $f_{\text{cd}}$, fraction of gas with $T < 0.5 T_{\text{vir}}$ and $\rho > 10^{19}$ M$_\odot$ Mpc$^{-3}$ that is available for star formation. The straight lines represent mean regression analyses of $f_c$ and $f_{\text{cd}}$ with the logarithm of halo mass. Right: Mass-weighted mean H$_2$ fraction as a function of virial temperature for all halos at $z = 17.5$ with $T_{\text{vir}} > 400$ K and $f_{\text{cd}} < 0.1$ (empty circles) or $f_{\text{cd}} > 0.1$ (filled circles). The straight line marks the scaling of the temperature-dependent asymptotic molecular fraction.

The primordial fractional abundance of H$_2$ in the low-density IGM is small, $x_{H_2} \equiv [H_2/H] \approx 2 \times 10^{-6}$, as at $z > 100$ H$_2$ formation is inhibited because the required intermediaries, either H$_2^+$ or H$^-$, are destroyed by CMB photons. Most of the gas in the simulation therefore cools by adiabatic expansion. Within collapsing minihalos, however, gas densities and temperatures are large enough that H$_2$ formation is catalyzed by H$^-$ ions through the associative detachment reaction H$^+$H$^- \rightarrow$ H$_2$+e$^-$, and the molecular
fraction increases at the rate $dx_{\text{H}_2}/dt \propto x_e n_{\text{HI}} T_{\text{vir}}^{0.88}$, where $x_e$ is the number of electrons per hydrogen atom. For $T_{\text{vir}} \lesssim 10^3$ K, the free electrons left over from recombination are depleted in the denser regions, and the production of H$_2$ stalls at a temperature-dependent asymptotic molecular fraction $x_{\text{H}_2} \approx 10^{-8} T_{\text{vir}}^{1.5} \ln(1 + t/t_{\text{rec}})$, where $t_{\text{rec}}$ is the hydrogen recombination time-scale (Tegmark et al. 1997). A typical H$_2$ fraction in excess of 200 times the primordial value is therefore produced after the collapse of structures with virial temperatures of order $10^3$ K. This is large enough to efficiently cool the gas and allow it to collapse within a Hubble time unless significant heating occurs during this phase (Abel et al. 2000; Yoshida et al. 2003).

Fig. 19 (left panel) shows the fraction of cold gas within the virial radius as a function of halo mass for all the halos identified at redshift 17.5. Following Machacek et al. (2001), we define $f_c$ as the fraction of gas with temperature $< 0.5 T_{\text{vir}}$ and density $> 1000$ times the background (this is the halo gas that is able to cool below the virial temperature because of H$_2$), and $f_{\text{cd}}$ as the fraction of gas with temperature $< 0.5 T_{\text{vir}}$ and (physical) density $> 10^{19}$ M$_\odot$ Mpc$^{-3}$ (this is the self-gravitating gas available for star formation). As in Machacek et al. (2001), we find that both $f_c$ and $f_{\text{cd}}$ are correlated with halo mass. The threshold for significant baryonic condensation (non-zero $f_{\text{cd}}$) is approximately $5 \times 10^5$ M$_\odot$ at these redshifts (Haiman et al. 1996). Also depicted in Fig. 19 (right panel) is the mass-weighted mean molecular fraction of all halos with $T_{\text{vir}} > 400$ K. Filled circles represent halos with $f_{\text{cd}} > 0.1$, while open circles represent the others. The straight line marks the scaling of the asymptotic molecular fraction in the electron-depletion transition regime. The maximum gas density reached at redshift 15 in the most refined region of our simulation is $4 \times 10^5$ cm$^{-3}$ (corresponding to an overdensity of $3 \times 10^8$): within this cold pocket the excited states of H$_2$ are in LTE and the cooling time is nearly independent of density.

4.3. 21cm signatures of the neutral IGM

It has long been known that neutral hydrogen in the diffuse IGM and in gravitationally collapsed structures may be directly detectable at frequencies corresponding to the redshifted 21cm line of hydrogen (Field 1959; Sunyaev & Zel’dovich 1975; Hogan & Rees 1979; see Furlanetto et al. 2006 for a recent review). The emission or absorption of 21cm photons from neutral gas is governed by the spin temperature $T_S$, defined as

$$n_1/n_0 = 3 \exp(-T_*/T_S).$$

Here $n_0$ and $n_1$ are the number densities of hydrogen atoms in the singlet and triplet $n = 1$ hyperfine levels, and $T_*$ = 0.068 K is the temperature corresponding to the energy difference between the levels. To produce an absorption or emission signature against the CMB, the spin temperature must differ from the temperature of the CMB, $T = 2.73 (1+z)$ K. At $30 \lesssim z \lesssim 200$, prior to the appearance of non-linear baryonic objects, the IGM cools adiabatically faster than the CMB, spin-exchange collisions between hydrogen atoms couple $T_2$ to the kinetic temperature $T_k$ of the cold gas, and cosmic hydrogen can be observed in absorption (Scott & Rees 1990; Loeb & Zaldarriaga 2004). At lower redshifts, the Hubble expansion rarefies the gas and makes collisions inefficient; the spin states go into equilibrium with the radiation, and as $T_S$ approaches $T$ the 21cm signal diminishes. It is the first luminous sources that make uncollapsed gas in the universe shine again in 21cm, by mixing the spin states either via Lyo scattering or via enhanced free electron-atom collisions (e.g. Madau et al. 1997; Tozzi et al. 2000; Nusser 2005).

While the atomic physics of the 21cm transition is well understood in the cosmological context, exact calculations of the radio signal expected during the era between the col-
The H I spin temperature is a weighted mean between $T_e$ and $T,$

$$T_S = \frac{T_e + T + yT_e}{1 + y},$$  \hspace{1cm} (4.77)

where coupling efficiency $y$ is the sum of three terms,

$$y = \frac{T_e}{A T_e} (C_H + C_e + C_p).$$  \hspace{1cm} (4.78)

Here $A = 2.85 \times 10^{-15} \text{s}^{-1}$ is the spontaneous emission rate and $C_H,$ $C_e,$ and $C_p$ are the de-excitation rates of the triplet due to collisions with neutral atoms, electrons, and protons. A fourth term must be added in the presence of ambient Lyα radiation, as intermediate transitions to the 2p level can mix the spin states and couple $T_S$ to $T_e,$ the “Wouthuysen-Field” effect (Wouthuysen 1952; Field 1958; Hirata 2006). In the absence of Lyα photons, to unlock the spin temperature of a neutral medium with (say) $T_e = 500 \text{K}$ from the CMB requires a collision rate $C_H > AT_e,$ corresponding to a baryon overdensity $\delta_b > 5[(1 + z)/20]^{-2}.$ Not only dense gas within virialized minihalos but also intergalactic filamentary structure heated by adiabatic compression or shock heating may then be observable in 21cm emission. A population of X-ray sources (“miniquasars”) turning on at early stages (e.g. Madau et al. 2004; Ricotti et al. 2005) may make even the low-density IGM visible in 21cm emission as structures develop in the pre-reionization era.

In Kuhlen et al. (2006) we used the same hydrodynamical simulations of early structure formation in a ΛCDM universe discussed in § 1.4.2 to investigate the spin temperature and 21cm brightness of the diffuse IGM prior to the epoch of cosmic reionization, at $10 < z < 20.$ The two-dimensional distribution of gas overdensity and spin temperature at $z = 17.5$ is shown in Figure 20 for a simulation with no radiation sources (“NS”) and one (“MQ”) in which a miniquasar powered by a 150 $M_\odot$ black hole turns on at redshift 21 within a host halo of mass $2 \times 10^6 M_\odot.$ The miniquasar shines at the Eddington rate and emits X-ray radiation with a power-law energy spectrum $\propto E^{-1}$ in the range $0.2 - 10 \text{keV}.$ The color coding in this phase diagram indicates the fraction of the simulated volume at a given $(\delta_b, T_S).$ In both runs we have assumed no Lyα mixing, so that the visibility of hydrogen at 21cm is entirely determined by collisions. Only gas with neutral fraction $> 90\%$ is shown in the figure. The low-density IGM in the NS run lies on the yellow $T_S = T = 50.4 \text{K}$ line: this is gas cooled by the Hubble expansion to $T_e \ll T$ that cannot unlock its spin states from the CMB and therefore remains invisible. At overdensities between a few and $\sim 200,$ H-H collisions become efficient and adiabatic compression and shocks from structure formation heats up the medium well above the radiation temperature. The coupling coefficient at this epoch is $y \sim \delta_b T_e^{-0.64};$ gas in this regime has $T < T_S \sim yT_e < T_e$ and appears in emission against the CMB (red and green swath). Some residual hydrogen with overdensity up to a few tens, however, is
still colder than the CMB, and is detectable in absorption. At higher densities, $y \gg 1$ and $T_S \rightarrow T_e$: the blue cooling branch follows the evolutionary tracks in the kinetic temperature-density plane of gas shock heated to virial values, $T_e = 2000 - 10^4 K$, which is subsequently cooling down to $\sim 100 K$ because of H$_2$ line emission.

The effect of the miniquasar on the spin temperature is clearly seen in the right panel of Figure 20. X-ray radiation drives the volume-averaged temperature and electron fraction ($x_e$) within the simulation box from $(8 K, 1.4 \times 10^{-4})$ to $(2800 K, 0.03)$, therefore producing a warm, weakly ionized medium (Kuhlen & Madau 2005). The H-H collision term for spin exchange in the low-density IGM increases on the average by a factor $350^{0.36} \sim 8$, while the e-H collision term grows to $C_e \sim 0.5 C_H$. Gas with $(\delta_b, T_e, x_e) = (1, 2800 K, 0.03)$ has coupling efficiency $y = 0.008$, spin temperature $T_S = 73 K > T$, and can now be detected in emission against the CMB. Within 150 comoving kpc from the source, the volume-averaged electron fraction rises above 10%, and e-H collisions dominates the coupling.

A beam of 21cm radiation passing through a neutral hydrogen patch having optical depth $\tau$ and spin temperature $T_S$ causes absorption and induces emission. In the comoving frame of the patch, the radiative transfer equation yields for the brightness temperature through the region: $T_b = T_e - \tau + T_S(1 - e^{-\tau})$. We have used our numerical simulations to perform 21cm radiation transport calculations, including the effect of peculiar velocities and local changes in spin temperature, gas density, and neutral hydrogen fraction. The resulting 21cm radio signal is shown in Figure 21 (lower panels), together with an image of the projected hydrogen spin temperature (upper panels): the latter highlights the abundance of structure within our simulation box on scales up to hundreds of kpc. Due to Hubble and peculiar velocity shifts not all of this structure contributes to the $\delta T_b$ map. In the NS simulation, coherent features in the IGM can be discerned in emission ($T_S > T, \delta T_b > 0$): this filamentary shock-heated structure is typ-
Figure 21. Projected (mass-weighted) spin temperature (upper panels, logarithmic scale) and 21cm differential brightness temperature (lower panels, composite linear scale) in a 0.5 Mpc simulation box for runs “NS” (left) and “MQ” (right) at $z = 17.5$. The location of the miniquasar is indicated by crosses in the right panels.

ically surrounded by mildly overdense gas that is still colder than the CMB and appears in absorption ($T_S < T, \delta T_b < 0$). The covering factor of material with $\delta T_b \leq -10$ mK is 1.7%, comparable to that of material with $\delta T_b \geq +10$ mK: only about 1% of the pixels are brighter than +40 mK. While low-density gas (black color in the left-lower panel) remains invisible against the CMB in the NS run, the entire box glows in 21cm after being irradiated by X-rays. The fraction of sky emitting with $\delta T_b > (+10, +20, +30, +50, +100)$ mK is now (0.57,0.31,0.19,0.1,0.035).

The above calculations show that, even in the absence of external heating sources, spin exchange by H-H collisions can make filamentary structures in the IGM (heated by adiabatic compression or shock heating) observable in 21cm emission at redshifts $z \lesssim 20$. Some cold gas with overdensities in the range 5-100 is still detectable in absorption at a level of $\delta T_b \lesssim -10$ mK, with a signal that grows as $T_S^{-1}$ and covers a few percent of the sky. X-ray radiation from miniquasars preheats the IGM to a few thousand kelvins and increases the electron fraction: this boosts both the H-H and the e-H collisional coupling between $T_S$ and $T_e$, making even low-density gas visible in 21cm emission well before the universe is significantly reionized. Any absorption signal has disappeared, and as much as 30% of the sky is now shining with $\delta T_b \gtrsim +20$ mK. As pointed out by Nusser (2005), the enhanced e-H coupling makes the spin temperature very sensitive to the free-electron fraction: the latter is also a tracer of the H$_2$ molecular fraction in the IGM.
Since hierarchical clustering theories provide a well-defined framework in which the history of baryonic material can be tracked through cosmic time, probing the reionization epoch may then help constrain competing models for the formation of cosmic structures. Quite apart from uncertainties in the primordial power spectrum on small scales, however, it is the astrophysics of baryons that makes us unable to predict when reionization actually occurred. Consider the following illustrative example:

Hydrogen photo-ionization requires more than one photon above 13.6 eV per hydrogen atom: of order $t/t_{\text{rec}} \sim 10$ (where $t_{\text{rec}}$ is the volume-averaged hydrogen recombination timescale) extra photons appear to be needed to keep the gas in overdense regions and filaments ionized against radiative recombinations (Gnedin 2000; Madau et al. 1999). A ‘typical’ stellar population produces during its lifetime about 4000 Lyman continuum (ionizing) photons per stellar proton. A fraction $f \sim 0.25\%$ of cosmic baryons must then condense into stars to supply the requisite ultraviolet flux. This estimate assumes a standard (Salpeter) initial mass function (IMF), which determines the relative abundances of hot, high mass stars versus cold, low mass ones. The very first generation of stars (‘Population III’) must have formed, however, out of unmagnetized metal-free gas: characteristics, these, which may have led to a ‘top-heavy’ IMF biased towards very massive stars (i.e. stars a few hundred times more massive than the Sun), quite different from the present-day Galactic case. Pop III stars emit about $10^5$ Lyman continuum photons per stellar baryon (Bromm et al. 2001), approximately 25 times more than a standard stellar population. A corresponding smaller fraction of cosmic baryons would have to collapse then into Pop III stars to reionize the universe, $f \sim 10^{-4}$. There are of course further complications. Since, at zero metallicity, mass loss through radiatively-driven stellar winds is expected to be negligible, Pop III stars may actually die losing only a small fraction of their mass. If they retain their large mass until death, stars with masses $140 \lesssim m_\ast \lesssim 260$ M$_\odot$ will encounter the electron-positron pair instability and disappear in a giant nuclear-powered explosion (Fryer et al. 2001), leaving no compact remnants and polluting the universe with the first heavy elements. In still heavier stars, however, oxygen and silicon burning is unable to drive an explosion, and complete collapse to a black hole will occur instead (Bond et al. 1984). Thin disk accretion onto a Schwarzschild black hole releases about 50 MeV per baryon. The conversion of a trace amount of the total baryonic mass into early black holes, $f \sim 3 \times 10^{-6}$, would then suffice to at least partially ionize and reheat the universe.

The above discussion should make it clear that, despite much recent progress in our understanding of the formation of early cosmic structure and the high-redshift universe, the astrophysics of first light remains one of the missing links in galaxy formation and evolution studies. We are left very uncertain about the whole era from $10^8$ to $10^9$ yr – the epoch of the first galaxies, stars, supernovae, and massive black holes. Some of the issues reviewed in these lectures are likely to remain a topic of lively controversy until the launch of the James Webb Space Telescope (JWST), ideally suited to image the earliest generation of stars in the universe. If the first massive black hole form in pregalactic systems at very high redshifts, they will be incorporated through a series of mergers into larger and larger halos, sink to the center owing to dynamical friction, accrete a fraction of the gas in the merger remnant to become supermassive, and form binary systems (Volonteri et al. 2003). Their coalescence would be signaled by the emission of low-frequency gravitational waves detectable by the planned Laser Interferometer Space Antenna (LISA). An alternative way to probe the end of the dark ages and discriminate between different reionization histories is through 21cm tomography. Prior to the epoch
of full reionization, 21cm spectral features will display angular structure as well as structure in redshift space due to inhomogeneities in the gas density field, hydrogen ionized fraction, and spin temperature. Radio maps will show a patchwork (both in angle and in frequency) of emission signals from H I zones modulated by H II regions where no signal is detectable against the CMB (Ciardi & Madau 2003). The search at 21cm for the epoch of first light has become one of the main science drivers for the next generation of radio arrays.

While many of the cosmological puzzles we have discussed can be tackled directly by studying distant objects, it has also become clear that many of today’s “observables” within the Milky Way and nearby galaxies relate to events occurring at very high redshifts, during and soon after the epoch of reionization. In this sense, galaxies in the Local Group (“near-field cosmology”) can provide a crucial diagnostic link to the physical processes that govern structure formation and evolution in the early universe (“far-field cosmology”). It is now well established, for example, that the hierarchical mergers that form the halos surrounding galaxies are rather inefficient, leaving substantial amounts of stripped halo cores or “subhalos” orbiting within these systems (see Fig. 22). Small halos collapse at high redshift when the universe is very dense, so their central densities are correspondingly high. When these merge into larger hosts, their high densities allow them to resist the strong tidal forces that acts to destroy them. Gravitational interactions appear to unbind most of the mass associated with the merged progenitors, but a significant fraction of these small halos survives as distinct substructure.

The Via Lactea simulation has recently shown that, in the standard CDM paradigm, galaxy halos should be filled with tens of thousands subhalos that appear to have no optically luminous counterpart: this is more than an order of magnitude larger than found in previous simulations. Their cumulative mass function is well-fit by $N(>M_{\text{sub}}) \propto M_{\text{sub}}^{-1}$ down to $M_{\text{sub}} = 4 \times 10^6 M_\odot$. Sub-substructure is apparent in all the larger satellites, and a few dark matter lumps are now resolved even in the solar vicinity. In Via Lactea, the number of dark satellites with peak circular velocities above 5 km s$^{-1}$ (10 km s$^{-1}$) exceeds 800 (120). As shown in Figure 23, such finding appears to exacerbate the so-called “missing satellite problem”, the large mismatch between the twenty or so dwarf satellite galaxies observed around the Milky Way and the predicted large number of CDM subhalos (Moore et al. 1999; Klypin et al. 1999). Solutions involving feedback mechanisms that make halo substructure very inefficient in forming stars offer a possible way out (e.g. Bullock et al. 2000; Kravtsov et al. 2004; Moore et al. 2006). Even if most dark matter satellites have no optically luminous counterparts, the substructure population may be detectable via flux ratio anomalies in strong gravitational lenses (Metcalf & Madau 2001), through its effects on stellar streams (Ibata et al. 2002), or possibly via $\gamma$-rays from dark matter annihilation in their cores (e.g. Bergstrom et al. 1999; Colafrancesco et al. 2006). We are coming into a new era of galaxy formation and evolution studies, in which fossil signatures accessible today within nearby galaxy halos will allow us to probe back to early epochs, and in which the basic building blocks of galaxies will become recognizable in the near-field. Understanding galaxy formation is largely about understanding the survival of substructure and baryon dissipation within the CDM hierarchy.

Acknowledgements

I would like to thank my collaborators, Jiürg Diemand and Michael Kuhlen, for innumerable discussions and for their years of effort on the science presented here. It is my
Figure 22. Projected dark matter density-squared map of the Via Lactea halo at the present epoch. The image covers an area of $800 \times 600$ kpc, and the projection goes through a 600 kpc-deep cuboid containing a total of 110 million particles. The logarithmic color scale covers 20 decades in density-square.

pleasure to thank the organizers of “The emission line universe” for their hospitality and patience in waiting for this proceeding, and all the students for making this a very enjoyable winter school. Support for this work was provided by NASA grant NNG04GK85G.
Figure 23. Left: Cumulative peak circular velocity function for all subhalos within Via Lactea’s $r_{\text{vir}}$ (upper curve) and for the subpopulation within the inner $0.1 r_{\text{vir}} \text{ (lower curve).}$ Solid line with points: observed number of dwarf galaxy satellites around the Milky Way. Right: Same plotted versus virial temperature $T_{\text{vir}}$.

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