Lecture 28
The First Atoms, Molecules and Stars

1. Reionization and the First Stars
2. The First Atoms and Molecules
3. Formation of the First Stars

References
Barkana & Loeb, Repts Prog Phys, 70 627 2007
Lepp, Stencil & Dalgarno, J Phys B 35 57 2002
1. Reionization and the First Stars

Observations of the Ly$\alpha$ forest and especially the GP troughs for high-$z$ quasars indicate that H I reionization occurred before $z = 6$ and for He II somewhat later.

Observations of other high-$z$ Ly$\alpha$ absorption indicate that the degree of reionization varies for $z = 5-6$
Cartoon of Reionization by the First Stars
Barkana & Loeb (2007)

Observations of high-z quasars (Lec27) suggest that reionization was complete just above $z \sim 7$
2008 WMAP image of the CMB fluctuations
\[ \langle T \rangle = 2.725 \text{ K} \quad \text{red } +2\times10^{-4}\text{K} \quad \text{blue } -2\times10^{-4}\text{K} \]
These fluctuations, seen above at \( z \sim 1200 \) (330,000 yr), grow until, somewhere between \( z \sim 10 -100 \) (13.5 Myr - 375 Myr), they produce the first stars.
Star Formation and $\Lambda$CDM Simulations

Stars are presumed to form in high-density knots shown in this $\Lambda$CDM simulation at $z = 17$.

Massive new stars ionize and heat the gas.
Miralda-Escude, Science 300 1907 2003

neutral fraction (blue)  atomic fraction (orange) temperature (green $\sim 10^4$ K)
2. The First Atoms and Molecules

The physical conditions close to recombination are given by the mean cosmological hydrogen density and the CMB temperature:

\[ n_H = (1 - Y) \frac{\rho_{cr}}{m_H} \Omega_B (1 + z)^3 \approx 1.6 \times 10^{-7} \text{ cm}^{-3} (1 + z)^3 \]

\[ T_{\text{rad}} = 2.728(1 + z) \]

For \( z = 1200 \) (~ 330,000) years ago, these are:

\[ n_H \approx 275 \text{ cm}^{-3} \quad T = 3000 \text{ K} \]

These are fairly mild conditions, e.g., thermal collisional ionization of H and He is suppressed, so recombination can occur. But going back to \( z = 3000 \) (84,000 yrs), \( n_H \sim 4000 \text{ cm}^{-3} \) and \( T \sim 8000 \text{ K} \), which allows for collisional ionization.
The First Elements and Atoms
(The beginning of chemistry)

Big Bang nucleosynthesis produced these stable nuclides:

<table>
<thead>
<tr>
<th>nuclide</th>
<th>abundance</th>
<th>IPs (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1.0</td>
<td>13.60</td>
</tr>
<tr>
<td>D</td>
<td>$\sim2\times10^{-5}$</td>
<td>13.60</td>
</tr>
<tr>
<td>$^3\text{He}$</td>
<td>$\sim10^{-5}$</td>
<td>13.60</td>
</tr>
<tr>
<td>He</td>
<td>0.06</td>
<td>24.59, 54.42</td>
</tr>
<tr>
<td>$^7\text{Li}$</td>
<td>$\sim10^{-10}$</td>
<td>5.39, 75.64, 122.5</td>
</tr>
</tbody>
</table>

Starting with the Big Bang, the nuclei were stripped and the dominant ions were the ones with the highest charge: $\text{H}^+$, $\text{He}^{2+}$, and $\text{Li}^{3+}$. With time, the ions remained in chemical equilibrium, and those with the largest IPs were the first to disappear, starting with $\text{Li}^{3+}$, then $\text{Li}^{2+}$, $\text{He}^{2+}$ and $\text{He}^+$. **He was the first atom to recombine.**
H and He Recombination

- Detailed multi-level treatment of H and He atoms.
- Recombination of H occurs near $z = 1300$.
- $H^+$ freezes out at $x(H^+) \sim 10^{-3}$
- $H_2$ freezes out at $x(H_2) \sim 4 \times 10^{-6}$

Blow-up just before recombination showing effect of He recombination on the electron abundance
Recombination timescales lengthen with decreasing $z$, and some $\text{H}^+$, $\text{He}^+$ and $\text{Li}^+$ are frozen into the dark ages. The residual ionization level is $\sim 10^{-4}$. 

Recombination Including D and Li
Lepp, Stancil & Dalgarno (2002)
Formation of $\text{H}_2$

Starting from warm (< 3000 K) and moderately dense (275 cm$^{-3}$) atomic hydrogen and helium gas without dust grains, molecules can form by weak radiative processes, some of which discussed in Sec. 3 of Lec15.

The first molecule produced at the onset of cosmic recombination was the molecular ion $\text{HeH}^+$, soon followed by $\text{H}_2^+$

\[
\begin{align*}
\text{He}^+ + \text{H} & \rightarrow \text{HeH}^+ + h\nu \quad k \approx 2 \times 10^{-16} \text{ cm}^3\text{s}^{-1} \quad \text{(at 3000 K)} \\
\text{He} + \text{H}^+ & \rightarrow \text{HeH}^+ + h\nu \quad k \approx 4 \times 10^{-17} \text{ cm}^3\text{s}^{-1} \\
\text{H}^+ + \text{H} & \rightarrow \text{H}_2^+ \quad k \approx 2 \times 10^{-16} \text{ cm}^3\text{s}^{-1}
\end{align*}
\]

These ions are destroyed by dissociative recombination, photodissociation and by reaction with H to form $\text{H}_2^+$:
H$_2^+$ /HeH$^+$ and H$^-$ Formation of H$_2$

HeH$^+$ + H $\rightarrow$ H$_2^+$ + He \hspace{1cm} k \approx 1.3 \times 10^{-9} \text{ cm}^3\text{s}^{-1} \hspace{1cm} \text{(at 3000K)}

H$_2^+$ + H $\rightarrow$ H$^+$ + H$_2$ \hspace{1cm} k \approx 6 \times 10^{-10} \text{ cm}^3\text{s}^{-1}

Just as important as this HeH$^+/H_2^+$ route is formation of H$_2$ from H$-$:

e$^- + H $\rightarrow$ H$^-$ + h$\nu$ \hspace{1cm} k \approx 2 \times 10^{-15} \text{ cm}^3\text{s}^{-1} \hspace{1cm} \text{(at 3000 K)}

H$^-$ + H $\rightarrow$ H$_2$ + e \hspace{1cm} k \approx 1.2 \times 10^{-9} \text{ cm}^3\text{s}^{-1}

Lastly, HD can be formed by similar sets of reactions, but unlike the highly forbidden reaction, H + H $\rightarrow$ H$_2$ + h$\nu$, the direct radiative association of H and D is allowed but weak:

H + D $\rightarrow$ HD + h$\nu$ \hspace{1cm} k \approx 8 \times 10^{-26} \text{ cm}^3\text{s}^{-1}
**Destruction of H$_2^+$, HeH$^+$, and H$^-$**

These ions are all formed by weak radiative association with H and then H$_2$ is formed by a fast reaction with another H

\[
\begin{align*}
H^+ & \quad H_2^+ \\
H_2^+ + H & \rightarrow HeH^+ + H \rightarrow H_2 \\
e & \quad H^- \\
\rightarrow & \text{ destruction by } h\nu \text{ in all cases} \\
& \quad \text{by e for } H_2^+ \text{ and } HeH^+ \text{ and by } H^+ \text{ for } H^- 
\end{align*}
\]

The thresholds for photo-destruction are:

\[
\begin{align*}
D(H_2^+) &= 2.65 \text{ eV} \quad 4680 \text{ Å} \\
D(HeH^+) &= 2.03 \text{ eV} \quad 6110 \text{ Å} \\
B(H^-) &= 0.754 \text{ eV} \quad 16400 \text{ Å} 
\end{align*}
\]

CMB radiation destroys H$^-$ at recombination, so the H$^-$ route to H$_2$ is relatively weak until smaller $z \sim 500$. 

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Three-Body Formation

In Lecture 15 three-body formation was mentioned as a way of synthesizing $\text{H}_2$ in dense regions like cool stellar atmospheres and the disk of YSOs:

$$3\text{H} \rightarrow \text{H}_2 + \text{H} \quad 2\text{H} + \text{H}_2 \rightarrow 2 \text{H}_2$$

These reactions also play a role when gas inside DM halos becomes dense. Cooling by $\text{H}_2$ then regulates the temperature in these cores. The inverses of these three-body reactions may also destroy $\text{H}_2$ by collisional dissociation.

Similarly, evaluations of the role of reactions based on the mean density after recombination will not hold once star formation has started. For example, the first stars will generate UV radiation that will destroy $\text{H}_2^+$ and HeH+ (as well as $\text{H}_2$) and photoionize H from excited levels.
These results go together with the figure in slide 9 for atoms. The most abundant species in decreasing order are:

\[ \text{H : He : H}^+ : \text{D : H}_2 : \text{HD} = 1 : 0.08 : 4 \times 10^{-4} : 4 \times 10^{-5} : 10^{-5} : 2 \times 10^{-8} \]
Milky May and Cosmic Molecule Formation

The key distinctions between contemporary and primeval molecule formation are the presence in the former case of (1) “metals” and (2) ionizing radiation in the form of stellar UV and cosmic rays.

The metals permit the formation of H₂ on grains. They also provide for the presence of O and other heavy atoms, so that OH and other hydrides form (with the help of H⁺ and H₃⁺), which then leads to molecules like CO and H₂O.

Cosmic molecule formation is a much slower process because it relies on weak radiative-association reactions to form H₂⁺, HeH+ and H⁻, which have very small abundances in local gas. On the other hand, cosmic star formation takes a long until the fluctuations grow big enough.
Significance of Molecular Abundances

• The central role of molecules is to cool the gas.
• The temperature is critical for the growth of fluctuations.
• If we assume that the Jeans criterion is a valid one for the early universe, it would predict that the first stars (or clusters of stars) would have been very massive.

\[ M_J \approx 12M_{\text{sun}} \, T^{3/2}n_H^{-1/2} \]

i.e., the Jeans mass is very sensitive to the temperature.

Using the conditions just after recombination \( (T = 3000 \, \text{K}, n_H = 200 \, \text{cm}^{-3}) \) leads to masses \( \sim 10^5 \, M_{\text{sun}} \).

• On collapse, the density would increase and promote molecule formation and cooling.

Fragmentation might occur as the Jeans mass decreases.

• These arguments are meant for illustration only: At recombination the CMB fluctuations are too small to collapse of gas clouds and form stars.
Unless T > 8,000 K, the main coolants are H$_2$ and HD. The greater cooling efficiency of HD (arising from its finite dipole moment) makes up for its low abundance.
Effect of HD Cooling


Fig. 2.— Evolution of the gas temperature (top) and molecular fractions (bottom) for an isobarically cooling gas. The gas is assumed to be fully ionized initially, with a temperature of $T = 50,000$ K. We run two cases with initial densities of $n_H = 1$ and $100$ cm$^{-3}$. The dashed lines in the top panel are for runs without HD cooling. The effect of HD cooling can be seen in the temperature and chemical evolution at $t > 10^5$ yr. In the bottom panel, we also show the fraction of $H_2^+$ ionic molecules.
3. The Formation of the First Stars

• The seeds that eventually lead to stars and galaxies are the fluctuations imprinted in the CMB.
• The dynamics of both the dark matter (DM) and the baryons have to be considered.
• Dark matter halos are the sites of star formation.
• The baryon collapse inside halos is governed by the thermal-chemical properties of the gas, including shocks.
• An analog with local star formation: baryon core - DM halo, with molecule formation playing a key role.
• This model of star formation is developed by generalizing the $\Lambda$CDM simulations to include the necessary atomic and molecular physics required to treat the formation of molecules and their thermal consequences.
• Examples of these simulations from CfA follow:
The growth of fluctuations eventually becomes nonlinear, and this point can be used to date the first stars at $z \sim 65$, or 30 Myr after the Big Bang.

The simulations support a “bottom-up” scenario, starting from tiny CMB fluctuations and ending with Milky-Way like galaxies at $z \sim 11$.

Naoz et al. MNRAS 373 L98 2006
High Resolution Simulation of One Halo
With Loads of Physics (Yoshida et al. 2006)

• Simulation at $z = 15$ in a 0.3 Mpc cube with 60 $M_{\odot}$ resolution
• focus on a single DM halo of 600,000 $M_{\text{sun}}$
• central part of top right panel has 300 $M_{\text{sun}}$ and diameter $\sim 1$ pc and is collapsing
• collapsing core does not fragment nor form a disk (low ang. mom.)
• estimated stellar mass $\sim 300$ $M_{\text{sun}}$
Evolution of Seed Physical Properties
Yoshida et al. 2006

A-C low to high H$_2$ density cooling
D. 3-body formation; conversion to H$_2$ is complete
E. cooling limited by trapping
F. collision-induced cooling
G. H$_2$ dissociation for T < 2000 K.
Simulation Including Ionizing Radiation: HII Region of the First Star $z = 26$


gas density weighted by ionization
Simulated Evolution of the First Star
Yoshida et al. 2007

The estimated mass of the first star is now reduced to \( \sim 40 \, M_{\text{sun}} \) -- a massive rather than a very massive star.
Change in DM evolution over 100 Myr, including effects of the ionizing radiation from the first star formed in halo A. A second generation star forms in nearby halo C under changed physical conditions. More generally, the time from the first star to complete reionization is several hundred Myr.
Evolution of the Second Generation Star
Yoshida et al. 2007

density

temperature

molecular fraction

ratio to BEM mass
Summary

• The simulation of early star formation from baryonic cores inside dark matter halos involves the complicated atomic and molecular and radiation physics of a cooling and chemically active collapsing gas cloud.
• The results are incomplete, in part because present simulations can only treat small regions of the pre-IGM.
• Although the results are not yet definitive, they are convincing in indicating that stars (and presumably galaxies) can form at moderately-high redshifts.
• An important and obvious goal of the observations is to attempt to find quasars at $z > 6.3$.
• Other goals include using $\gamma$-ray bursts as light sources to probe the IGM and to detect the 21-cm emission from the dark ages and the epoch of recombination.