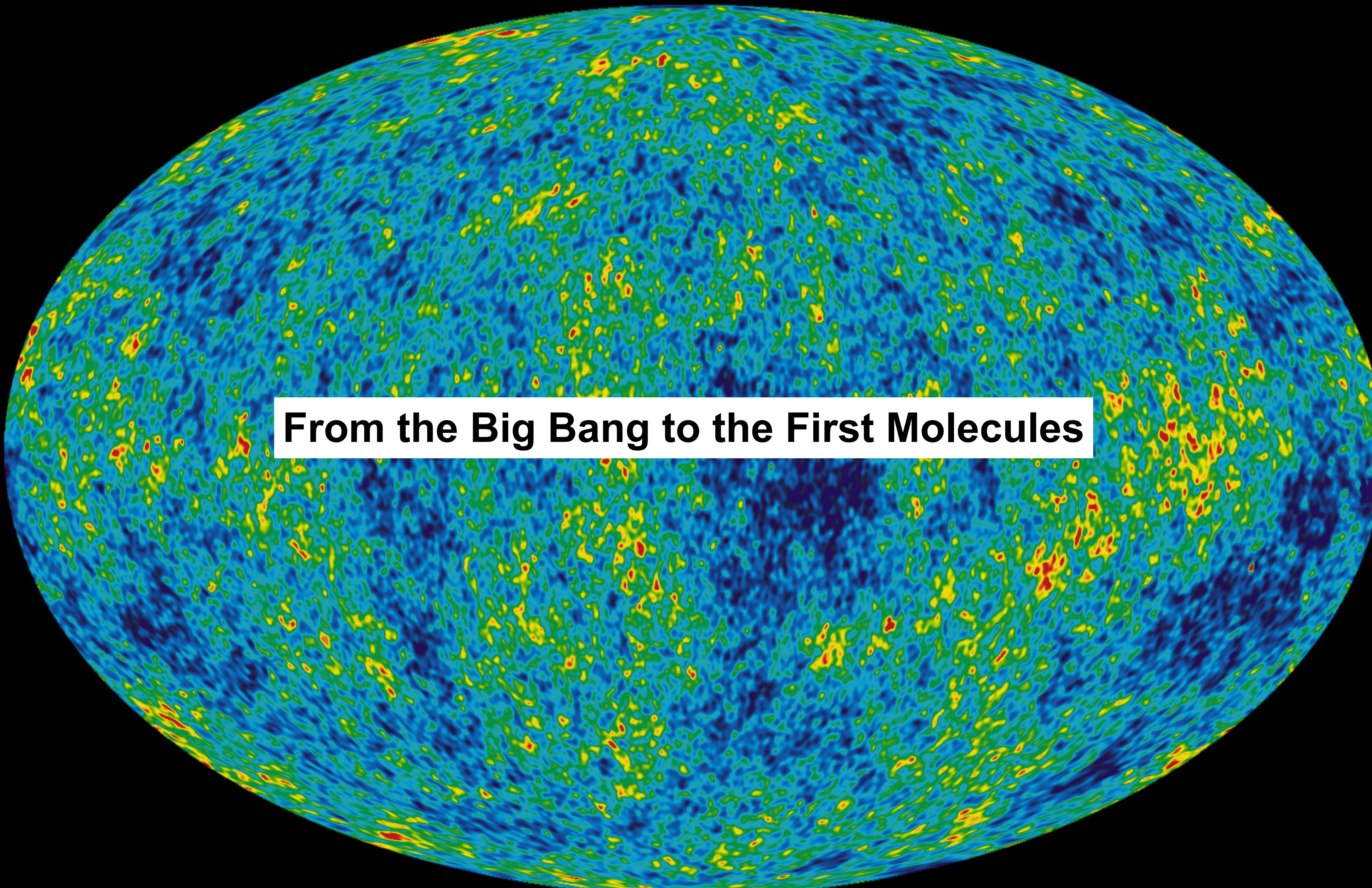
From the Big Bang to the First Molecules



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

PART I

Most galaxies are redshifted

Redshift:

(blueshift for z<0)

$$z = \frac{\lambda_{observed} - \lambda_{emitted}}{\lambda_{emitted}}$$

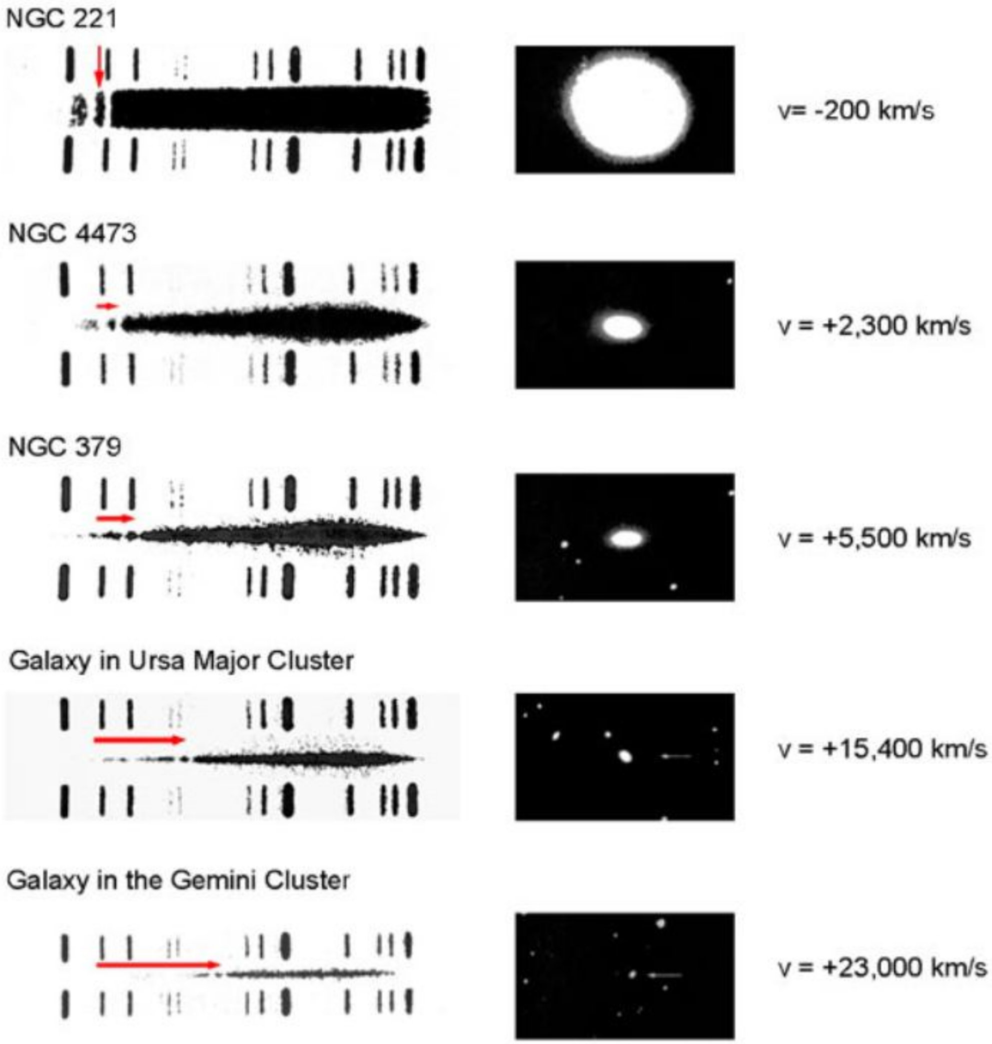
1912-14: Vesto Slipher (Lowell Obs.) was first to find that M31 Andromeda galaxy is blue-shifted: V = - 300 km/s

1917–25: Slipher had observed the spectral lines of 40 galaxies: nearly all were **redshifted**

Edwin Hubble interprets redshift as **non-relativistic Doppler shift** to determine velocities:

$$\Delta\lambda/\lambda = z = \frac{v}{c}$$

Spectrographic observations in the 1920s



Historic spectra of selected galaxies as taken by Milton Humason at the Mout Wilson Observatory in the 1930s. (Credit: Humason, 1936, The Astrophysical Journal, 83:10)

Arrows above the spectra point at the H and K lines of calcium and show the amounts these lines are displaced to the red. The comparison spectra are of helium.

The Universe is Expanding

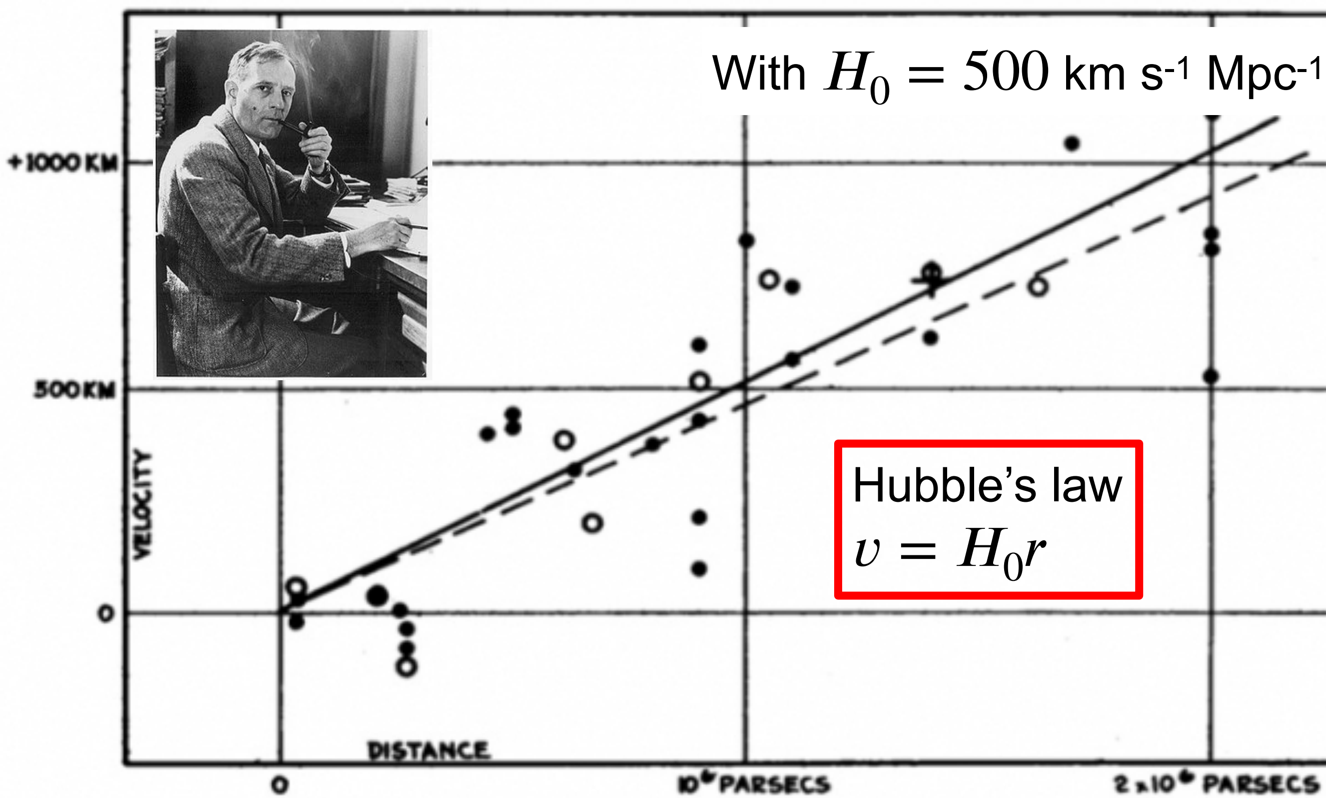


FIGURE 1

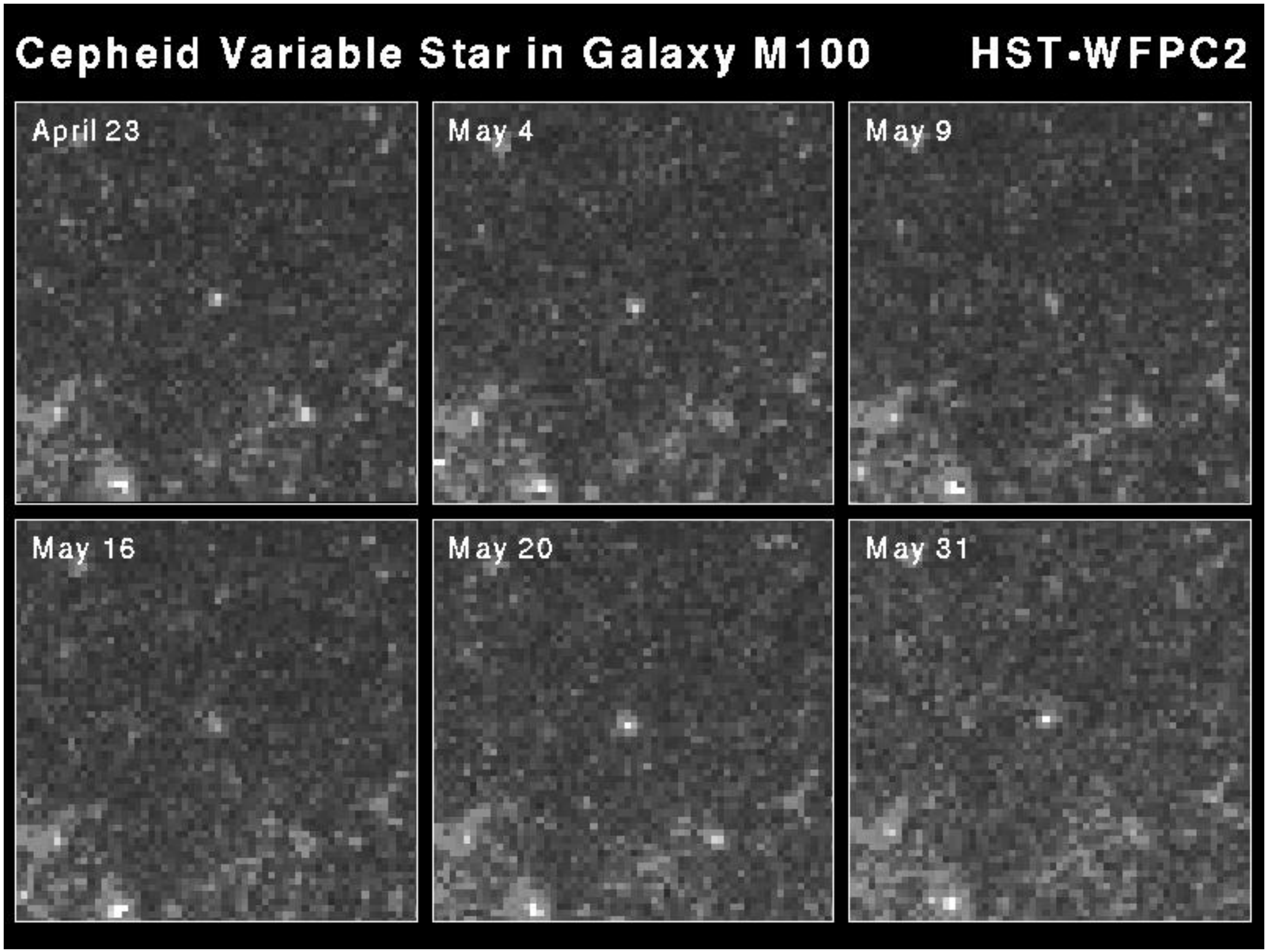
Velocity-Distance Relation among Extra-Galactic Nebulae.

Edwin Hubble, PNAS, vol. 15 no. 3, pp.168-173 (1929)

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

Cepheids as standard candles

Cepheids are luminous stars with a pulsation period of days or weeks.

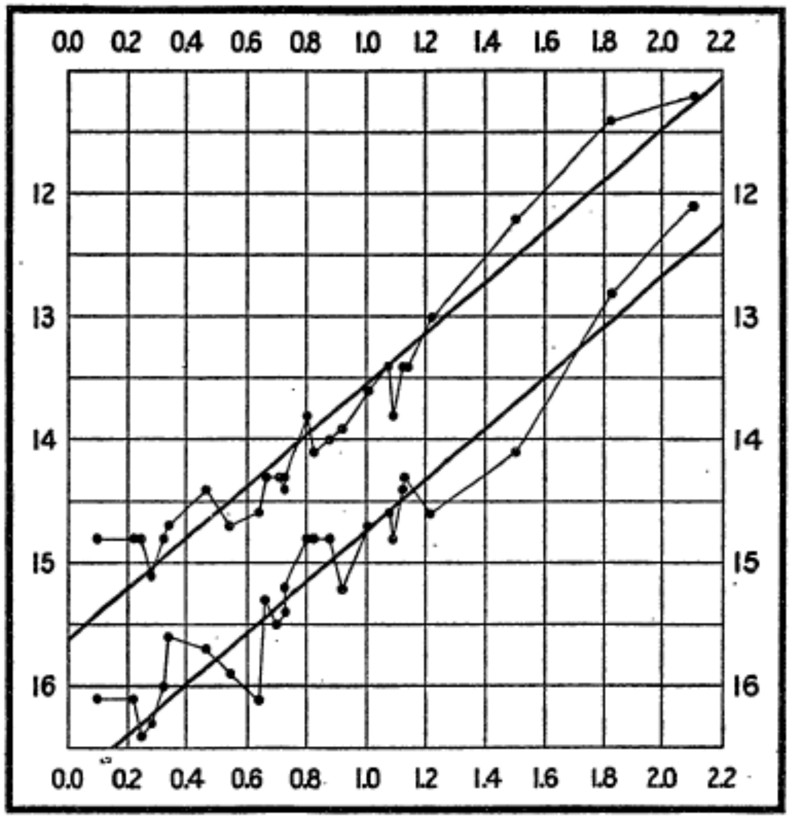


Cepheids as Standard Candles

HARVARD COLLEGE OBSERVATORY.

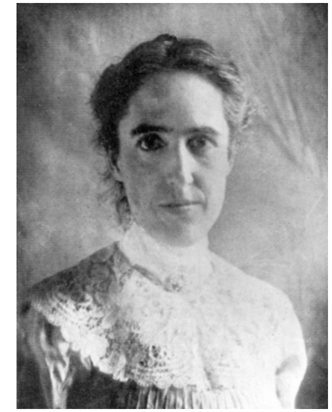
CIRCULAR 173.

PERIODS OF 25 VARIABLE STARS IN THE SMALL MAGELLANIC CLOUD.



Brightness of minima and maxima (magnitudes)

Pulsation period (days)



Henrietta Swan Leavitt
(1868 – 1921)

Apparent magnitude m < — > Absolute magnitude M and Distance d:

$$d = 10^{(m-M+5)/5}$$

Problem: extinction and calibration

Henrietta Swan Leavitt (Harvard College Obs.): Cepheids' pulsating stars show a period-luminosity relation

Cepheids as Standard Candles

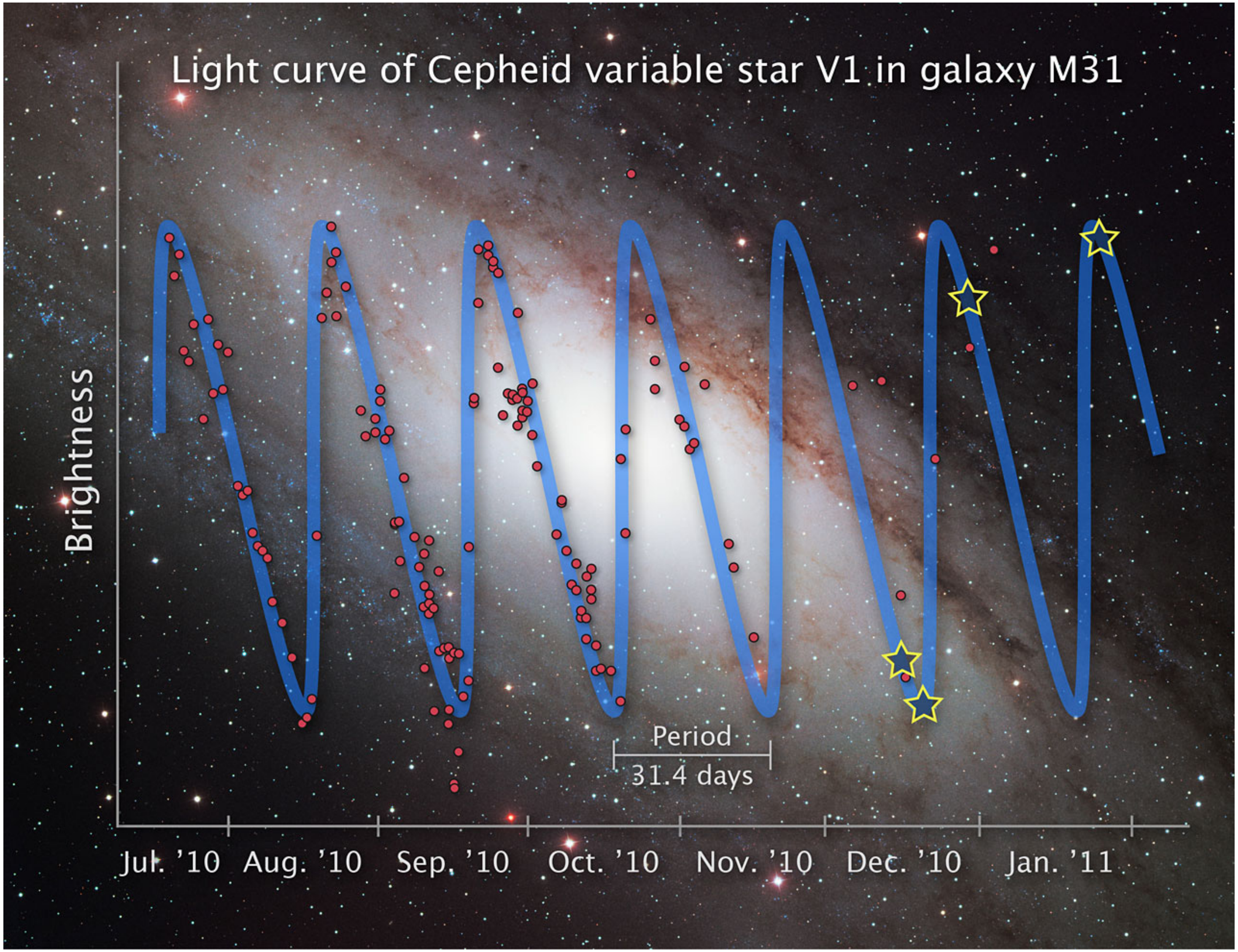
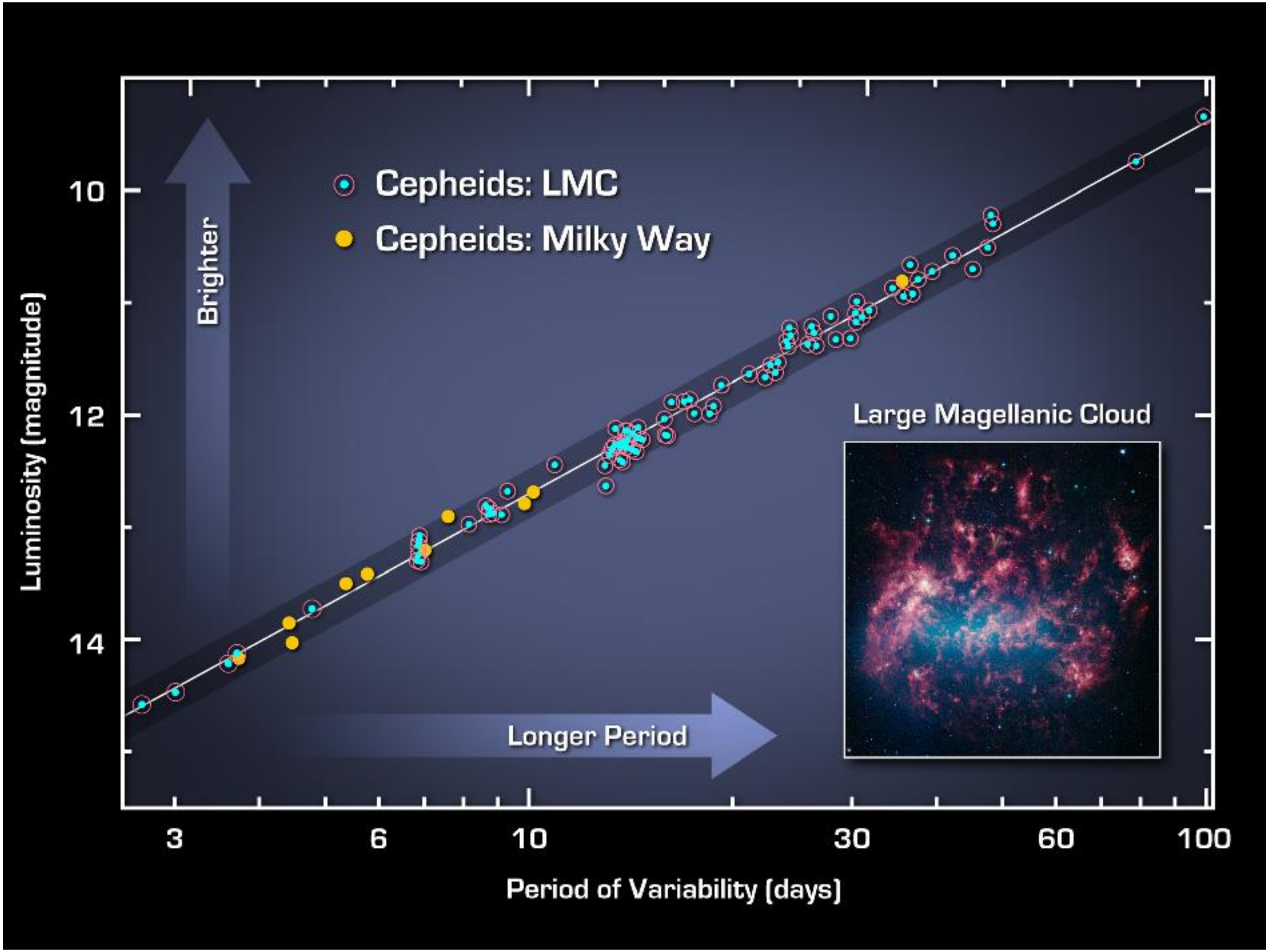


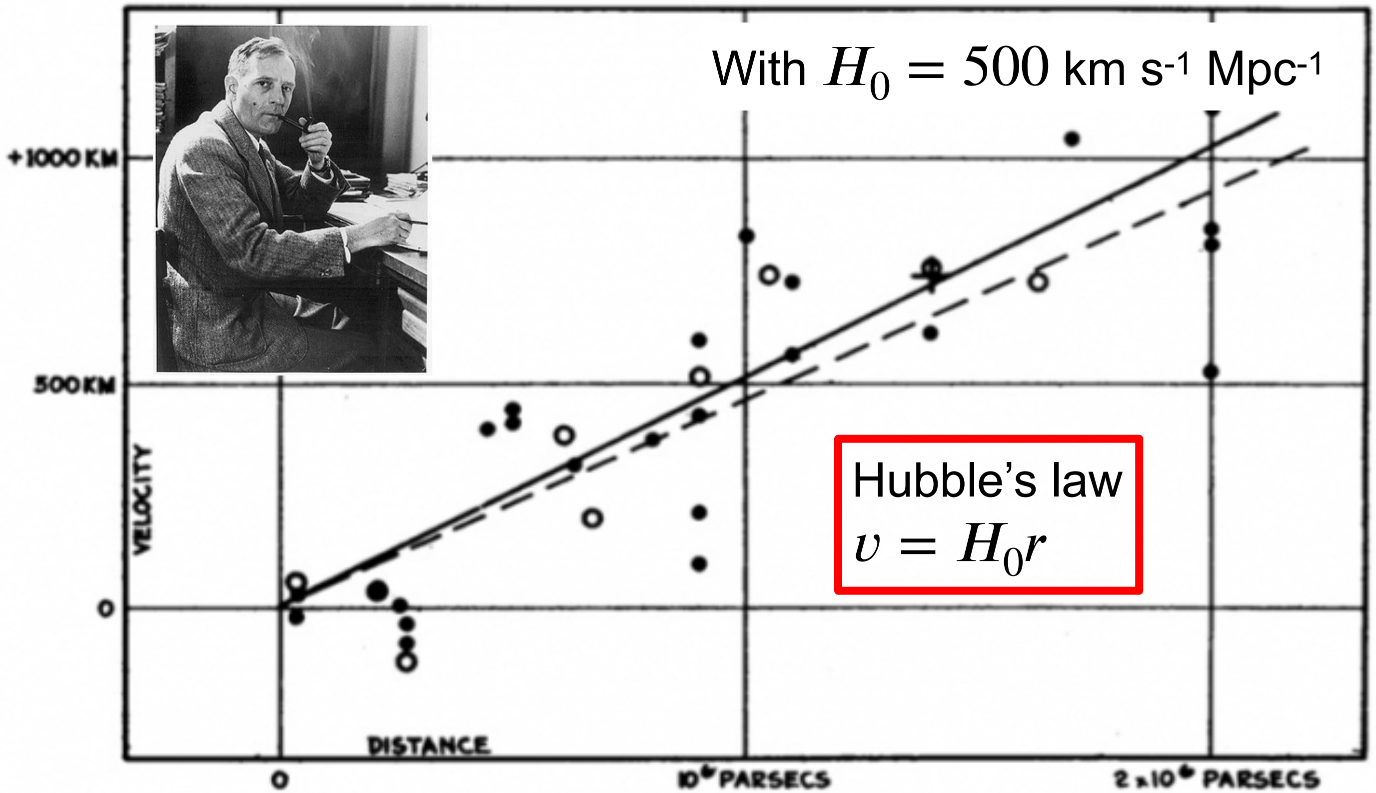
Image: Hubble Space Telescope and American Association of Variable Star Observers (AAVSO)

Cepheids as standard candles: period vs luminosity depends on stellar metallicity



Spitzer observations. Image Credit: NASA

The Universe is Expanding



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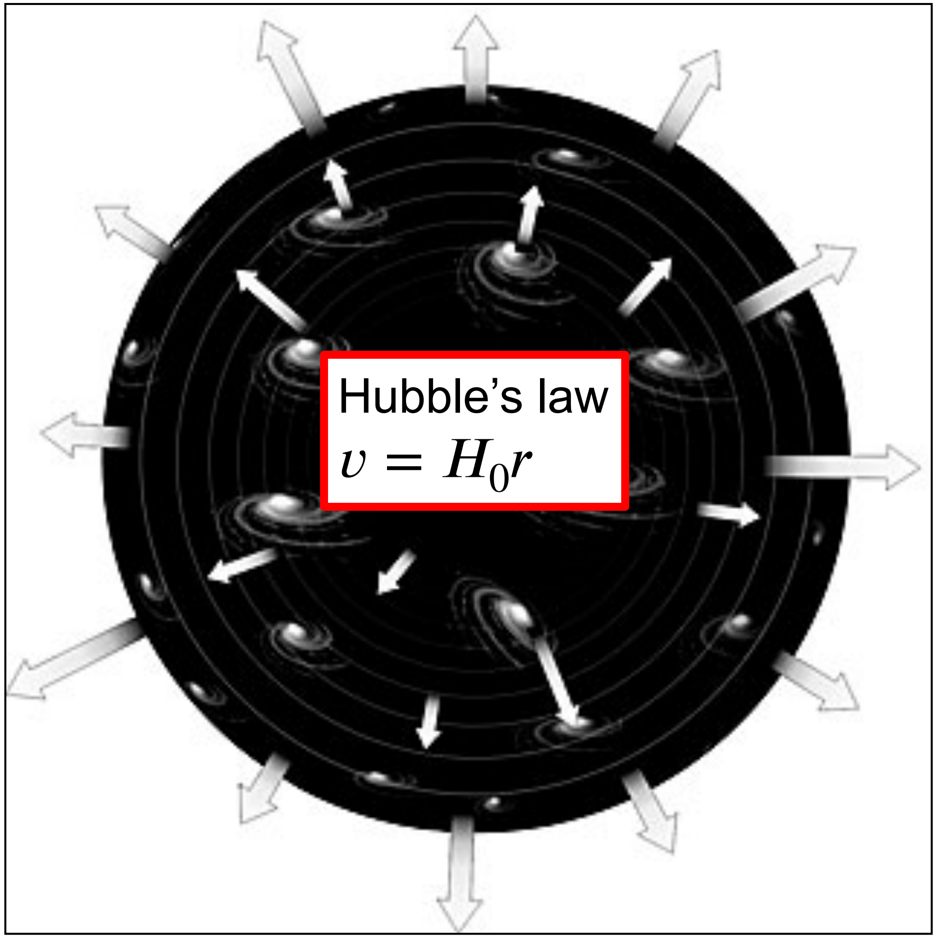
Consequences of Hubble's Observation



If H_0 constant, density is decreasing with time, and the age of the Universe (Hubble time) is:

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

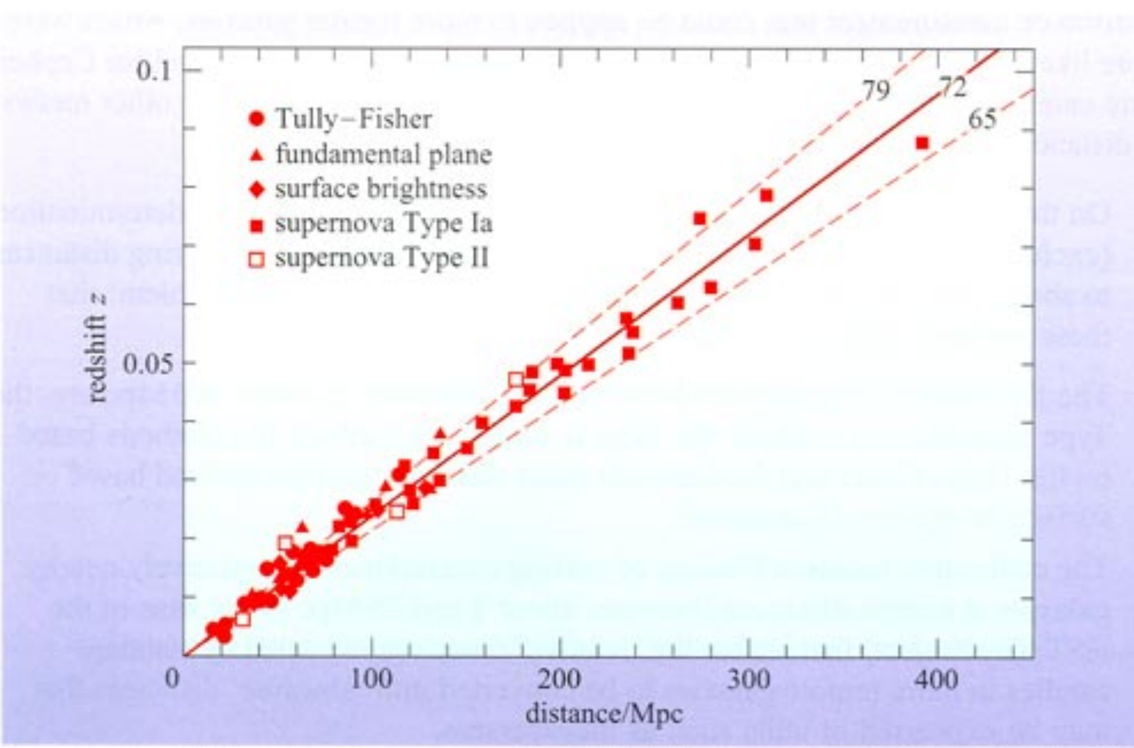
With $H_0 = 500$ km s^{-1} Mpc^{-1}

$t_0 \sim 2 \times 10^9$ yr or only 2 Gyr

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

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

Modern determinations of H_0



Date published	Hubble constant (km/s)/Mpc	Observer
2013-03-21	67.80 ±0.77	Planck Mission
2012-12-20	69.32 ±0.80	WMAP (9-years)
2010	$70.4^{+1.3}_{-1.4}$	WMAP (7-years), combined with other measurements.
2010	71.0 ±2.5	WMAP only (7-years).
2009-02	70.1 ±1.3	WMAP (5-years). combined with other measurements.
2009-02	$71.9^{+2.6}_{-2.7}$	WMAP only (5-years)
2006-08	$77.6^{+14.9}_{-12.5}$	Chandra X-ray Observatory
2007	$70.4^{+1.5}_{-1.6}$	WMAP (3-years)
2001-05	72 ±8	Hubble Space Telescope
prior to 1996	50–90 (est.)	
1958	75 (est.)	Allan Sandage

Source: Wikipedia

Age of the Universe: $t_0 = 1 / H_0$

$$H_0 = 67.8 \frac{\text{km/s}}{\text{Mpc}} = \frac{67.8 \text{ km/s}}{3.1\text{x } 10^{19} \text{ km}} = 2.2 \text{ x } 10^{-18} \text{ s}^{-1}$$

$t_0 = 4.55 \text{ x } 10^{17} \text{ s} = 14.5 \text{ x } 10^{9} \text{ yr}$

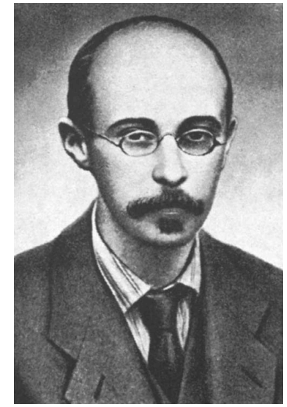
Expansion makes H_0 variable. Currently, H_0 = 7% / Gyr

The Big Bang

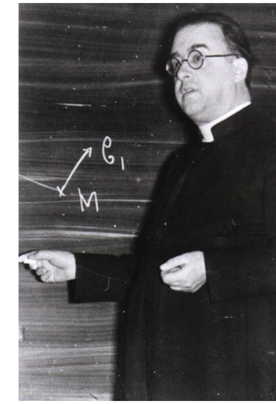
Friedmann 1922: Idea of an expanding universe that contained moving matter in the context of general relativity. Friedmann equations describing the expansion.

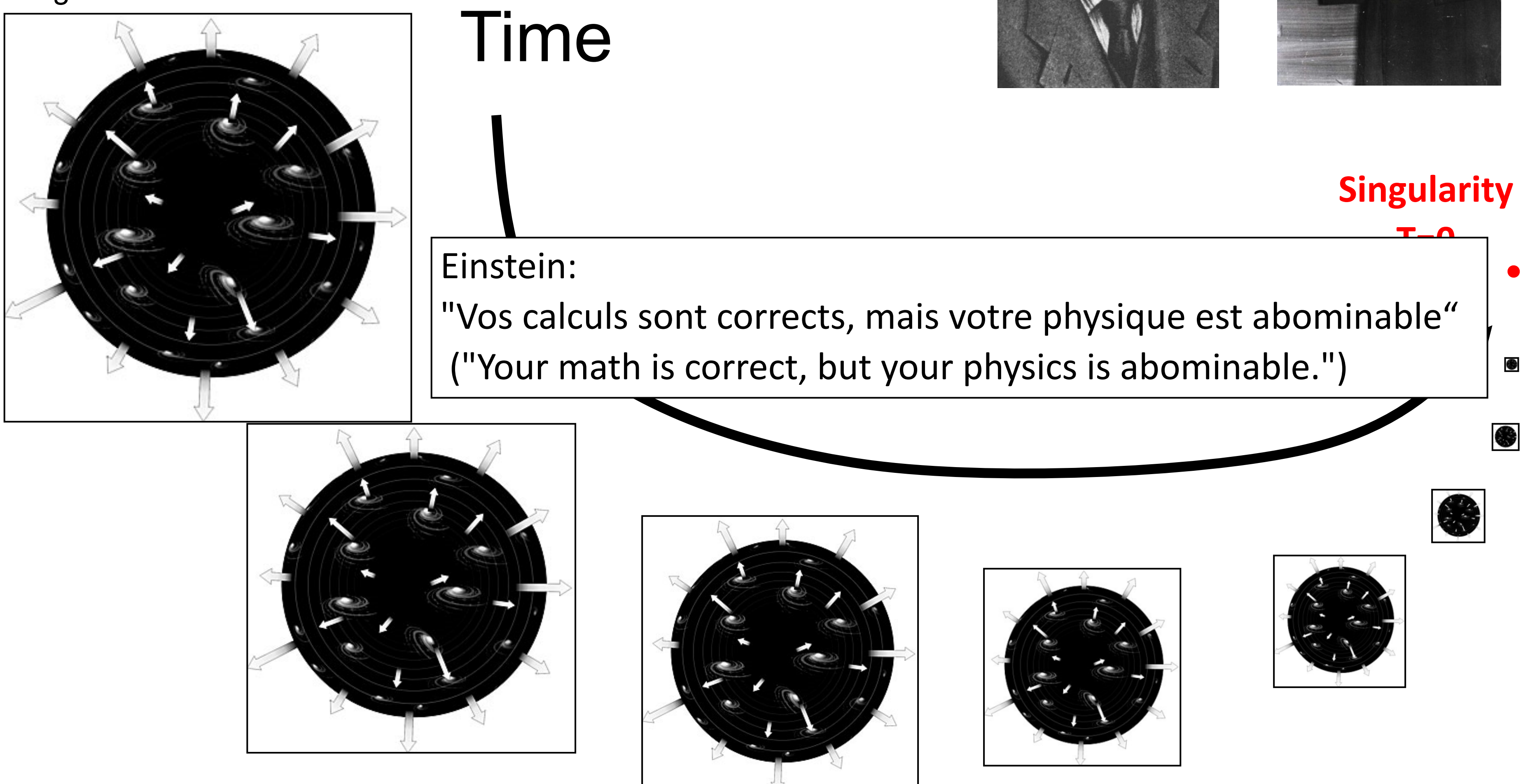
Lemaitre 1927: A homogeneous Universe of constant mass and growing radius accounting for the radial velocity of extragalactic nebula

Alex Friedmann



Georges Lemaitre





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

Steady-State Model

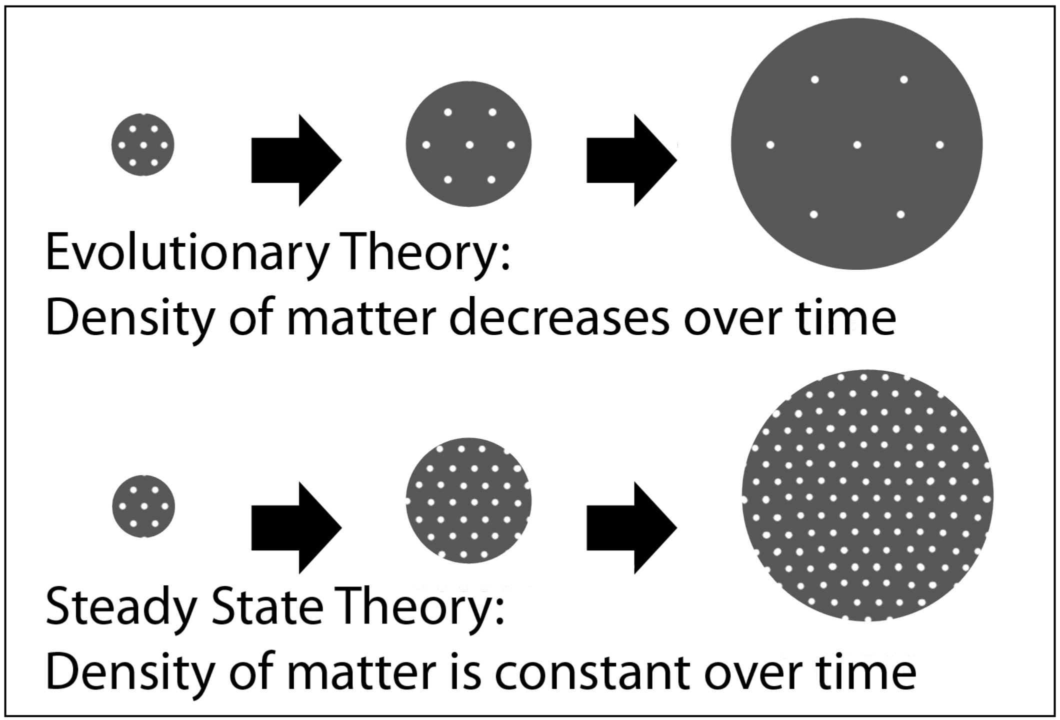
Fred Hoyle

Density of matter in expanding universe does not change.

Requires continuous creation of matter!

Thomas Gold

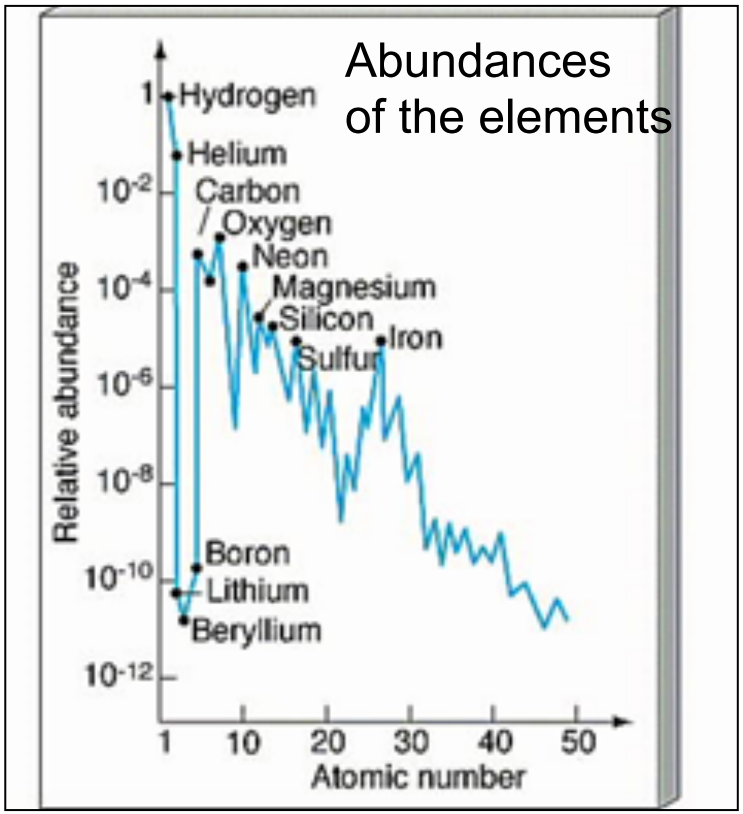
Herman Bondi

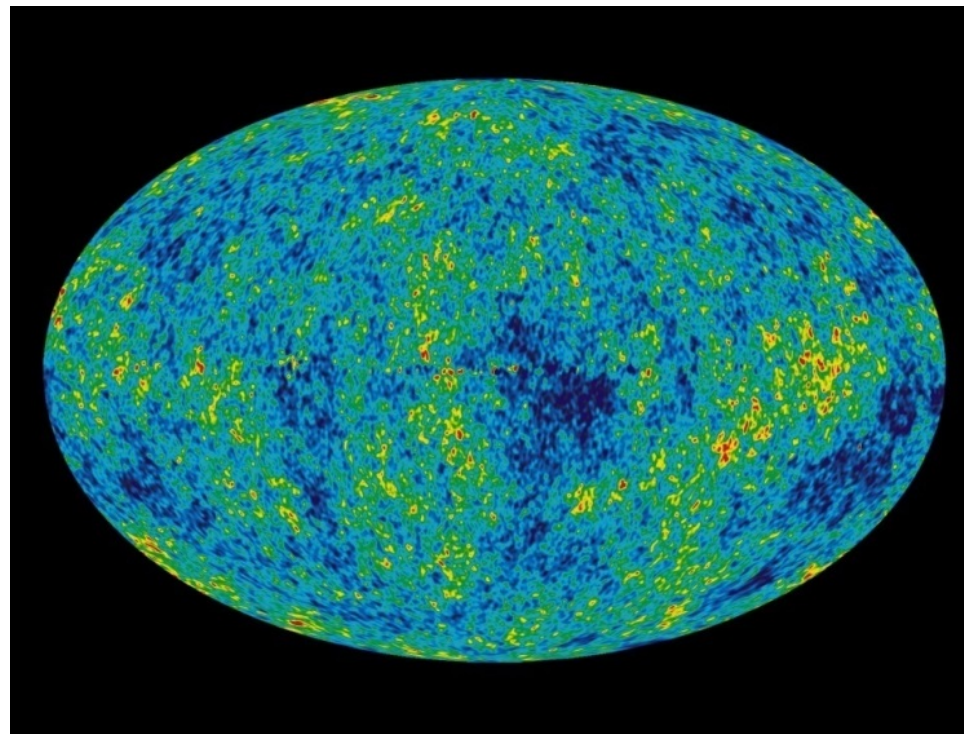


Creation of 1 hydrogen atom per m^3 per billion years

The downfall of the Steady-State model:

The Cosmic Microwave Background and Big Bang Nucleosynthesis (BBN)





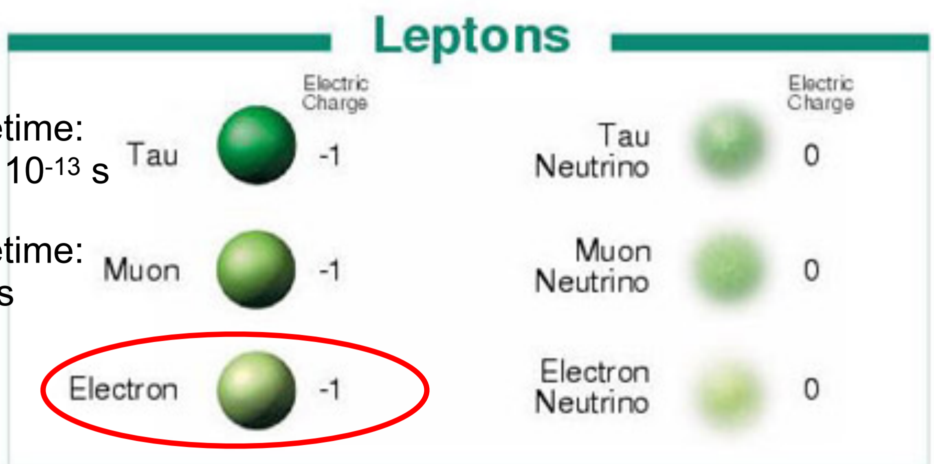
Standard Model: Elementary Particles

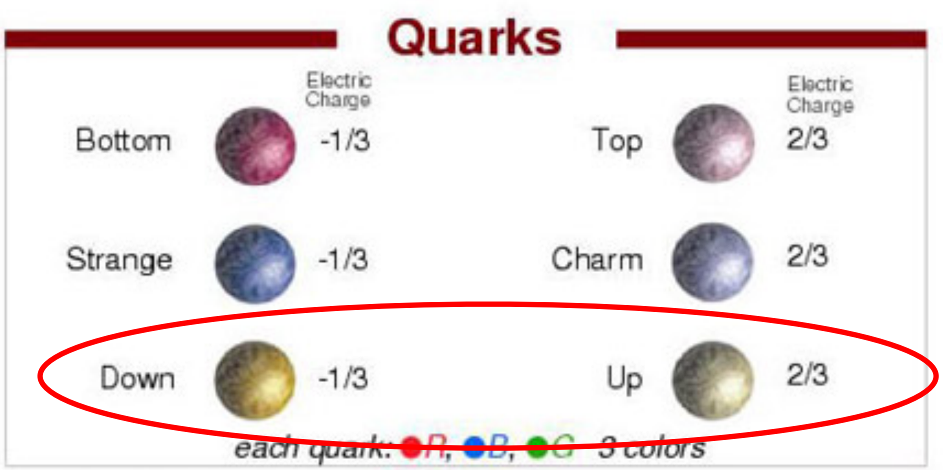
Describes 3 of the 4 known fundamental forces (electromagnetic, weak, and strong interactions) and all elementary particles.

Current formulation finalized in mid-1970s (confirmation of quarks).

Lifetime: 3×10^{-13} s

Lifetime: 2 μs





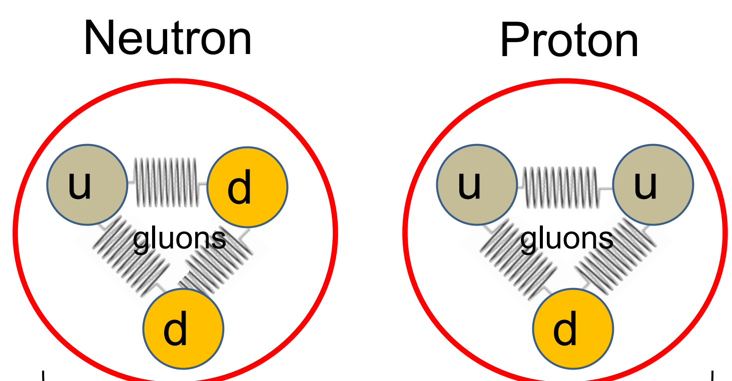
Mesons
(made out of 2 quarks)

Pions, Kaons, etc.…

Baryons
(made out of 3 quarks)

Protons, Neutrons, etc …

Hadrons



Nucleons

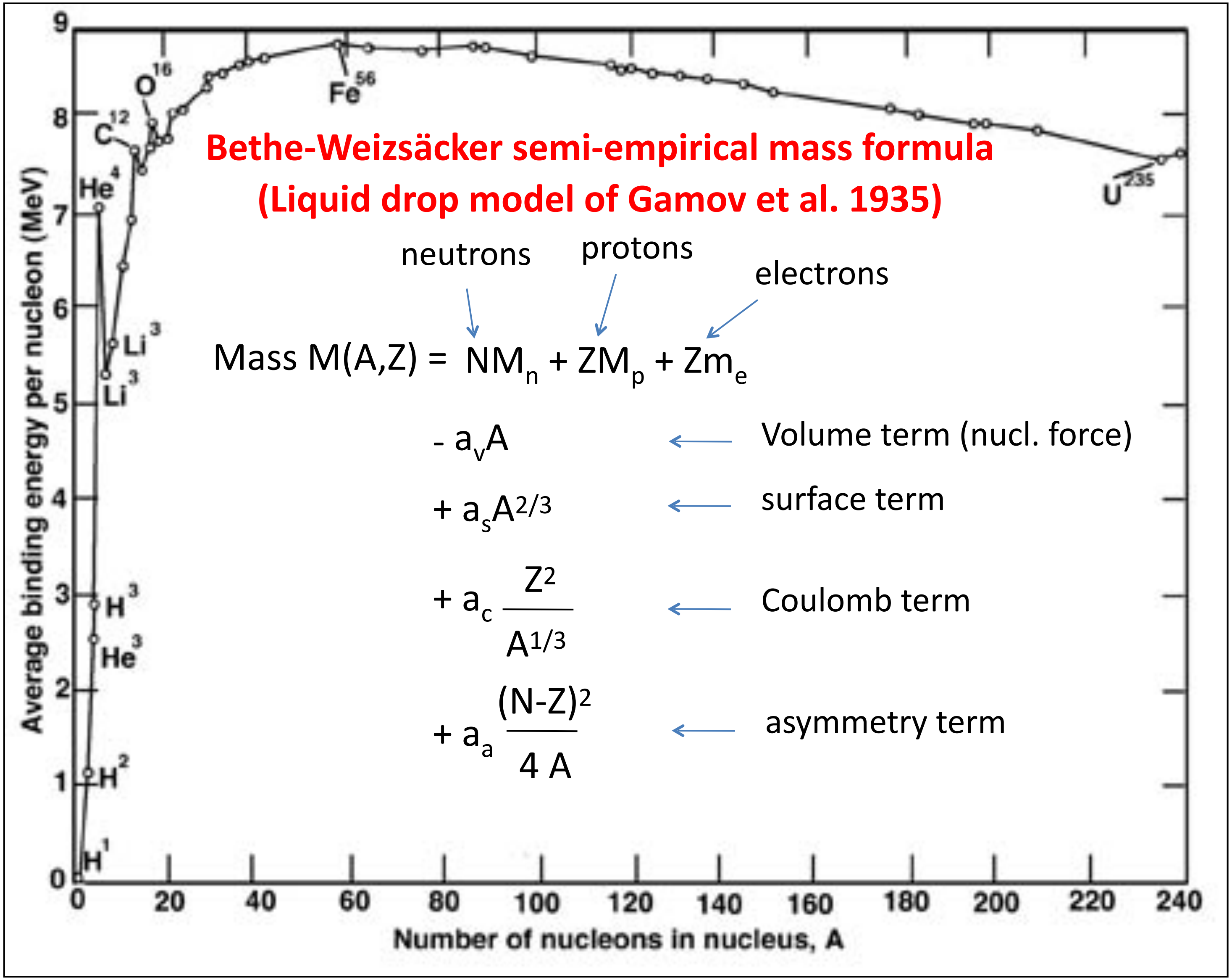
Standard Model: Fundamental Forces

Force	Acts on	Particles experiencing	Exchange particle	Coupling constant	Strength
Strong	Color	Quarks, Gluons	Gluons	α_S	1
Electromagnetic	Electric charge	Electrically charged	Photon	α	1/137
Weak	Flavor	Quarks, Leptons	W^+, W^-, Z^0	α_W	10^{-6}
Gravitation	Mass	All	(Graviton)	α_g	10^{-39}

→ 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)

Everything you need to know about Nuclear Physics



Bethe-Weizsäcker semi-empirical mass formula
(Liquid drop model of Gamov et al. 1935)

neutrons, protons, electrons

$$\text{Mass } M(A,Z) = \underbrace{NM_n}_{\text{neutrons}} + \underbrace{ZM_p}_{\text{protons}} + \underbrace{Zm_e}_{\text{electrons}}$$

$- a_v A$ ← Volume term (nucl. force)

$+ a_s A^{2/3}$ ← surface term

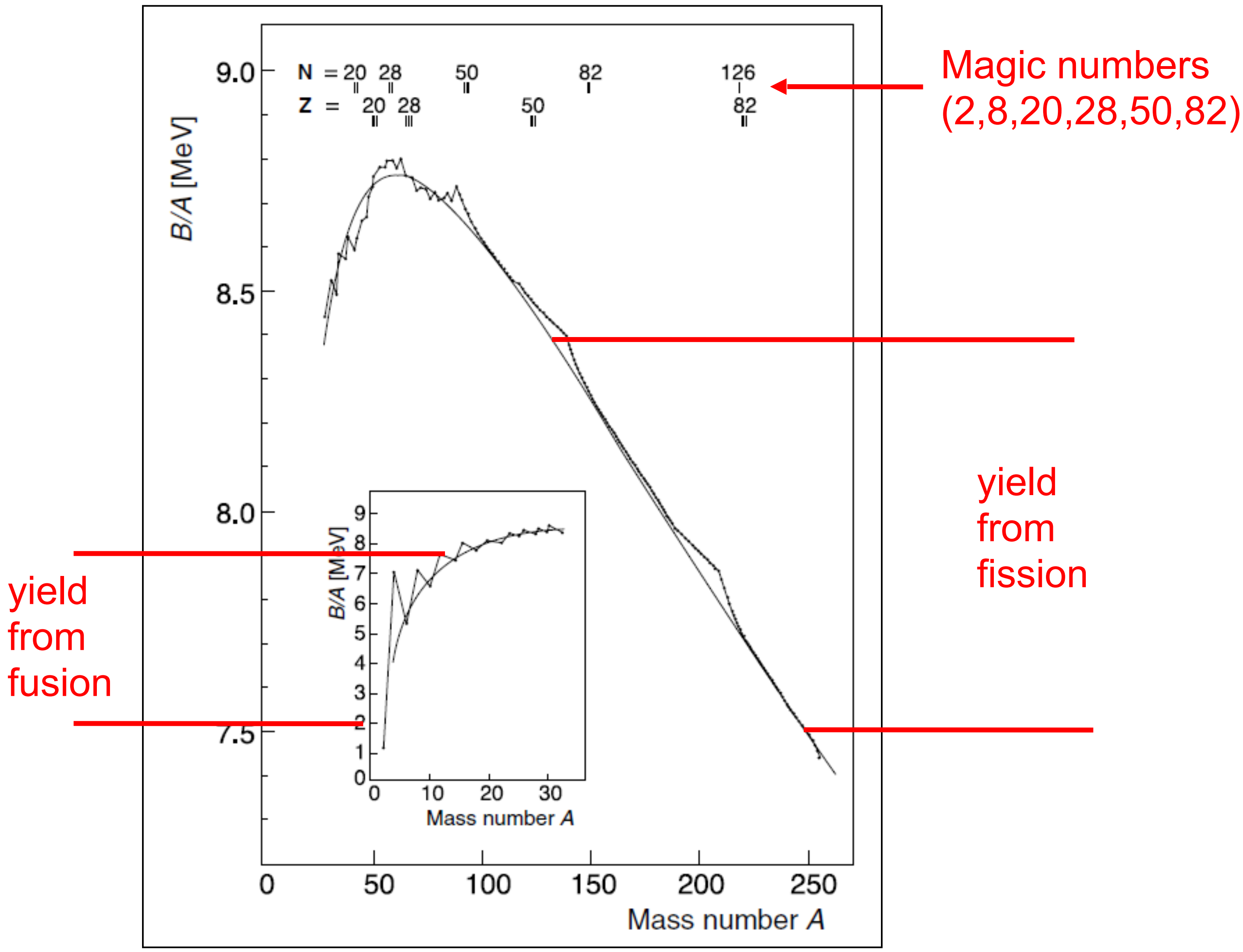
$+ a_c \dfrac{Z^2}{A^{1/3}}$ ← Coulomb term

$+ a_a \dfrac{(N-Z)^2}{4\,A}$ ← asymmetry term

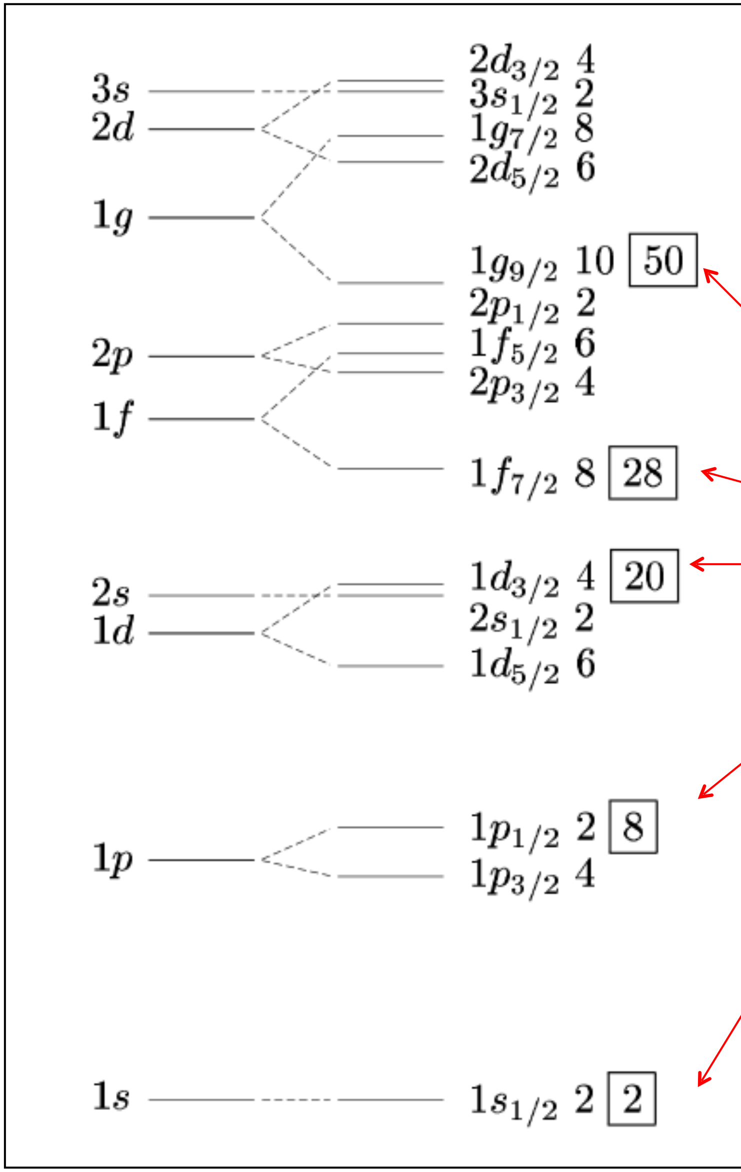
Good approximation for atomic masses

Fails to explain the existence of magic nuclei (requires nuclear shell model)

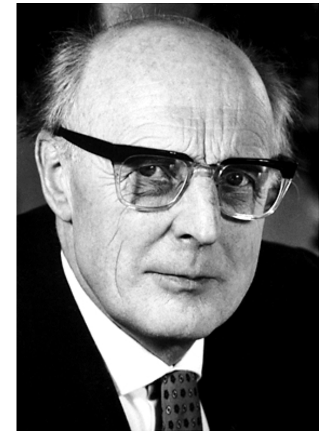
Semi-Empirical Mass Formula



Nuclear Shell Model (1949)



Maria Goeppert Mayer
(1906 – 1972)



Johannes Hans D. Jensen
(1906 – 1972)

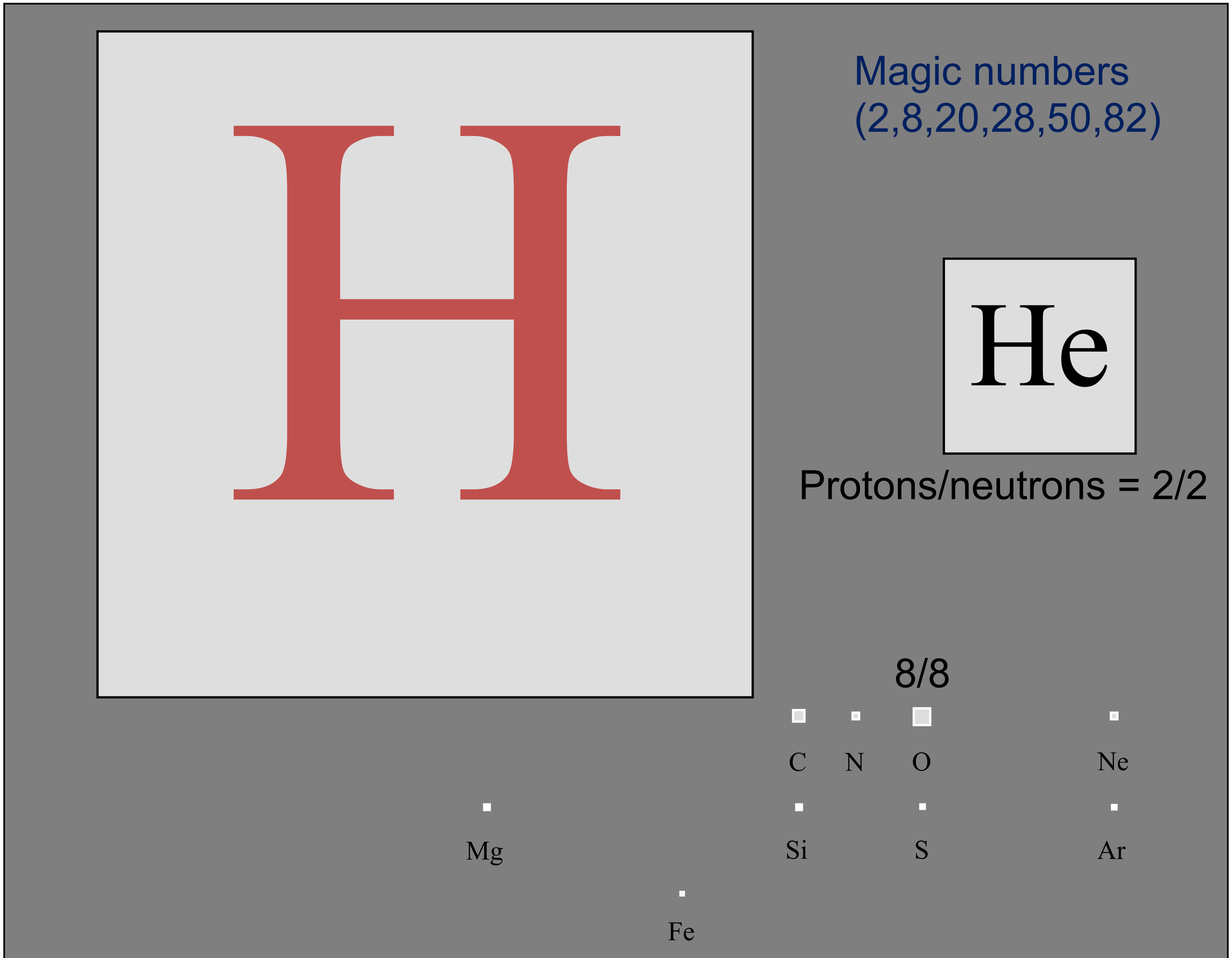
Magic
Numbers

Model of atomic nuclei (Pauli exclusion principle)

Similar to atomic shell model for e-: filled shell results in better stability

1963 Nobel Prize in Physics (M. Goeppert Mayer and J. Hans D. Jensen)

Astronomer's Periodic Table



26/30 (magic number 28)

Timeline: The First Second of the Universe

Time

Temp.

10^{30} K

< 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

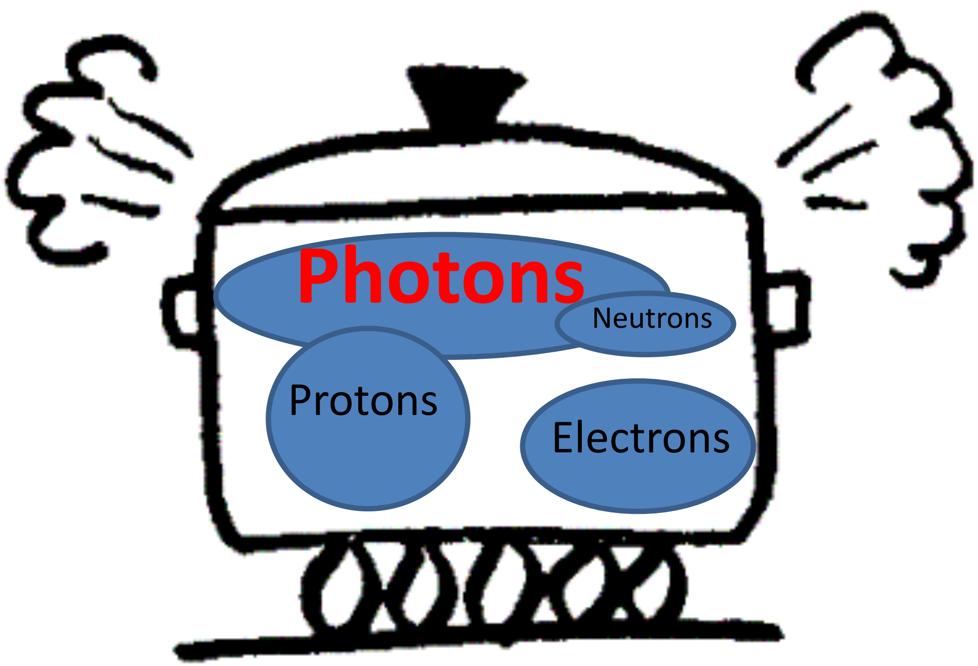
10^{10} K

Ingredients in the fist second after Big Bang

Time after Big Bang: 0.1 - 1 s

Temperature: 10^{10} K (≈ 0.86 MeV)

Photons, neutron, protons, electrons ….



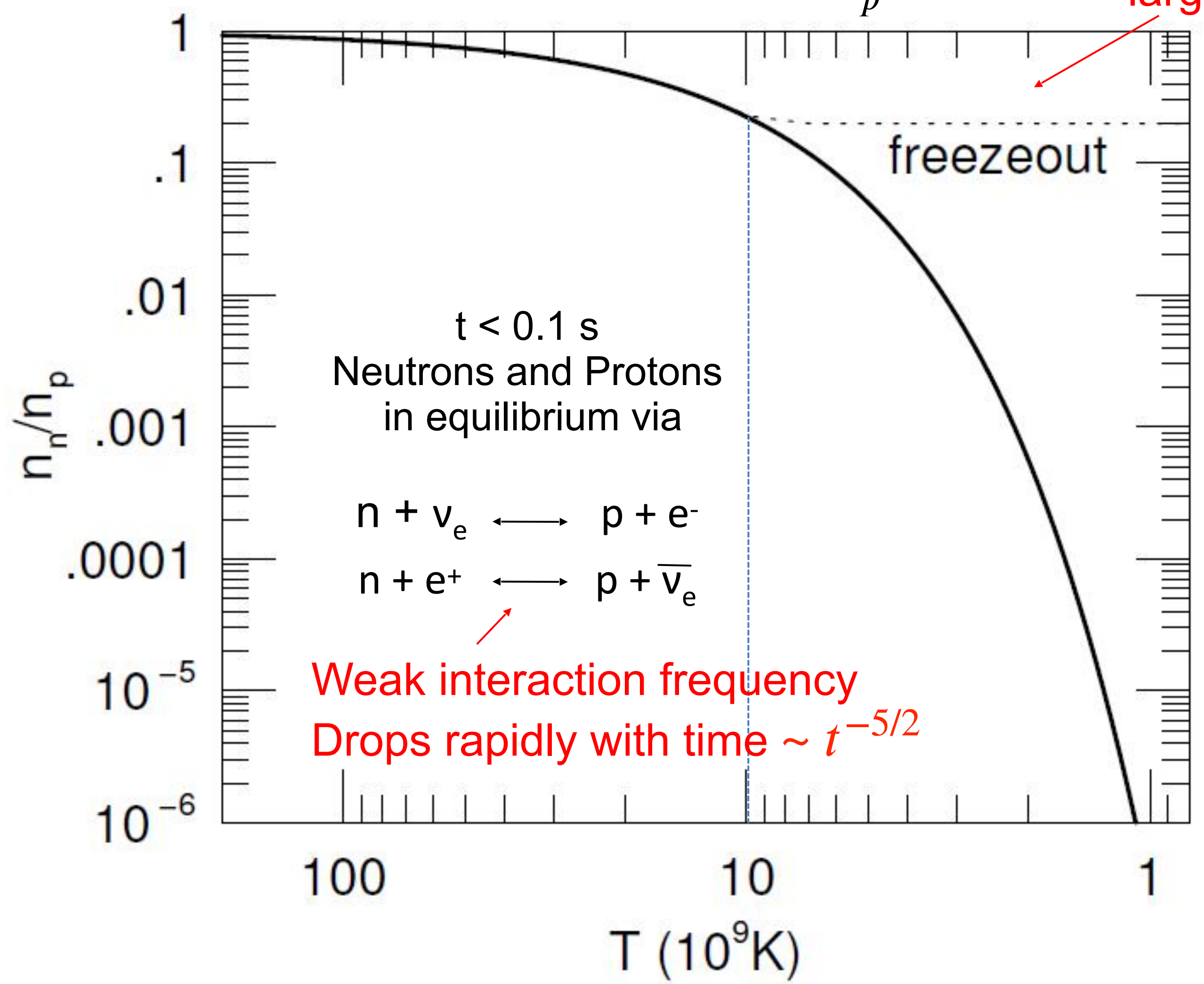
How did it end up here?

Helium mass fraction Y=0.24

Neutron/Proton Freeze-out

$Q_n = m_n c^2 - m_p c^2 = 1.29$ MeV => $\dfrac{n_n}{n_p} = e^{-\frac{Q_n}{kT}}$

Interaction time scale larger than Hubble time



Free neutrons live for 880 s and decay:

$n \longleftrightarrow p + e^- + \bar{\nu}_e$

$\boxed{\dfrac{[n]}{[p]} \sim 1/7}$

Big Bang Nucleosynthesis (BBN): Ways to form Deuterium

Occurred at t ~ 10 s to 20 min (D atoms can survive)

has to overcome Coulomb force

weak interaction

1) $p + p \longrightarrow D + e^{+} + \nu_e$

2) $n + n \longrightarrow D + e^{-} + \bar{\nu}_e$

3) $p + n \longrightarrow D + \gamma$

Good approximation:

all neutrons are used up to form deuterium via Reaction 3)

BBN: Beyond Deuterium

$$D + p \longleftrightarrow {}^3He + \gamma$$
$$D + n \longleftrightarrow {}^3H + \gamma$$

$$D + D \longleftrightarrow {}^4He + \gamma$$

$$D + D \longleftrightarrow {}^3H + p$$
$$D + D \longleftrightarrow {}^3He + n$$

$${}^3He + p \longleftrightarrow {}^4He + \gamma$$
$${}^3He + n \longleftrightarrow {}^4He + \gamma$$
$${}^3H + D \longleftrightarrow {}^4He + n$$
$${}^3He + D \longleftrightarrow {}^4He + p$$

all D, ^3He, ^3H rapidly converted to ^4He

BBN: helium yield approximation

1) Neutron/proton freeze-out at 10^{10} K with $\frac{[n]}{[p]} \approx 1/7$

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

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

Estimate primordial helium mass fraction Y_p

Sample of primordial matter:
10 protons and 2 neutrons

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

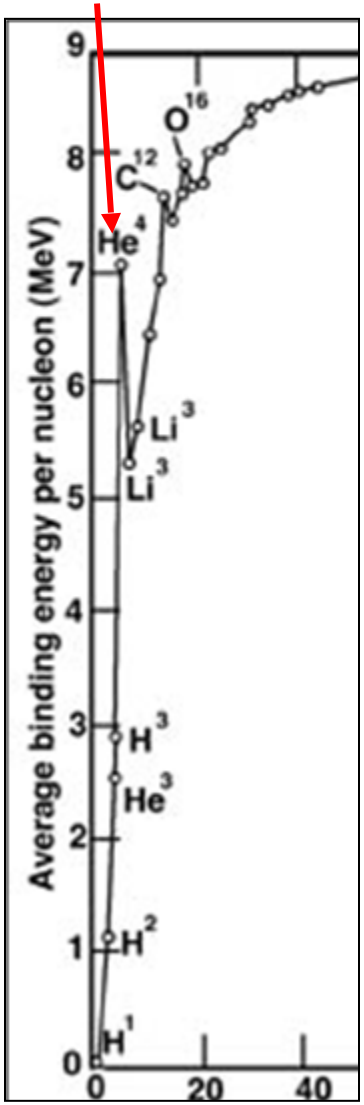
Helium mass fraction: $\mathbf{Y} \approx \frac{M_{He}}{M_{He} + 8M_p} = \frac{4}{4+8} = \mathbf{0.33}$

Y = 0.24 in reality

(take into account neutron lifetime)

Nucleosynthesis Roadblocks

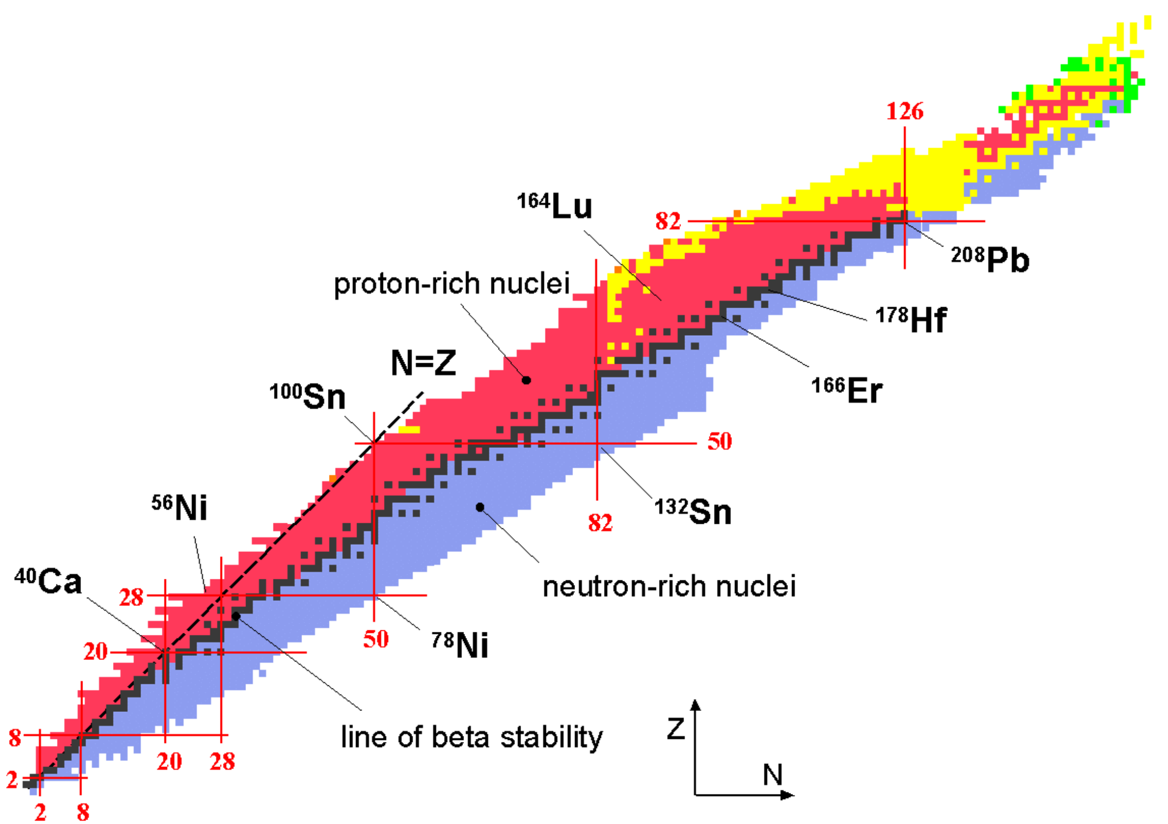
^{4}He very stable



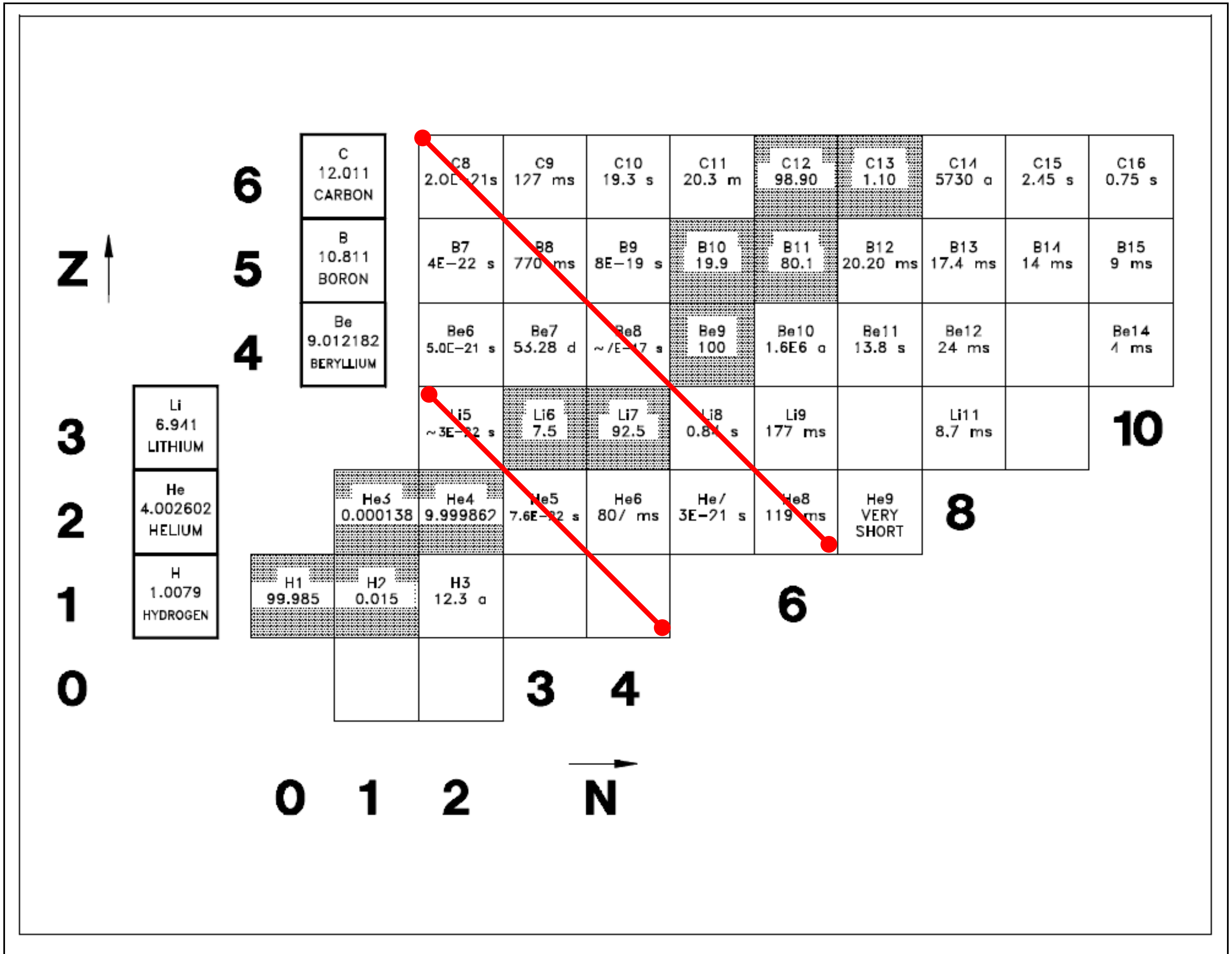
Universe filled with protons and ^{4}He:

$$p + {}^4He \longrightarrow {}^5Li + \gamma$$

$$^4He + {}^4He \longrightarrow {}^8Be + \gamma$$



Mass-5 and Mass-8 instabilities



Big Bang Nucleosynthesis

(the „alphabetical article“ or „αβγ-paper“)

Letters to the Editor

PUBLICATION of brief reports of important discoveries in physics may be secured by addressing them to this department. The closing date for this department is five weeks prior to the date of issue. No proof will be sent to the authors. The Board of Editors does not hold itself responsible for the opinions expressed by the correspondents. Communications should not exceed 600 words in length.

The Origin of Chemical Elements

R. A. Alpher*
Applied Physics Laboratory, The Johns Hopkins University, Silver Spring, Maryland
AND
H. Bethe
Cornell University, Ithaca, New York
AND
G. Gamow
The George Washington University, Washington, D. C.
February 18, 1948

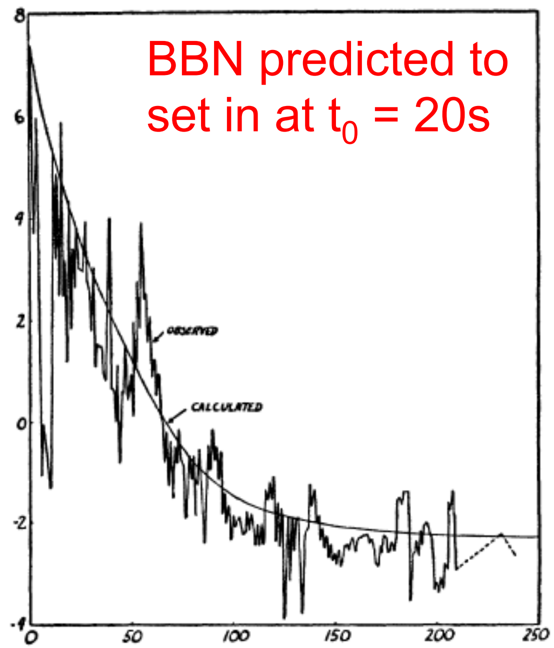


Fig. 1.
Log of relative abundance
Atomic weight

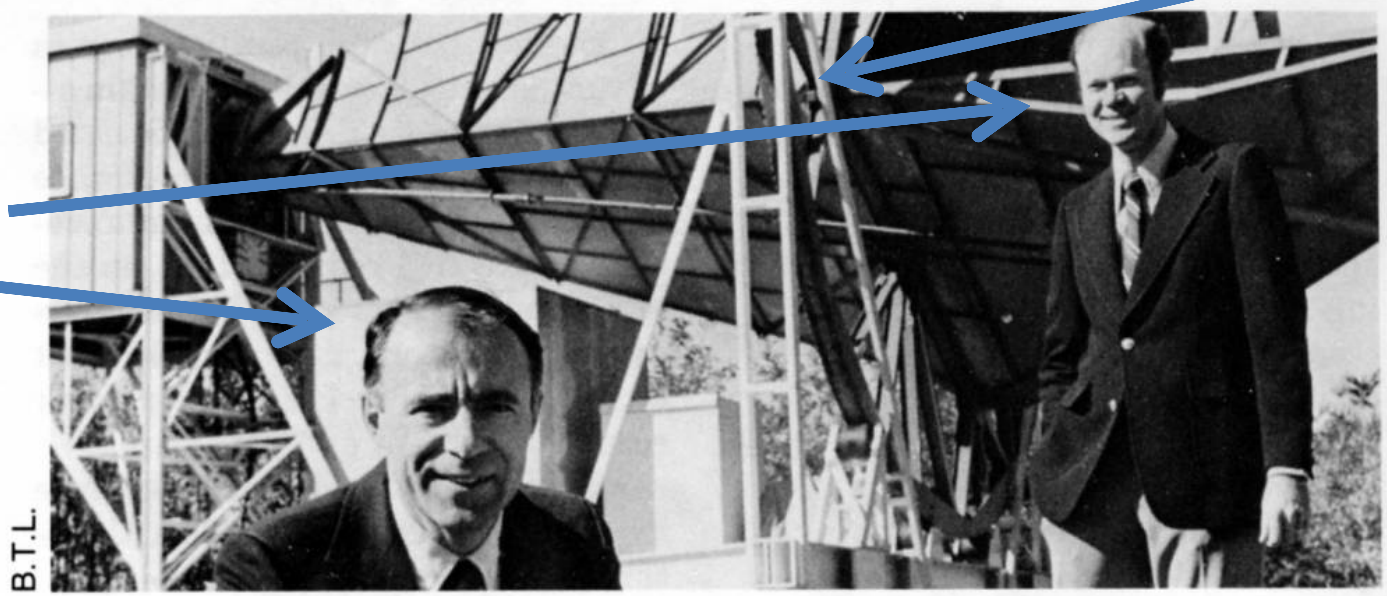
“It seemed unfair to the Greek alphabet to have the article signed by Alpher and Gamow only, and so the name of Dr. Hans A. Bethe (*in absentia*) was inserted in preparing the manuscript for print. Dr. Bethe, who received a copy of the manuscript, did not object, and, as a matter of fact, was quite helpful in subsequent discussions. There was, however, a rumor that later, when the alpha, beta, gamma theory went temporarily on the rocks, Dr. Bethe seriously considered changing his name to Zacharias.”

G. Gamov

The Cosmic Microwave Background and Big Bang Nucleosynthesis (BBN)

Microwave antenna

Nobel Prize 1978



Penzias (left) and Wilson. "A small discrepancy led them to the grandest of all possible answers."

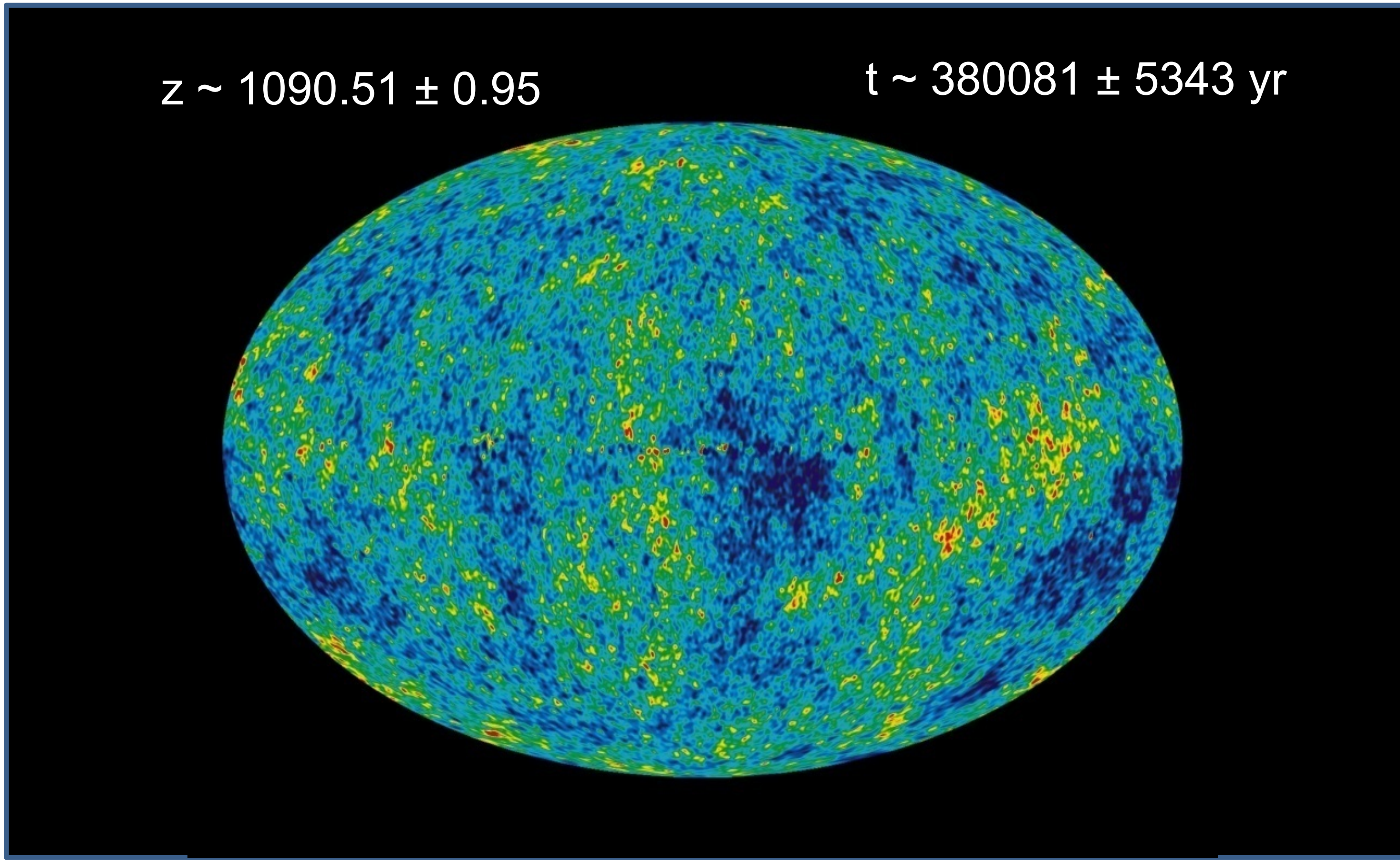
Nobel Prize 2019

Intense isotropic background at a wavelength of 7cm

Interpreted as Big Bang signature by R.H. Dicke and J. Peebles

The last scattering surface

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



At T = 380 000 yr (after recombination) matter and radiation de-couple

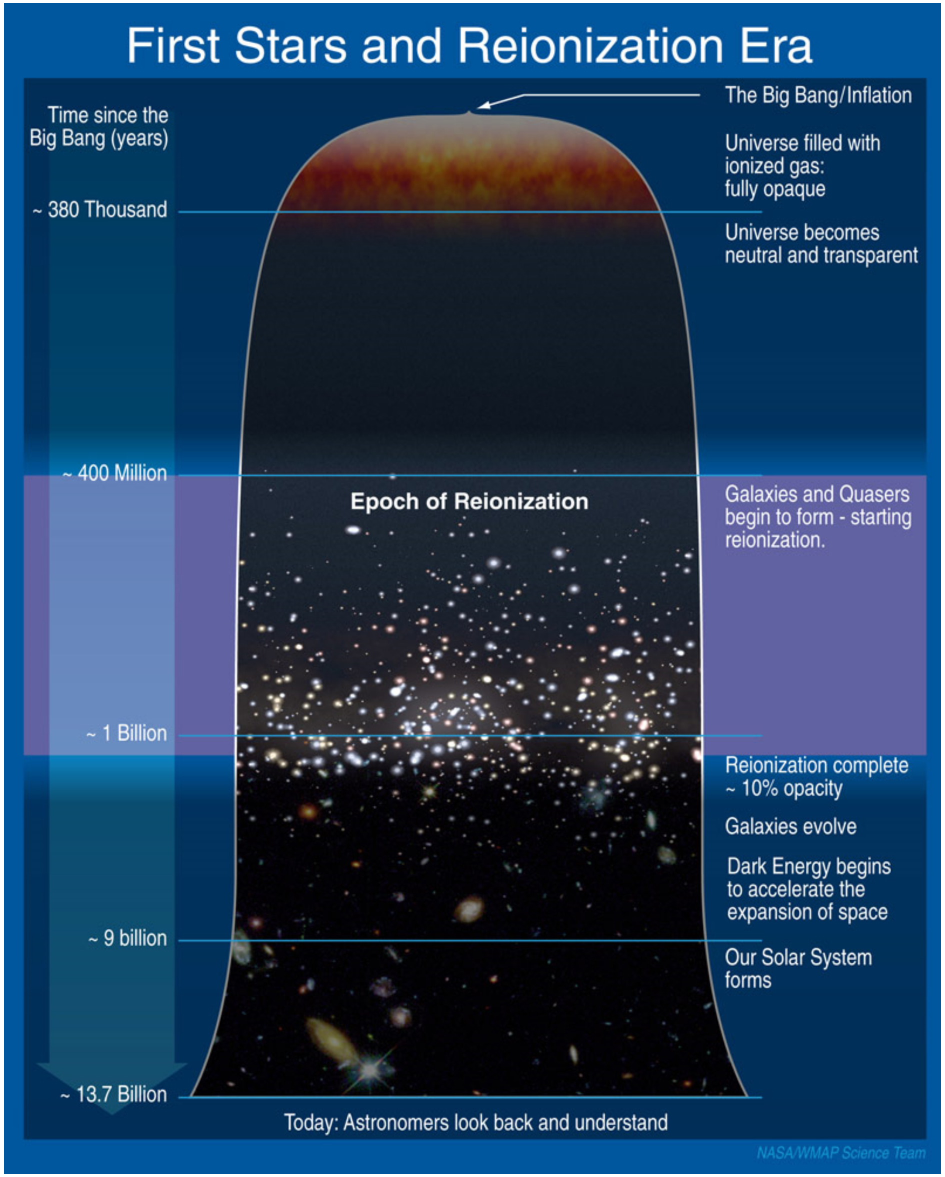
Density fluctuations on the order of 10^{-5}

PART II

Timeline

10000 K

30 K



First molecules

First stars

Recombination
t < 380000 yr

Ionization potentials [in eV]

	1st	2nd	3rd	4th
H	13.6			
He	**24.6**	54.4		
Li	5.4	75.6	122.5	

$Li^{3+} + e \rightarrow Li^{2+} + \gamma$

$Li^{2+} + e \rightarrow Li^{+} + \gamma$

$Li^{+} + e \rightarrow Li + \gamma$

$He^{2+} + e \rightarrow He^{+} + \gamma$

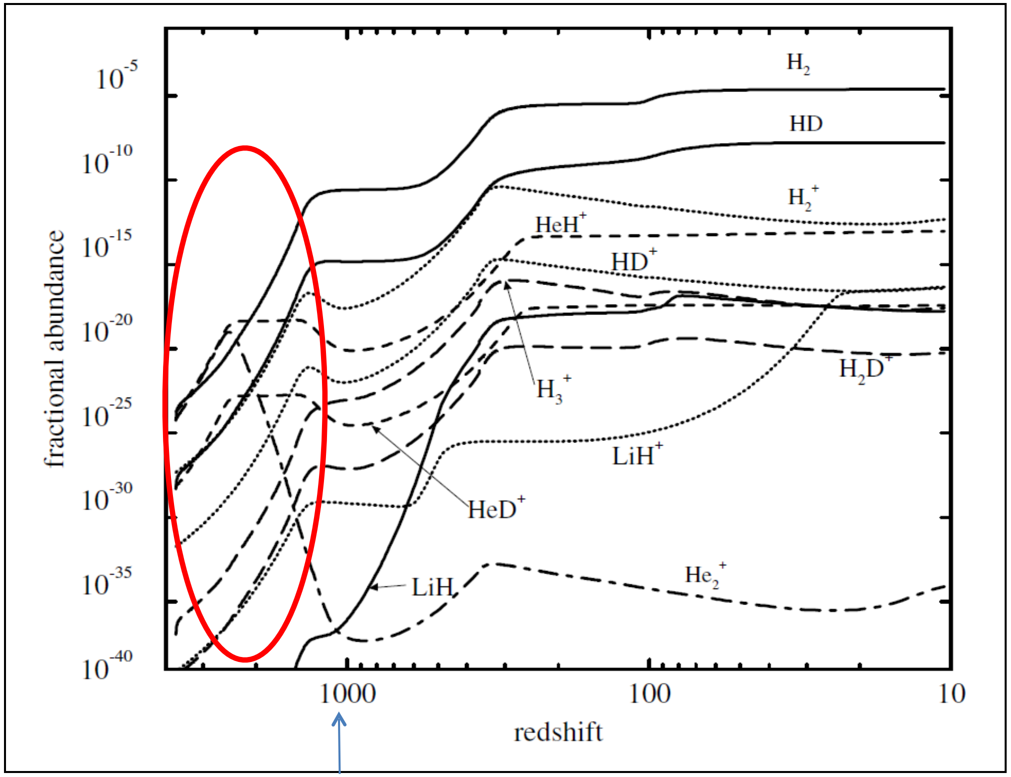
$He^{+} + e \rightarrow \mathbf{He} + \gamma$

$H^{+} + e \rightarrow \mathbf{H} + \gamma$

He^{+} recombines first to form the first neutral atoms **He**

H^{+} recombines second to form **neutral H**

Formation of Molecules (z > 1000)



T = 380000yr

The First Molecule: HeH^+

$$\begin{aligned} \mathrm{He} + \mathrm{H}^+ &\rightarrow \mathrm{HeH}^+ + \gamma\,, \\ \mathrm{He} + \mathrm{He}^+ &\rightarrow \mathrm{He}_2^+ + \gamma\,. \end{aligned}$$

The first neutral molecule: H_2

$$\begin{aligned} \mathrm{HeH}^+ + \mathrm{H} &\rightarrow \mathrm{H}_2^+ + \mathrm{He}, \\ \mathrm{H}_2^+ + \mathrm{H} &\rightarrow \mathrm{H}_2 + \mathrm{H}^+, \end{aligned}$$

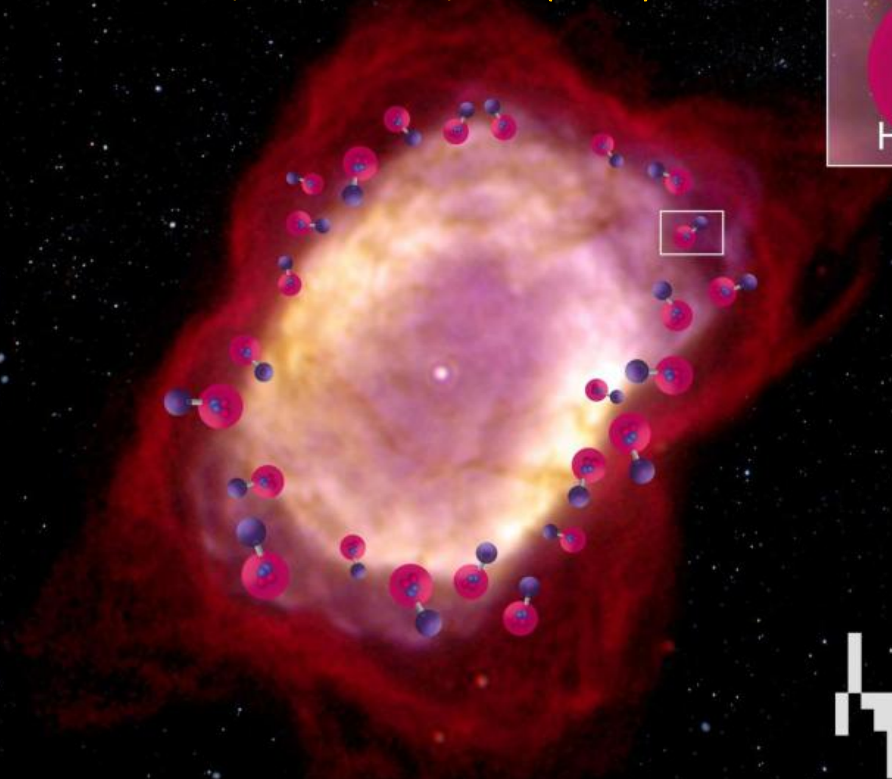
Lepp, Stancil, Dalgarno, J. Phys. B., At. Mol. Opt. Phys 35 (2002) R57-R80

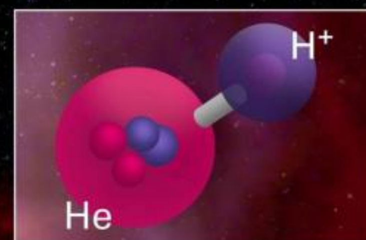
Recent astronomical detection of HeH^+

Güsten et al, Nature 568, 357 (2019)

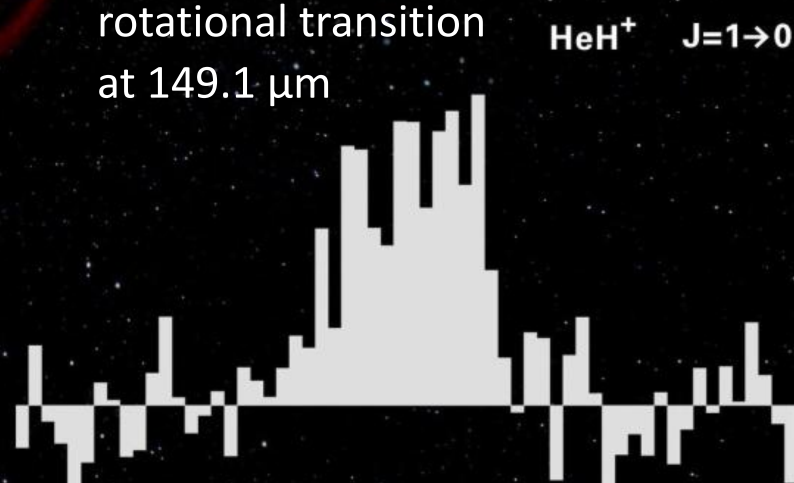
First Molecule detected!

(But: in a planetary nebula)

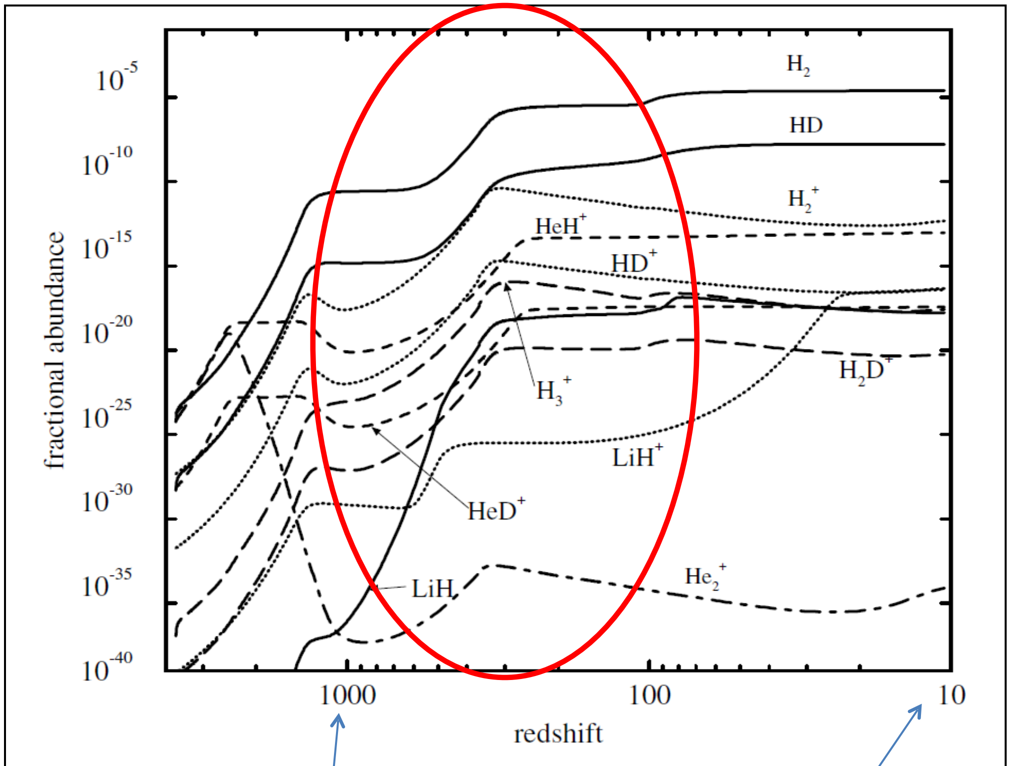




Ground state
rotational transition
at 149.1 µm



Formation of Molecules (1000> z > 100)



t = 380000yr

t = 480 x10⁶ yr

More hydrogen: the H_2^+ channel

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

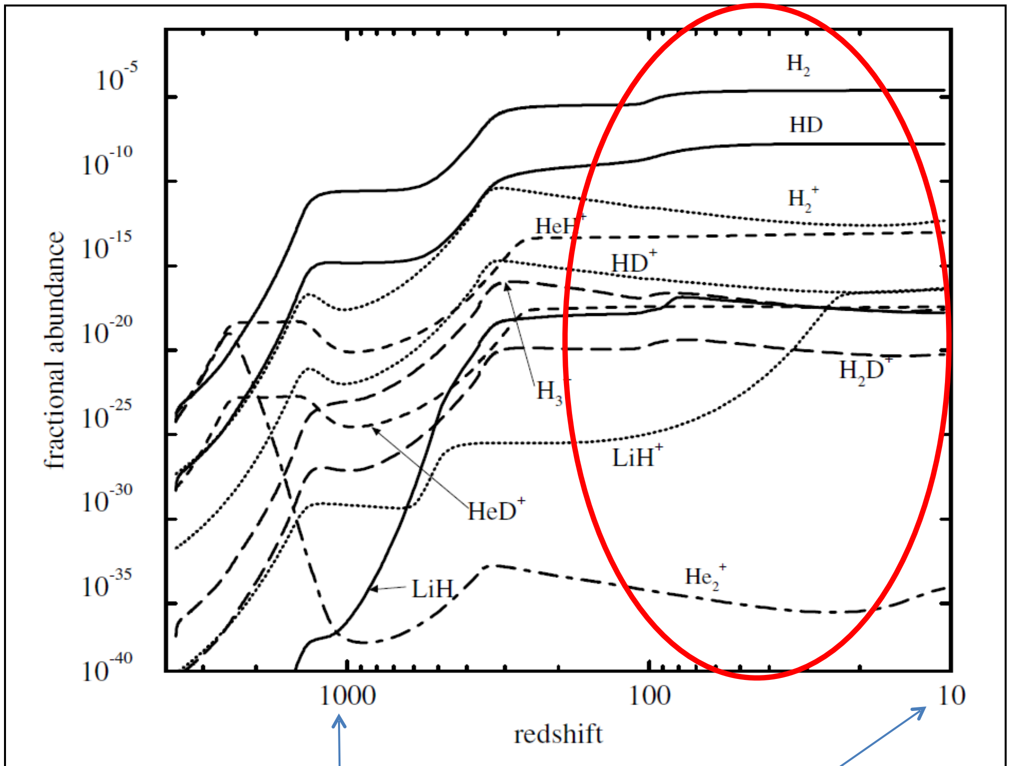
More molecules:

D_2^+ , H_3^+, H_2D^+, D_2H^+, D_3^+

HeH^+, HeD^+, He_2^+

LiH^+, LiD^+, LiD, LiH^+

Formation of Molecules (z < 100)



T = 380000yr

t = 480 x10^6 years

The H^- channel:

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

Binding energy 0.75 eV

$$H^- + H \rightarrow H_2 + e^-.$$

H_2 associative detachment

Nobel Prize 2019

Peebles, P.J.E. and Dicke, R.H. (1968) *Astrophys. J.*, **154**, 891–908.

Peebles and Dicke find H^- channel more proficient than H_2^+ channel

H^- in Space: Source of the Sun's Opacity

Photodetachment

$H^- + \gamma \longrightarrow H + e$

This process happens in the **photosphere**, and it is responsible for the suns' opacity. (Otherwise the Sun would be transparent).

NEGATIVE IONS OF HYDROGEN AND THE OPACITY OF STELLAR ATMOSPHERES

RUPERT WILDT

ABSTRACT

Astrophysical Journal, vol. 90, p.611 (1939)

Stars and Metallicity*

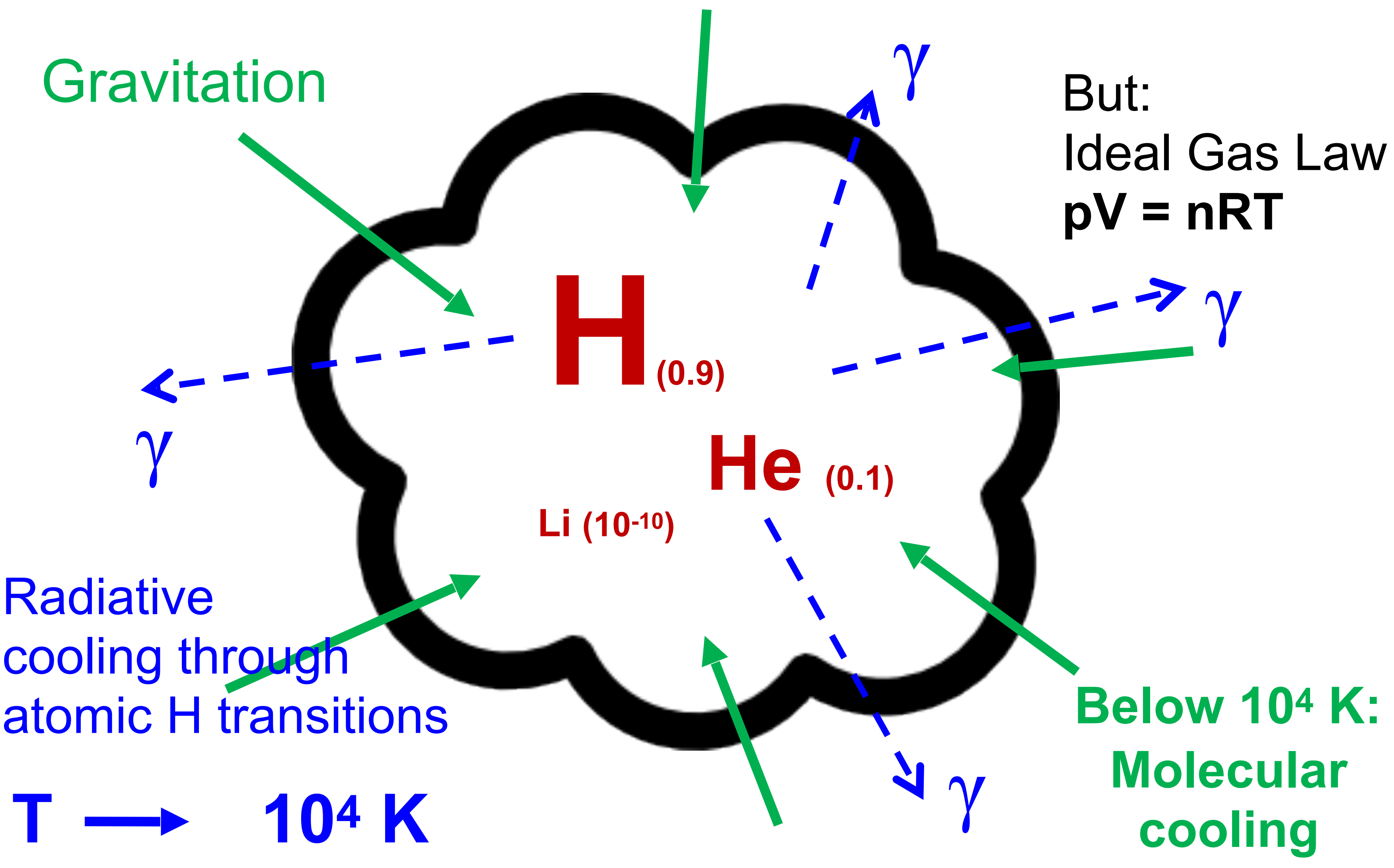
Population I stars : **Metal-rich stars**, formed out of clouds that were enriched by previous generations
(example: our Sun)

Population II stars : **Metal-poor stars**, formed out of clouds that have been contaminated by the first generation of stars
(example: galactic halo stars)

Population III stars : **Metal-free stars.**

*Metals in astronomy: anything heavier than He

The Onset of Star Formation in the Early Universe



Cooling through Rovibrational Transitions of H_2

Through collisions H atoms transfer some of their energy to H_2

Kinetic energy

vibrations, rotations

$$\mathbf{H(Ek) + H_2(v,R) \rightarrow H(Ek\text{-}\Delta) + H_2(v',R')}$$

The excited H_2 radiates that energy out of the cloud

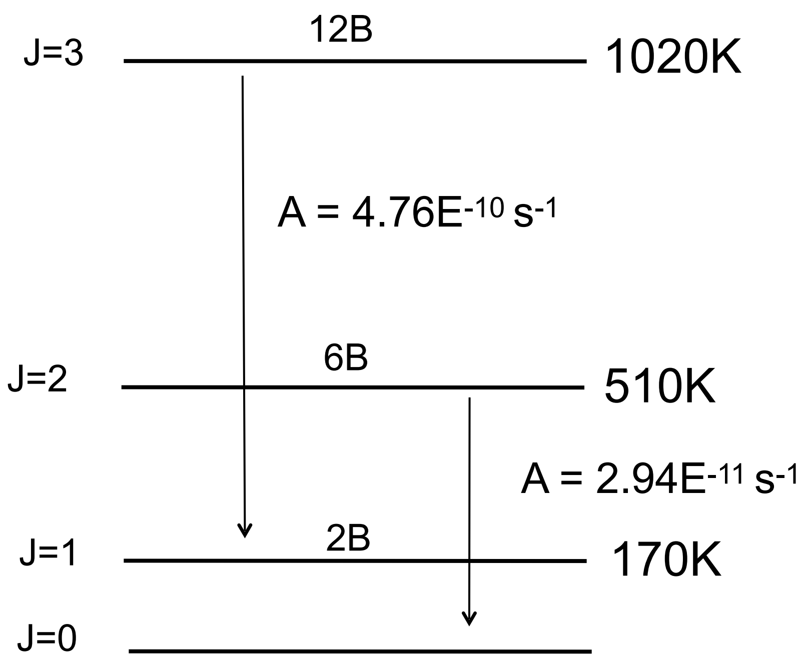
$$\mathbf{H_2(v',R') \rightarrow H_2(v,R) + photon(s)}$$

Primordial Cooling: H_2 and HD

H_2

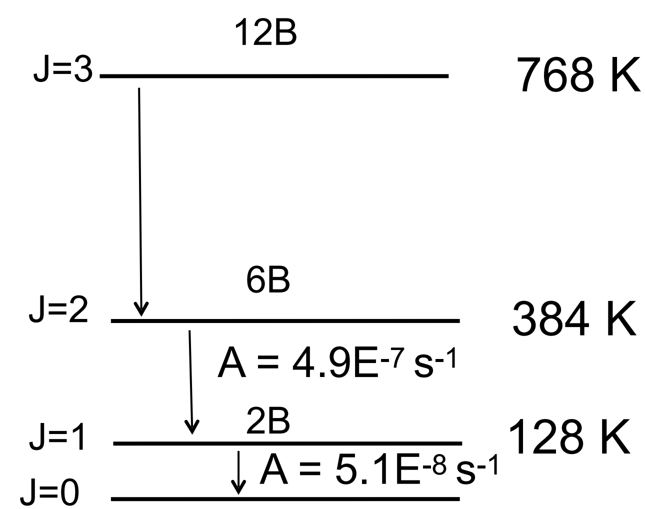
$E = B\,J\,(J+1)$

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



HD

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



Deuterium Fractionation

TABLE IV. Dissociation energies of the hydrogen molecule in cm^{-1}.

	H_2	HD	D_2
Theory	36 118.049	36 405.763	36 748.345
Experiment	36 118.11 ± 0.08[a]	36 406.2 ± 0.4[b]	36 748.3 ± 0.1[c]
Discrepancy	0.06 ± 0.08	0.4 ± 0.4	0.0 ± 0.1

[a]Reference 4.
[b]Reference 18.
[c]Reference 7.

Kolos and Rychlewski, J.Chem. Phys. 98, 3960 (1993)

H_2: 4.47792 eV
HD: 4.51359 eV

$\Delta E = 0.0357$ eV = 413.9 K

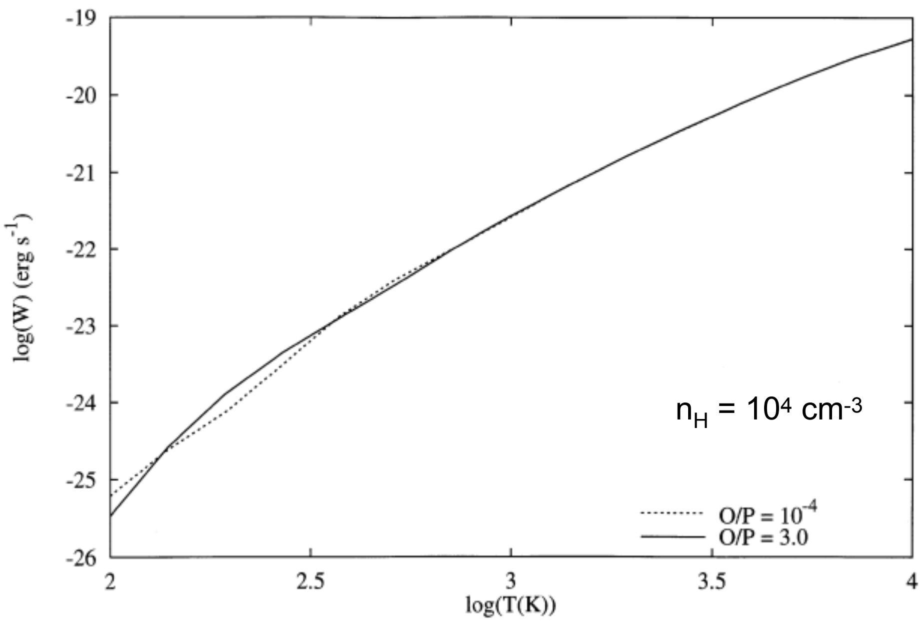
$$H_2 + D^+ \longrightarrow HD + H^+$$

D insertion into molecules preferred at low temperatures

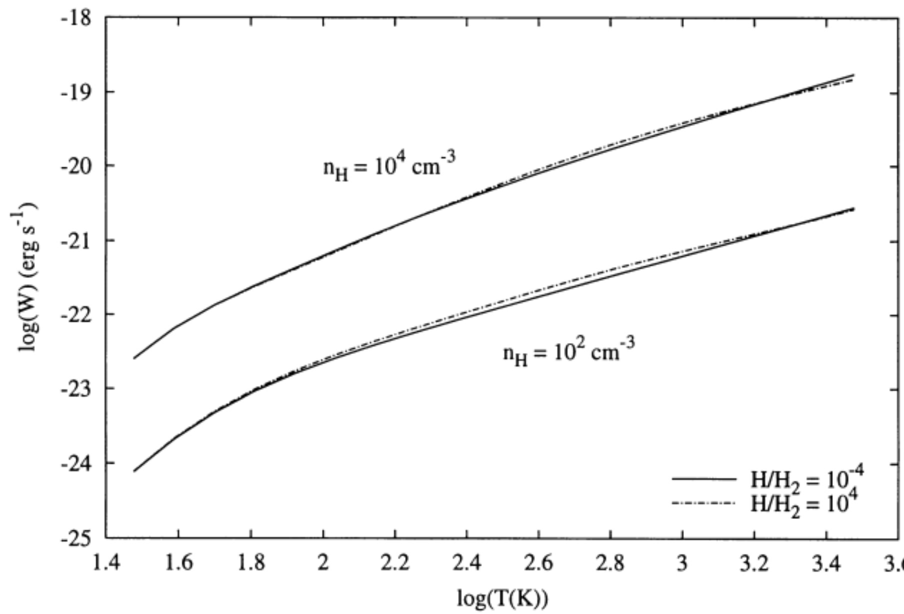
$\longrightarrow$ overabundance of deuterated molecules

H_2 vs. HD cooling function

H_2

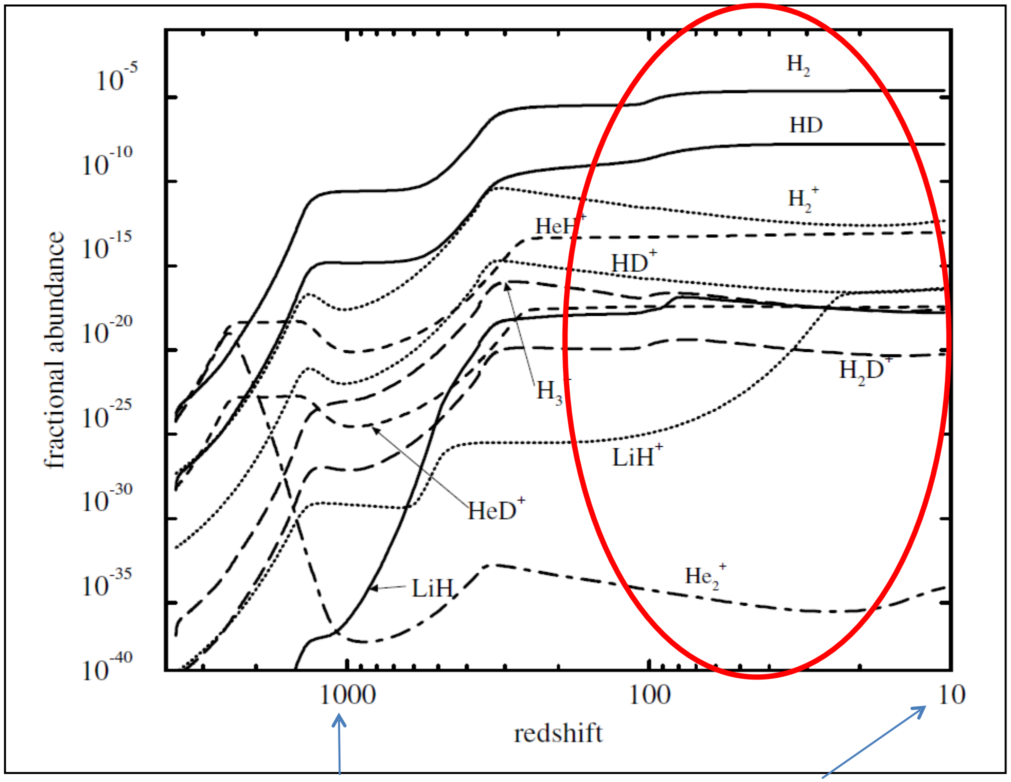


HD



HD is a much more efficient coolant at low temperature!

Formation of Molecules (z < 100)



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Binding energy 0.75 eV

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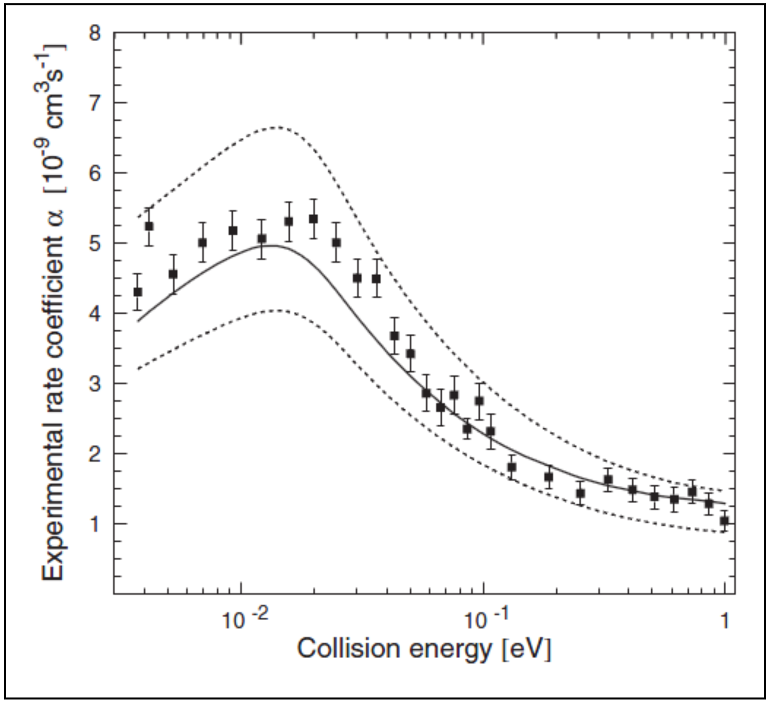
H_2 associative detachment

Protogalaxy Formation in the Early Universe

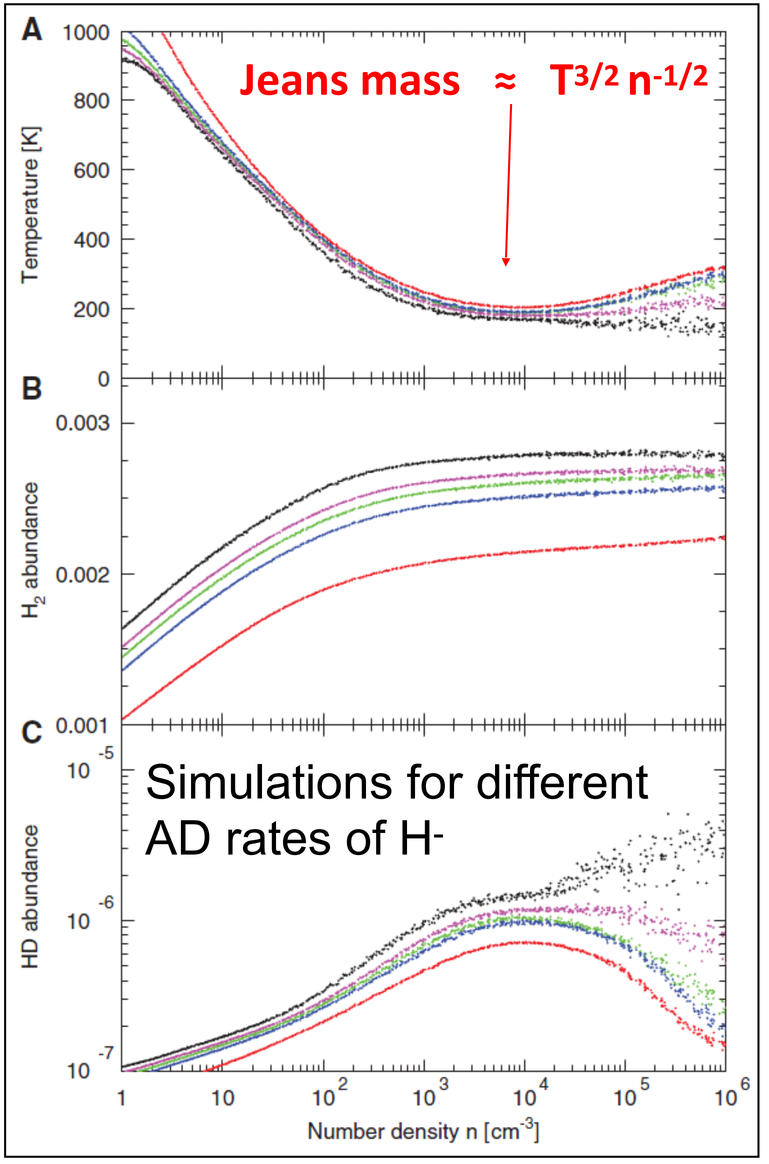
H_2 associative detachment AD

$$H^- + H \rightarrow H_2 + e^- .$$



Kreckel et al., Science **329**, 69 (2010)

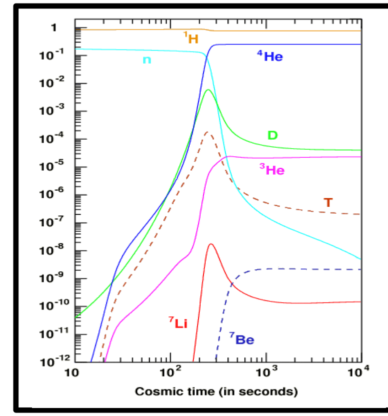
The mass of the first stars can be determined more precisely



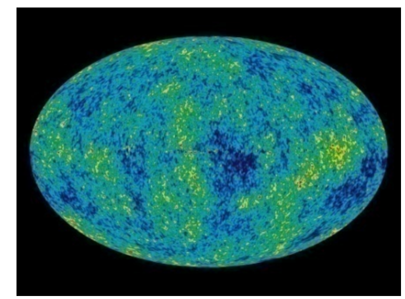
Simulation: Simon Glover

Summary

At times **t = 3- 20 minutes, nuclear physics** dominates at MeV energies (T ~ 10^{10}K). Big Bang Nuleosynthesis model reproduces the elemental abundances accurately.

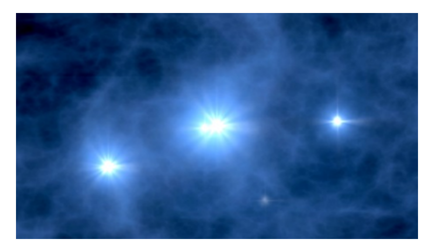


Just before **t ~ 380 000 yr**, protons and electrons recombine and the Universe becomes transparent. Temperatures are around
T ~10000K, energies around **1eV**.
The first molecules form shortly thereafter!



Dark ages

Around t ~ 400 x 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 reviews:

S. Lepp, P.C. Stancil, A. Dalgarno
"Atomic and molecular processes in the early Universe"
J. Phys. B.: At. Mol. Opt. Phys. **35** (2002) R57-R80

Galli, Daniele; Palla, Francesco
"The Dawn of Chemistry"
Annual Review of Astronomy and Astrophysics,
vol. 51, issue 1, pp. 163-206 (2013)