From the Big Bang to the First Molecules
Outline

Part I

- Historic Remarks: why we believe in the Big Bang
- Some particle physics
- The first second
- Some basic Nuclear Physics
- Big Bang Nucleosynthesis

Part II

- The First Molecules
- The Role of Molecules for the Formation of the First Stars
The Universe is Expanding

- Distance estimated using the variability of Cepheid stars and their apparent brightness
- Velocity determined through the measured red shift

Hubble’s law

\[ v = H_0 r \]

With \( H_0 = 500 \text{ km s}^{-1} \text{ Mpc}^{-1} \)

Consequences of Hubble’s Observation

Assume constant $H_0$, density decreasing with time:

$$t_0 = \frac{r}{v} = \frac{r}{H_0 r} = H_0^{-1}$$

$t_0$: Approximate age of the Universe (Hubble time)

With $H_0 = 500 \text{ km s}^{-1} \text{ Mpc}^{-1}$

$$t_0 \approx 2 \times 10^9 \text{ yr}$$

Initial Hubble constant wrong (500 km s$^{-1}$/Mpc$^{-1}$), Universe younger than Earth!

(Age of the Earth: ca. 4.5 billion years)
Big Bang

Georges Lemaitre  George Gamov

Time

Einstein:
"Vos calculs sont corrects, mais votre physique est abominable"
("Your math is correct, but your physics is abominable.")
Steady-State Model

The universe, by Heaven's decree
Was never formed in time gone by,
But is, has been, shall ever be—
For so say Bondi, Gold and I.
Stay, O Cosmos, O Cosmos, stay the same!
We the Steady State proclaim!

Written by Gamov

Fred Hoyle
Herman Bondi
Thomas Gold

1946
Big Bang vs. Steady-State Model

Evolutionary Theory:
Density of matter decreases over time

Steady State Theory:
Density of matter is constant over time

Steady State Model:
Requires the creation of 1 hydrogen atom per m$^3$ per billion years
The downfall of the Steady-State model:

The Cosmic Microwave Background and
Big Bang Nucleosynthesis (BBN)
Standard Model: Elementary Particles

**Mesons**
(made out of 2 quarks)

Pions, Kaons, etc.

**Baryons**
(made out of 3 quarks)

Protons, Neutrons, etc.

**Hadrons**

**Mesons** (made out of 2 quarks)

Pions, Kaons, etc.

**Baryons** (made out of 3 quarks)

Protons, Neutrons, etc.

**Nucleons**

Electrons

[Image of electron, muon, and tau particles with their electric charges]

**Quarks**

- Bottom: Electric Charge -1/3
- Strange: Electric Charge -1/3
- Down: Electric Charge -1/3
- Top: Electric Charge 2/3
- Charm: Electric Charge 2/3

**Nucleons**

Proton

[Image of proton with quarks and gluons]

Neutron

[Image of neutron with quarks and gluons]
**Fundamental Forces**

<table>
<thead>
<tr>
<th>Force</th>
<th>Acts on</th>
<th>Particles experiencing</th>
<th>Exchange particle</th>
<th>Coupling constant</th>
<th>Strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strong</td>
<td>Color</td>
<td>Quarks, Gluons</td>
<td>Gluons</td>
<td>$\alpha_s$</td>
<td>1</td>
</tr>
<tr>
<td>Electromagnetic</td>
<td>Electric charge</td>
<td>Electrically charged</td>
<td>Photon</td>
<td>$\alpha$</td>
<td>1/137</td>
</tr>
<tr>
<td>Weak</td>
<td>Flavor</td>
<td>Quarks, Leptons</td>
<td>$W^+, W^-, Z^0$</td>
<td>$\alpha_w$</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>Gravitation</td>
<td>Mass</td>
<td>All</td>
<td>(Graviton)</td>
<td>$\alpha_g$</td>
<td>$10^{-39}$</td>
</tr>
</tbody>
</table>

Gravitation is extremely weak, but has a very long range
irrelevant on atomic scale, very important on astronomical scales

Neutrinos only experience the weak force (and gravity)
Timeline: The First Second of the Universe

Time

- $< 10^{-37}$ s: Universe is filled with high energy density, expanding, cooling
- $10^{-37}$ s: **Inflation**, the Universe expands exponentially
- $< 10^{-11}$ s: The Universe is filled with a **Quark-Gluon plasma**, elementary particles are being created and destroyed continuously
  - **Baryogenesis**: creates in imbalance in the matter / antimatter ratio of 100,000,001 to 100,000,000 → the universe is matter-dominated
- $10^{-6}$ s: Quarks and Gluons combine, **Protons and Neutrons (Baryons) form** and annihilate immediately, leaving $10^{-10}$ of the initial baryons due to the matter / antimatter imbalance
- $1$ s: **Electrons and positrons (leptons) form**, annihilate, leaving $10^{-10}$ of the leptons as electrons

Temp.

- $10^{30}$ K
- $10^{10}$ K
Neutron/Proton Freezeout

\[ Q_n = m_n c^2 - m_p c^2 = 1.29 \text{ MeV} \]

Interaction time scale larger than Hubble time

Neutrons and Protons in equilibrium via

\[ \begin{align*}
  n + \nu_e & \leftrightarrow p + e^- \\
  n + e^+ & \leftrightarrow p + \nu_e \\
  [n] \quad [p] & \sim 0.2
\end{align*} \]
Ingredients 1 Second after Big Bang

Time after Big Bang: 1 s
Temperature: $10^{10}$ K ($\approx 0.86$ MeV)
Neutron/proton ratio 0.2
Everything you need to know about Nuclear Physics

Bethe-Weizsäcker semi-empirical mass formula
(Liquid drop model 1935)

\[ M(A,Z) = NM_n + ZM_p + Zm_e \]

- \( a_v A \) \hspace{1cm} \text{Volume term (nucl. force)}
- \( a_s A^{2/3} \) \hspace{1cm} \text{Surface term}
- \( a_c \frac{Z^2}{A^{1/3}} \) \hspace{1cm} \text{Coulomb term}
- \( a_a \frac{(N-Z)^2}{4A} \) \hspace{1cm} \text{Asymmetry term}

\( a_v = 15.67 \text{ MeV/c}^2 \)
\( a_s = 17.23 \text{ MeV/c}^2 \)
\( a_c = 0.714 \text{ MeV/c}^2 \)
\( a_a = 93.15 \text{ MeV/c}^2 \)
Contributions to the binding energy per nucleon
Solar Abundances

\[ M(A,Z) = N M_n + Z M_p + Z m_e - a_v A + a_s A^{2/3} + a_c \frac{Z^2}{A^{1/3}} + a_a \frac{(N-Z)^2}{4 A} + \frac{\delta}{A^{1/2}} \]

with \( \delta = \)
-11.2 MeV/c^2 for Z gerade and N gerade
0 MeV/c^2 for A ungerade
+11.2 MeV/c^2 for Z ungerade and N ungerade

Abundance of Si is normalized to 10^6
Semi-Empirical Mass Formula

Magic numbers (2, 8, 20, 28, 50, 82)

yield from fusion

yield from fission
Nuclear Shell Model

3s 2d 1g 2p 1f 2s 1d 1p 1s

\[
\begin{align*}
3s & \rightarrow 2d_{3/2} 4 \\
2d & \rightarrow 3s_{1/2} 2, 1g_{7/2} 8, 2d_{5/2} 6 \\
1g & \rightarrow 1g_{9/2} 10, 2p_{1/2} 2 \\
2p & \rightarrow 1f_{5/2} 6, 2p_{3/2} 4 \\
1f & \rightarrow 1f_{7/2} 8 \\
2s & \rightarrow 1d_{3/2} 4, 2s_{1/2} 2, 1d_{5/2} 6 \\
1d & \rightarrow 1p_{1/2} 2, 1p_{3/2} 4 \\
1p & \rightarrow 1s_{1/2} 2 \\
1s & \rightarrow 
\end{align*}
\]

- Magic Numbers:
  - 2, 8, 20, 28, 50
Astronomer’s Periodic Table

Magic numbers (2, 8, 20, 28, 50, 82)
Big Bang Nucleosynthesis (BBN): Ways to form Deuterium

1) \( p + p \rightarrow D + e^+ + \nu_e \)
2) \( n + n \rightarrow D + e^- + \bar{\nu}_e \)
3) \( p + n \rightarrow D + \gamma \)

has to overcome Coulomb force
weak interaction

Good approximation:
all neutrons are used up to form deuterium via Reaction 3)
BBN: Beyond Deuterium

\[
\begin{align*}
D + p & \quad \leftrightarrow \quad ^3\text{He} + \gamma \\
D + n & \quad \leftrightarrow \quad ^3\text{H} + \gamma \\
D + D & \quad \leftrightarrow \quad ^4\text{He} + \gamma \\
D + D & \quad \leftrightarrow \quad ^3\text{H} + p \\
D + D & \quad \leftrightarrow \quad ^3\text{He} + n \\
^3\text{He} + p & \quad \leftrightarrow \quad ^4\text{He} + \gamma \\
^3\text{He} + n & \quad \leftrightarrow \quad ^4\text{He} + \gamma \\
^3\text{H} + D & \quad \leftrightarrow \quad ^4\text{He} + n \\
^3\text{He} + D & \quad \leftrightarrow \quad ^4\text{He} + p \\
\end{align*}
\]

all D, ^3\text{He}, ^3\text{H} rapidly converted to ^4\text{He}
BBN: helium yield approximation

1) Neutron/proton freezeout at $10^{10}$ K with $\frac{[n]}{[p]} \approx 0.2$

2) All neutrons converted to deuterons via $n + p \rightarrow D + \gamma$

3) All deuterons end up as $^4\text{He}$ via various nuclear reaction paths

Estimate primordial helium mass fraction $Y_p$

Sample of primordial matter:
10 protons and 2 neutrons

2), 3) Yields 1 $^4\text{He}$ and 8 protons

$Y_{\text{max}} \approx 0.33$ (0.24 in reality)
Nucleosynthesis Roadblocks

Universe filled with protons and $^4\text{He}$:

\[ p + ^4\text{He} \rightarrow ^5\text{Li} + \gamma \]
\[ ^4\text{He} + ^4\text{He} \rightarrow ^8\text{Be} + \gamma \]
Mass-5 and Mass-8 instabilities
BBN predictions (t = 3 - 20 min)
# Recombination

\( T < 380000 \text{ yr} \)

Ionization potentials [in eV]

<table>
<thead>
<tr>
<th></th>
<th>1(^{st})</th>
<th>2(^{nd})</th>
<th>3(^{rd})</th>
<th>4(^{th})</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>13.6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>He</td>
<td>24.6</td>
<td>54.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Li</td>
<td>5.4</td>
<td>75.6</td>
<td>122.5</td>
<td></td>
</tr>
</tbody>
</table>

\[
\begin{align*}
\text{Li}^{3+} + e & \rightarrow \text{Li}^{2+} + \gamma \\
\text{Li}^{2+} + e & \rightarrow \text{Li}^{+} + \gamma \\
\text{Li}^{+} + e & \rightarrow \text{Li} + \gamma \\
\text{He}^{2+} + e & \rightarrow \text{He}^{+} + \gamma \\
\text{He}^{+} + e & \rightarrow \text{He} + \gamma \\
\text{H}^{+} + e & \rightarrow \text{H} + \gamma
\end{align*}
\]

He\(^{+}\) recombines first to form the first neutral atoms \(\text{He}\)

\(\text{H}^{+}\) recombines second to form \textit{neutral H}
The last scattering surface

Before $z > 1090$ : Matter and radiation highly coupled
(Compton scattering with free electrons)

$z \sim 1090.51 \pm 0.95 \quad T \sim 380081 \pm 5343 \text{ yr}$

At $T = 380,000 \text{ yr}$ (after recombination) matter and radiation de-couple

Density fluctuations on the order of $10^{-5}$
Conclusions

We live in a Universe that:

• Is expanding,
• Seems to have developed out of a very high density “primal nucleus” about 14 billions years ago,
• Is rather isotropic on large scales,
• Has a hierarchy of gravitationally dominated structures on smaller scales (galaxy clusters, galaxies, stars, planets),
• Is totally out of thermal equilibrium (very few heavy nuclei),
• Is filled uniformly with the remnants of Big Bang blackbody radiation,
PART II

Timeline

First Stars and Reionization Era

- The Big Bang/Inflation
  - Universe filled with ionized gas: fully opaque
  - Universe becomes neutral and transparent
- Epoch of Reionization
  - Galaxies and Quasars begin to form - starting reionization.
- Reionization complete
  - ~ 10% opacity
  - Galaxies evolve
  - Dark Energy begins to accelerate the expansion of space
- Our Solar System forms
- Today: Astronomers look back and understand

10000 K

30 K

First molecules
First stars
PART II

Formation of Molecules (z > 1000)

The First Molecules

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

The first neutral molecule: \( \text{H}_2 \)

\[
\begin{align*}
\text{HeH}^+ + \text{H} & \rightarrow \text{H}_2^+ + \text{He}, \\
\text{H}_2^+ + \text{H} & \rightarrow \text{H}_2 + \text{H}^+,
\end{align*}
\]

T = 380000yr

Formation of Molecules (1000 > z > 100)

More hydrogen: the $H_2^+$ channel

$$H^+ + H \rightarrow H_2^+ + \gamma,$$

$$H_2^+ + H \rightarrow H_2 + H^+,$$

More molecules:

$D_2^+, H_3^+, H_2D^+, D_2H^+, D_3^+, HeH^+, HeD^+, He_2^+$

$LiH^+, LiD^+, LiD, LiH^+$
Formation of Molecules ($z < 100$)

The $H^-$ channel:

$$H + e^- \rightarrow H^- + \gamma,$$

0.75 eV

$$H^- + H \rightarrow H_2 + e^-.$$
H⁻ in Space: Source of the Sun’s Opacity

Photodetachment
H⁻ + γ → H + e
The Onset of Star Formation in the Early Universe

Gravitation

Radiative cooling through atomic H transitions

\[ T \rightarrow 10^4 \text{ K} \]

But: Ideal Gas Law
\[ pV = nRT \]

Below 10^4 K: Molecular cooling

H^{(0.9)}

He^{(0.1)}

Li^{10^{-10}}
Cooling through Rovibrational Transitions of \( \text{H}_2 \)

Through collisions \( \text{H} \) atoms transfer some of their energy to \( \text{H}_2 \)

\[
\text{H(Ek)} + \text{H}_2(\nu,R) \rightarrow \text{H(Ek-}\Delta\text{)} + \text{H}_2(\nu',R')
\]

The excited \( \text{H}_2 \) radiates that energy out of the cloud

\[
\text{H}_2(\nu',R') \rightarrow \text{H}_2(\nu'',R'') + \text{photon}
\]
Primordial Cooling: $\text{H}_2$ and HD

$\text{H}_2$

Rotational constant: $B \sim 85K$
only $\Delta J \pm 2$ allowed

$E = B \, J \, (J+1)$

HD

Rotational constant: $B \sim 64K$
$\Delta J \pm 1$ allowed

$A = 4.76 \times 10^{-10} \text{ s}^{-1}$
$A = 2.94 \times 10^{-11} \text{ s}^{-1}$
$A = 4.9 \times 10^{-7} \text{ s}^{-1}$
$A = 5.1 \times 10^{-8} \text{ s}^{-1}$
Deuterium Fractionation

H\textsubscript{2}: 4.47792 eV
HD: 4.51359 eV

\[ \Delta E = 0.0357 \text{ eV} = 413.9 \text{ K} \]

\[ \text{H}_2 + \text{D}^+ \rightarrow \text{HD} + \text{H}^+ \]

D insertion into molecules preferred at low temperatures

overabundance of deuterated molecules


**Cooling functions**

Figure 3. The H\(_2\) cooling function, \(W\), relative to its value in thermal equilibrium, \(W_{LTE}\); \(n(H)/n(H_2) = 10^{-3}\) and \(n(ortho)/n(para) = 1\) were adopted in these calculations.

\[
W(H_2) = \frac{1}{n(H_2)} \sum_{\nu J, \nu' J'} (E_{\nu J} - E_{\nu' J'}) n_{\nu J} A(\nu J \rightarrow \nu' J') \quad (E_{\nu J} > E_{\nu' J'})
\]

[ in erg s\(^{-1}\) ]

\( \text{H}_2 \text{ vs. HD cooling} \)

HD is a much more efficient coolant at low temperature!
Is $H_3^+$ cooling ever important in primordial gas?

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Also considered:

$D_2^+, H_3^+, H_2D^+, D_2H^+, D_3^+$
$HeH^+, HeD^+, He_2^+$
$LiH^+, LiD^+, LiD, LiH^+$
Protogalaxy Formation in the Early Universe

$\text{H}_2$ associative detachment

$$\text{H}^- + \text{H} \rightarrow \text{H}_2 + \text{e}^-.$$
Summary

At times $t = 3-20$ minutes, nuclear physics dominates at MeV energies ($T \sim 10^{10}K$). Big Bang Nucleosynthesis models reproduce the elemental abundances very accurately.

Just before $t \sim 380,000$ yr, protons and electrons recombine and the Universe becomes transparent. Temperatures are around $T \sim 10,000K$, energies around $1eV$. The first molecules form shortly thereafter!

Dark ages

Around $t \sim 400 \times 10^6$ yr the First Stars are born. Molecular cooling (mainly $H_2$) is essential for the formation of the First Stars.
## Literature

### Cosmology:
Ryden, Barbara  
“Introduction to Cosmology”  
Pearson / Addison-Wesley

### Nuclear Physics:
Povh / Rith / Scholz / Zetsche  
“Particles and Nuclei: an introduction to the Physical Concepts”  
Springer

### Early Universe review:
S. Lepp, P.C. Stancil, A. Dalgarno  
“Atomic and molecular processes in the early Universe”  