The hot, early universe

Cosmology Block Course 2014

Simon Glover & Markus Pössel

Institut für Theoretische Astrophysik/Haus der Astronomie

30 July 2014

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Thermodynamics & statistics in an FLRW universe

- Up to now, matter in our universe has not interacted
- If we get back to sufficiently small $a(t)$ (as we must $\rightarrow$ singularity theorems!), we cannot have had separate galaxies
- Early universe: filled with plasma, colliding particles (atoms and photons, nucleons and nucleons) $\Rightarrow$ we need a description from thermodynamics and statistical physics!

When thermodynamics is simple and when it isn’t

Thermodynamics is simple when a system is in **thermal equilibrium**, and complicated when it isn’t.

(If not in equilibrium: fluid dynamics plus reaction kinetics – can be horribly complicated!)

In equilibrium, certain *thermodynamical quantities* can be introduced, which take on constant values throughout the system. Best-known of those: Temperature T and pressure p.

Equilibrium thermodynamics: given energy E, volume V, particle number N, calculate T, p.

Statistical basis for thermodynamics

Thermodynamics: Macrostates specified by thermodynamic variables like E, V, T, p, N.

Statistical mechanics: Microstates of particles (e.g. N particles making up a gas – each has a given momentum at a given time)

Entropy as a quantity to count microstates compatible with a macrostate:

$$S = k \cdot \log \Omega(E, V, N).$$

Systems in equilibrium

Entropy difference in terms of changing variables:

$$\mathrm{d}S = \frac{1}{T} \cdot \mathrm{d}E + \frac{p}{T} \cdot \mathrm{d}V$$

(this can be taken as *definitions* of T and p).
Re-write as first law of thermodynamics:

$$\mathrm{d}E = T \cdot \mathrm{d}S - p \cdot \mathrm{d}V$$

Systems that are not in equilibrium

Second law of thermodynamics: $\delta S \geq 0$, but never $\delta S < 0$. Entropy cannot decrease.

Two systems in contact so that $S = S_1 + S_2$, $V = V_1 + V_2$, $E = E_1 + E_2$:

$\mathrm{d}E_1 = -\mathrm{d}E_2$; $\mathrm{d}V_1 = -\mathrm{d}V_2$ so that

$$\mathrm{d}S = \left(\frac{1}{T_1} - \frac{1}{T_2}\right) \cdot \mathrm{d}E_1 + \left(\frac{p_1}{T_1} - \frac{p_2}{T_2}\right) \cdot \mathrm{d}V_1 \geq 0.$$

Second law means: at constant volume, $\mathrm{d}E_1 < 0$ if $T_1 > T_2$. At constant temperature, $\mathrm{d}V_1 > 0$ if $p_1 > p_2$. In thermodynamics equilibrium, $\mathrm{d}S = 0$, so $T_1 = T_2$, $p_1 = p_2$. All as expected.

Entropy density

Define the entropy density $s(T)$ by $S(T,V) = V\cdot s(T)$
(This works because entropy is extensive!).

Then for any adiabatic change,

$$\begin{aligned} \mathrm{d}(s(T)V) &= V\mathrm{d}s(T) + s(T)\mathrm{d}V = \mathrm{d}S(T,V) = \frac{\mathrm{d}(\rho c^2 V) + p\mathrm{d}V}{T} \\ &= \frac{Vc^2}{T}\frac{\mathrm{d}\rho}{\mathrm{d}T}\mathrm{d}T + \frac{(\rho c^2 + p)\mathrm{d}V}{T} \end{aligned}$$

This can only hold generally if the coefficients for $\mathrm{d}V$ are equal:

$$s(T) = \frac{\rho c^2 + p}{T}$$

(coefficients for $\mathrm{d}T$ give energy conservation).

Chemical potential

Additional contribution to entropy:

$$\mathrm{d}S = \frac{1}{T}\cdot\mathrm{d}E + \frac{p}{T}\cdot\mathrm{d}V - \sum_i \frac{\mu_i}{T}\mathrm{d}N_i$$

(this can be taken as the definition of the μ_i). New first law:

$$\mathrm{d}E = T\cdot\mathrm{d}S - p\cdot\mathrm{d}V + \sum_i \frac{\mu_i}{T}\mathrm{d}N_i$$

Chemical potential

Within the same system, in thermal equilibrium, reactions changing particle species 1 into 2 (and other way around), with $N_1 + N_2 = N$ =const.:

$$\mathrm{d}S = \frac{1}{T}(\mu_2 - \mu_1)\mathrm{d}N_1.$$

If $\mu_2 > \mu_1$, number of 1-particles increases! In full thermodynamic equilibrium, from $\mathrm{d}S = 0$, $\mu_1 = \mu_2$.

Distinguish between

- **thermal equilibrium** (T, p constant, μ_i can differ from equilibrium values)
- **chemical equilibrium** (μ_i have equilibrium values, T, p could differ)
- **thermodynamic equilibrium** (T, p, μ_i all have equilibrium values)

Multi-particle reactions:

Particle reaction

$$1 + 2 \leftrightarrow 3 + 4$$

(z.B. $H + \gamma \leftrightarrow p + e^-$, or nuclear reaction):

$\mathrm{d}N_1 = \mathrm{d}N_2 = -\mathrm{d}N_3 = -\mathrm{d}N_4$, then in thermal (not necessarily chemical!) equilibrium:

$$\mathrm{d}S = \frac{1}{T}(\mu_3 + \mu_4 - \mu_1 - \mu_2)\mathrm{d}N_1 \geq 0.$$

In equilibrium,

$$\mu_3 + \mu_4 = \mu_1 + \mu_2$$

(more generally: one such relation for each conserved quantum number: baryon number, lepton number, . . .)

Particles in thermal equilibrium

Grand-canonical example: E, V, N given — what is the equilibrium state? (Sum over quantum states, treat bosons and fermions differently).

Number density in momentum space cell $\mathrm{d}^3p = \mathrm{d}p_x \cdot \mathrm{d}p_y \cdot \mathrm{d}p_z$:

$$n(p_x, p_y, p_z) = \frac{g}{\exp\left([E(p)-\mu]/kT\right) \mp 1} \; \frac{\mathrm{d}^3p}{h^3}$$

with $E(p) = \sqrt{mc^2 + (pc)^2}$.

Integrate up to get total particle number density!

Highly relativistic particles 1/2

$kT > mc^2$, $kT > \mu$, $E \approx pc$:

Equipped with these formulae, it is straightforward to show that

$$n = \frac{8\pi}{(ch)^3}\,\zeta(3)\,g(kT)^3 \cdot \begin{cases} 1 & \text{bosons} \\ 3/4 & \text{fermions} \end{cases}$$

wIth $\zeta(3) = 1.2020569031$. The density for highly relativistic particles is

$$\rho c^2 = \frac{4\pi^5}{15(ch)^3}\,g(kT)^4 \cdot \begin{cases} 1 & \text{bosons} \\ 7/8 & \text{fermions} \end{cases}$$

For bosons, this is *Bose-Einstein statistics*, for fermions, *Fermi-Dirac statistics*.

Highly relativistic particles 2/2

Pressure:

$$p = \frac{1}{3}\rho c^2 \quad \text{(as for radiation!)}$$

Entropy density:

$$s(T) = \frac{4}{3}\frac{\rho c^2}{T} = \frac{16\pi^5}{45(ch)^3}\, gk(kT)^3 \cdot \begin{cases} 1 & \text{bosons} \\ 7/8 & \text{fermions} \end{cases}$$

Note that the chemical potential ν features nowhere in here – for highly relativistic particles, lots of particle-antiparticle pairs flying around, the chemical potential can be neglected!

Photons

Thermal photon gas: $g = 2$ (two polarizations), bosons, $m = 0$, $E = h\nu$, in thermal equilibrium $\mu = 0$:

Number density of photons with frequencies between ν and $\nu + \mathrm{d}\nu$ is

$$\frac{8\pi\nu^2/c^2}{\exp(h\nu/kT) - 1}\mathrm{d}\nu$$

Photons

$$\rho c^2 = \frac{8\pi h}{c^3} \int\limits_0^\infty \frac{\nu^3}{\exp(h\nu/kT) - 1}\, \mathrm{d}\nu$$

From the bosonic energy distribution, it follows that the number $n(m)$ of photons with energies greater or equal to $m \cdot kT$ is

$$n(m) = \frac{n}{2\zeta(3)} \int\limits_m^\infty \frac{x^2 \mathrm{d}x}{\exp(x) - 1}.$$

For instance, 10^{-9} of the photons have energies $> 26kT$, while 10^{-10} have energies $> 29kT$.

Non-relativistic particles

For non-relativistic particles, $mc^2 \gg kT$ and

$$E(p) \approx mc^2 + \frac{p^2}{2m}.$$

The number density is

$$n = \frac{g}{h^3}(2\pi\, m\, kT)^{3/2} \;\exp\left(-\frac{mc^2 - \mu}{kT}\right)$$

even when not in chemical equilibrium, the energy density is

$$\rho c^2 = n \cdot \left(mc^2 + \frac{3}{2}\, kT\right)$$

and the pressure

$$\mathrm{p} = n\, kT.$$

These last expressions are as expected.

Particle interactions and time scales

How many particle interactions (collisions) in a given situation? For non-relativistic particles in thermal (not necessarily chemical!) equilibrium, number densities n_1 and n_2, reduced mass $\mu = m_1 m_2/(m_1 + m_2)$, the collision rate density C is

$$C = n_1 n_2 \, \langle u\sigma(E)\rangle_u,$$

where the averaging is over a Maxwell-Boltzmann distribution for the relative velocity u, and $\sigma(E)$ is the cross section (= collision probability), with $E(u)$ the (velocity-dependent!) energy,

$$\langle u\sigma(E)\rangle_u = 4\pi \left(\frac{\bar{\mu}}{2\pi\, kT}\right)^{3/2} \int_0^\infty \exp\left(\frac{-\bar{\mu}u^2}{2kT}\right) \sigma(E)\, u^3 \, \mathrm{d}u.$$

Particle interactions and time scales

If $\sigma(E)$ is independent, or weakly dependent on E, the integral becomes

$$\langle u\sigma\rangle_u = \sigma\langle u\rangle_u. = \sigma\sqrt{\frac{8kT}{\pi\bar{\mu}}}$$

If one of the particle species is photons, we will approximate the collision rate by

$$C = n_1 n_2 \sigma c,$$

scaling, if necessary, with the fraction of photons with an energy larger than the reaction we're interested in.

Particle interactions and time scales

The number of reactions per particle of species 1 is

$$\Gamma = \frac{C}{n_1} = n_2 \, \langle u\sigma(E) \rangle_u,$$

which has physical dimension 1/time.

We compare this with the Hubble parameter

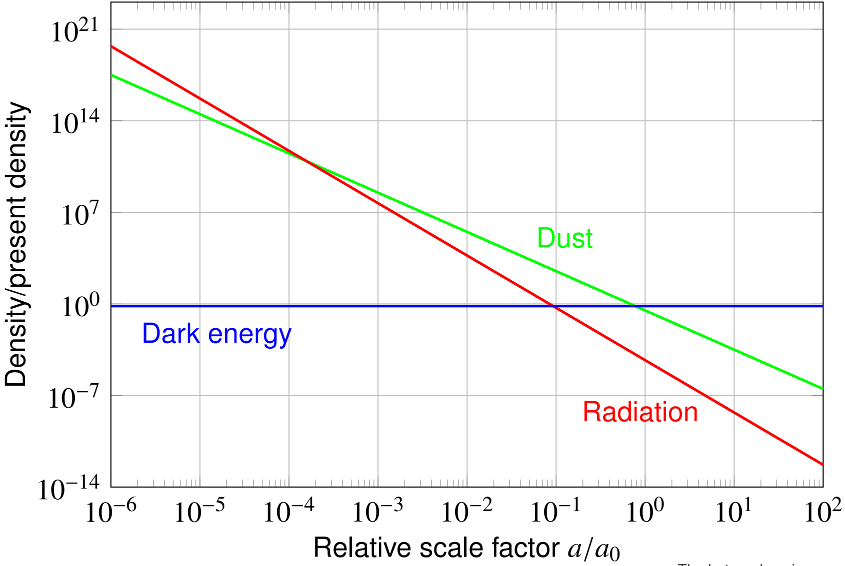
$$H(t) = \frac{\dot{a}}{a}$$

which is the ratio of the change of a to a itself, and thus a measure for the time it takes a to change significantly.

Local equlibrium vs. freeze-out

1. $\Gamma \gg H$ for reactions that establish thermal equilibrium: Local Thermal Equilibrium (LTE): Adiabatic (=isentropic) change from one temperature-dependent equilibrium to the next
2. $H \gg \Gamma$: Freeze-out – particle concentrations remain constant (or change because of decay, or alternative reactions). Temperature decouples.

For small $x = a/a_0$: Radiation dominates!



Radiation dominates

For early times, assume that the only significant contribution comes from radiation:

$$a = a_0 \sqrt{2\sqrt{\Omega_{r0}} H_0\, t}$$

so with $\Omega_{r0} = 5 \cdot 10^{-5}$ and $H_0 = 2.18 \cdot 10^{-18}$/s,

$$a = a_0 \cdot (1.76 \cdot 10^{-10}) \sqrt{\frac{t}{1\ s}}.$$

Hubble parameter goes as

$$H(t) = \frac{1}{2t}.$$

For the phase directly following radiation dominance

For later times assume the only significant contribution comes from the matter density,

$$a = a_0 \left(\frac{3}{2} \sqrt{\Omega_{m0}}\, H_0\, t \right)^{2/3},$$

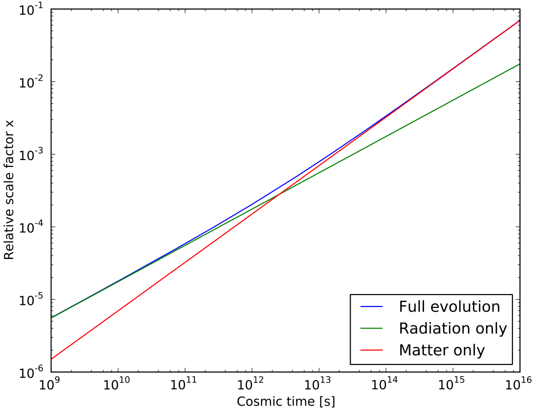
so with $\Omega_{m0} = 0.317$ and $H_0 = 2.18 \cdot 10^{-18}$/s,

$$a = a_0 \cdot (1.5 \cdot 10^{-12}) \left(\frac{t}{1\ s} \right)^{2/3}.$$

Hubble parameter goes as

$$H(t) = \frac{2}{3t}.$$

How does this compare to the exact treatment?



... works except for $t = 8 \cdot 10^{10} - 2 \cdot 10^{14}$ s = 6k – 300k years.

How does the energy distribution evolve?

At some time t_1, scale factor value $a(t_1)$, in some volume V_1, let the photon number between ν_1 and $\nu_1 + \mathrm{d}\nu_1$ be

$$V_1 \frac{8\pi(\nu_1)^2/c^3}{\exp(h\nu_1/kT_1) - 1} \mathrm{d}\nu_1.$$

At some later time t_2, the same photons are now spread out over a volume $V_2 = (x_{21})^3$ with $x_{21} = a(t_2)/a(t_1)$. They have been redshifted to $\nu_2 = \nu_1/x_{21}$, and their new frequency interval is $\mathrm{d}\nu_2 = \mathrm{d}\nu_1/x_{21}$.

How does the energy distribution evolve?

We can re-write the new number density in terms of the new frequency and interval values ν_2 and $\mathrm{d}\nu_2$; the x_{21} mostly cancel, which gives a new number density in the frequency interval $\nu_2 \ldots \nu_2 + \mathrm{d}\nu_2$ at time t_2 that is

$$\frac{8\pi(\nu_2)^2/c^3}{\exp(h\nu_2 x_2 1/kT_1) - 1}\mathrm{d}\nu_2.$$

This corresponds to the number of photons we would expect in the given frequency range for thermal radiation with temperature

$$T_2 = T_1 \cdot a(t_1)/a(t_2),$$

which for $a(t_2) > a(t_1)$ corresponds to lower temperature. Temperature scales as $\sim 1/a(t)$! Radiation remains Planckian!

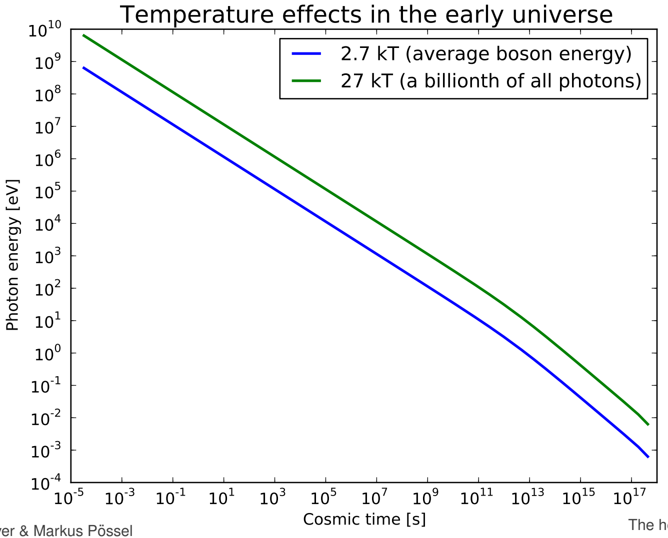
Photon number $\gg$ baryon number

Now it becomes important that the number of photons is so much larger than the baryon number (as you will estimate in the exercise):

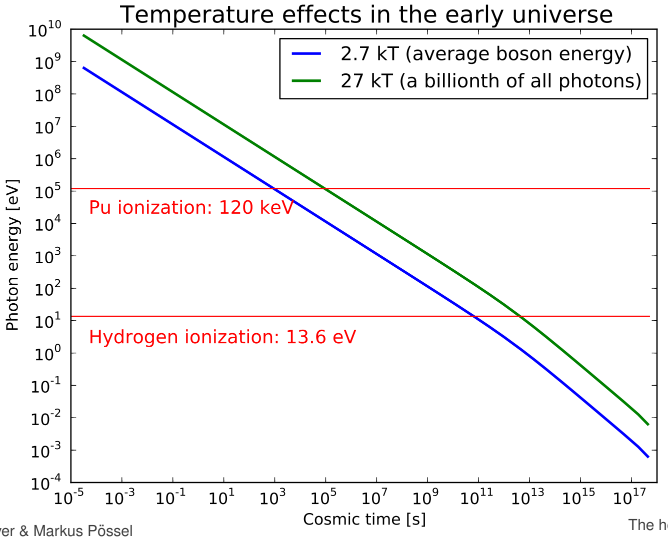
$$\eta = \frac{n_B}{n_\gamma} \approx 6 \cdot 10^{-10}.$$

Everything that's going on will take place in a photon bath! Even absorption reactions hardly matter – they will change the bath by at most 10^{-9}!

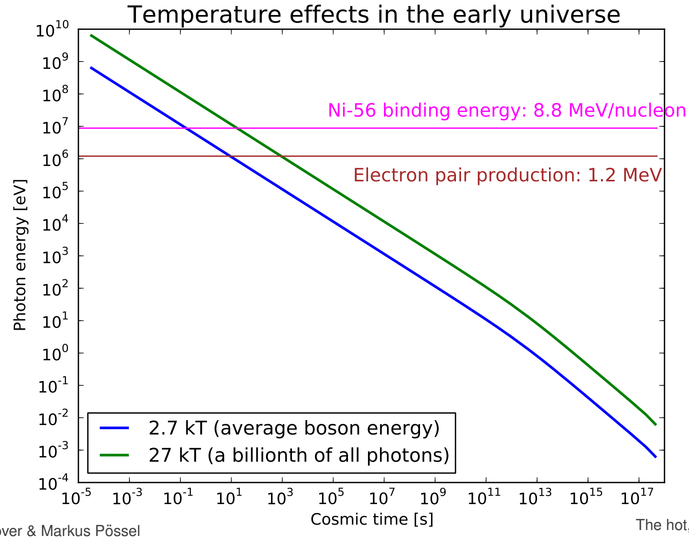
Photon energy over time



Photon energy over time



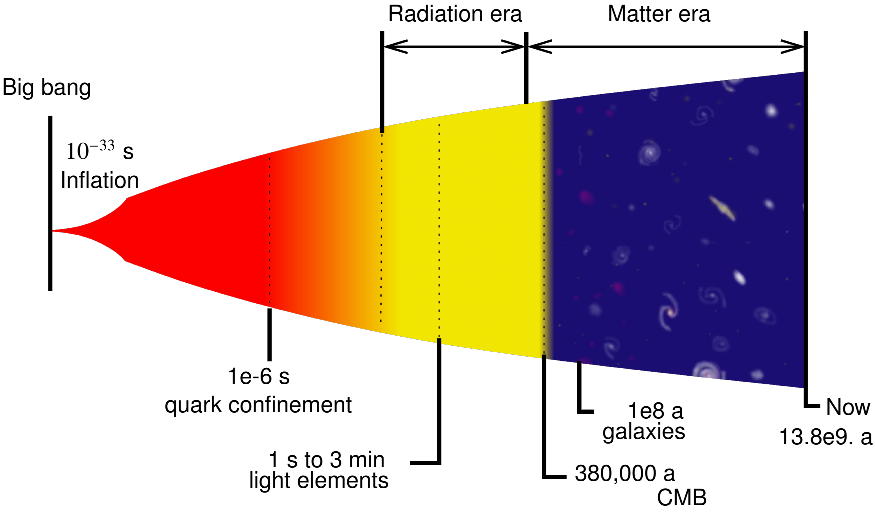
Photon energy over time



Reaction numbers?

You will calculate some reaction numbers (photon colliding with atom, or with nucleus) in the exercises today. Collision rates will not be a problem — as long as the photons carry sufficient energy to trigger a reaction (ionization, splitting a nucleus...)!

The big picture

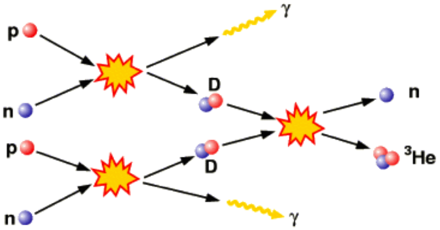


Where do we begin?

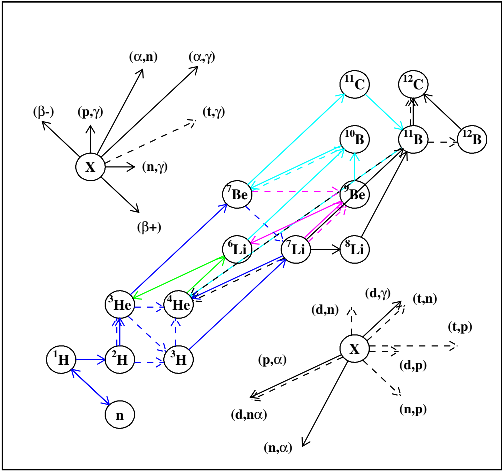
In this lecture, we trace temperature back until we have a sea of single nucleons (protons and neutrons). We leave earlier phases (inflation etc.) for later, namely for the last lecture.

Primordial nucleosynthesis

As we have seen, at about 1s of cosmic time, sufficient photon energy to tear apart the most stable nuclei (Ni-56).
Three-particle reactions much too uncommon (will occur in stars, but not here!), so nuclei have to be built from two-particle reactions.



Reaction network



Key: There is no stable element with $A = 5$! (Fig. from Coc 2012)

When can nucleosynthesis start?

All nucleosynthesis starts with deuterium production. Binding energy of Deuterium: $2.2 MeV$.

Nothing happens until the photon energy $27kT$ (this or more carried by $6 \cdot 10^{-10}$ of all photons!) goes below $2.2\ MeV$, which is ($k = 8.6 \cdot 10^{-5}\ eV/K$) at

$$T_D = 9.5 \cdot 10^8\ K$$

or

$$a/a_0 = T_0/T_D = 3 \cdot 10^{-9}$$

so

$$t = 290\ s.$$

...at which time, all neutrons are quickly built into ^4He; most stable configuration, gap at $A = 5$! But how many neutrons do we have in the first place?

How many neutrons do we have to start with?

Weak interactions between protons and neutrons:

$$n + \nu_e \leftrightarrow p + e^-$$

Reaction rate for these weak interactions is:

$$\sigma_w = 10^{-47}\, m^2 \left(\frac{kT}{1\, MeV}\right)^2$$

Estimating the reaction rate (similar to exercise), this works only while there is still pair production, and stops at

$$t \approx 1s, \quad kT \approx 0.8\, MeV.$$

How many neutrons do we have to start with?

$$n + \nu_e \leftrightarrow p + e^-$$

in equilibrium above or about $kT = 1\ MeV$ means that

$$\mu_n + \mu_{\nu_e} = \mu_p + \mu_{e^-} \quad \Rightarrow \mu_n = \mu_p$$

(where, as mentioned above, we have neglected μ for highly relativistic, pair-produced particles. But the non-relativistic number density was

$$n = \frac{g}{h^3}(2\pi\, m\, kT)^{3/2}\ \exp\left(-\frac{mc^2 - \mu}{kT}\right),$$

so

$$\frac{n_n}{n_p} = \left(\frac{m_n}{m_p}\right)^{3/2}\ \exp\left(-\frac{(m_n - m_p)c^2}{kT}\right).$$

How many neutrons do we have to start with?

$$\frac{n_n}{n_p} = \left(\frac{m_n}{m_p}\right)^{3/2} \exp\left(-\frac{(m_n - m_p)c^2}{kT}\right).$$

Inserting $kT = 0.8\ MeV$ and $(m_n - m_p)c^2 = 1.293\ MeV$, neglecting the pre-factor:

$$\frac{n_n}{n_p} = 0.198 \approx \frac{1}{5}$$

at $t = 1s$.

Problem: Neutrons decay, with half-life $611\ s$! Between $t = 1\ s$ and $t = 290\ s$, the number ratio has dropped from 1 neutron to 5 protons to

$$(1/2)^{290\ s/611\ s} \approx 0.72\ \text{ neutrons per proton} \approx \frac{1}{7}.$$

Helium fraction

With 2 neutron per 14 protons (1/7), you can make 1 ^{4}He plus 12 protons. Mass ratio between He and total mass is

$$Y = \frac{4}{16} = 25\%$$

. . . this is the fairly robust main prediction for big bang nucleosynthesis!

Time evolution

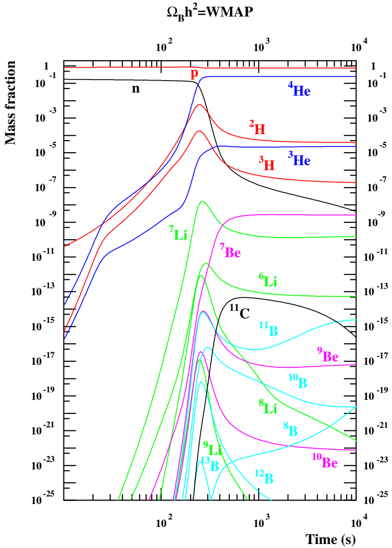


Fig. from Coc 2012

Comparing with observations

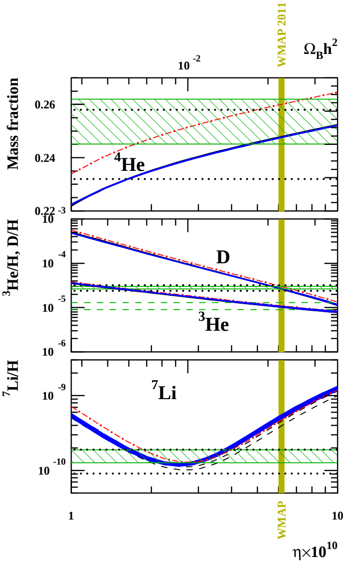


Image from Coc 2012

The cosmic background radiation

How do we get from the plasma state (hydrogen and helium nuclei, electrons, photons) to an atomic, transparent universe?

Reaction:

$$H + \gamma \leftrightarrow = p + e^-$$

As you will estimate in the exercises (at least the LHS), lots and lots of collisions – system will be in equilibrium!

In thermodynamic equilibrium, thermodynamic potentials add up:

$$\mu_H + \mu_\gamma = \mu_p + \mu_{e^-}.$$

. . . but μ_γ in chemical equilibrium is zero!

Photon chemical potential

But there are atomic reactions where either one or two photons can be produced:

$$A \rightarrow B + \gamma \quad \text{versus} \quad A \rightarrow B^* + \gamma,\ B^* \rightarrow A + \gamma.$$

This means

$$\mu_A = \mu_B + \mu_\gamma,$$

but also

$$\mu_A = \mu_{B^*} + \mu_\gamma = \mu_B + 2\mu_\gamma$$

$\Rightarrow$ this can only hold if $\mu_\gamma = 0$!

Equilibrium state for ionization

Since $\mu_\gamma = 0$, in equilibrium for the reaction $H + \gamma \leftrightarrow= p + e^-$,

$$\mu_H = \mu_p + \mu_{e^-}.$$

Our particles are all non-relativistic, so

$$n = \frac{g}{h^3}(2\pi\, m\, kT)^{3/2} \; \exp\left(-\frac{mc^2 - \mu}{kT}\right),$$

and with the $g_e = g_p = 2$ (spin $\pm 1/2$) and $g_H = 1 + 3 = 4$ (spin 0 plus spin 1), so

$$\frac{n_p n_e}{n_H} = \frac{(2\pi m_e kT)^{3/2}}{h^3}\left(\frac{m_p}{m_H}\right)^{3/2} \; \exp\left(-\frac{B}{kT}\right)$$

where $B = (m_p + m_e - m_H)c^2 = 13.6\ eV$ is the binding energy.

Equilibrium state for ionization

Charge neutrality means $n_e = n_p$. Define the *ionization fraction*

$$x_e \equiv \frac{n_e}{n_e + n_H},$$

so that

$$\frac{x_e^2}{1-x_e} = \frac{n_e}{n_H(n_e+n_H)} = \frac{n_e}{n_H n_b} = \frac{(2\pi m_e kT)^{3/2}}{n_B h^3}\left(\frac{m_p}{m_H}\right)^{3/2} \exp\left(-\frac{B}{kT}\right)$$

with n_b the baryon number density. But the number density is related to the modern value, and the present (CMB) temperature T_0, as

$$n_b(t) = n_{b0}\left(\frac{a_0}{a(t)}\right)^3 = n_{b0}\left(\frac{T}{T_0}\right)^3.$$

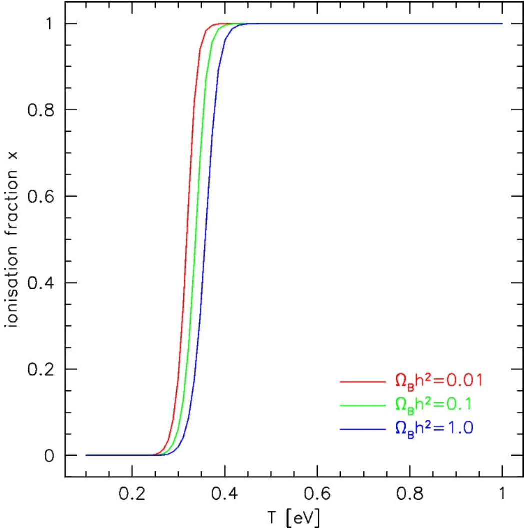
Equilibrium state for ionization

Inserting this into the equation, neglecting the m_p/m_H term,

$$\frac{x_e^2}{1-x_e} = \frac{1}{n_{b0}h^3}\left(\frac{2\pi m_e k}{T}\right)^{3/2} \exp\left(-\frac{B}{kT}\right)$$

$$= 8.78\cdot 10^{21}\left(\frac{1\ K}{T}\right)^{3/2} \exp\left(-\frac{1.6\cdot 10^5\ K}{T}\right)$$

Ionization fraction by temperature



Graph: M. Bartelmann

Recombination at what redshift?

From the previous graph, $T_{rec} \approx 0.3\ eV \approx 3500\ K$.
By scaling behaviour of T:

$$\frac{a(t_{rec})}{a_0} = \frac{T_0}{T_{rec}} = 7.8 \cdot 10^{-4} = \frac{1}{1+z}$$

so

$$z \approx 1280.$$

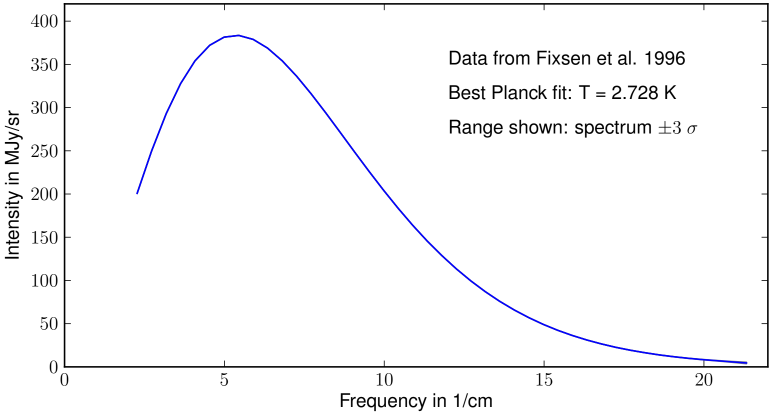
Using the “matter only” approximation

$$a = a_0 \left(\frac{3}{2} \sqrt{\Omega_{m0}}\, H_0\, t \right)^{2/3}$$

we get

$$t_{rec} = 376,000\ a.$$

Precision CMB: COBE-FIRAS (Mather et al.)



Data from Fixsen et al. 1996 via http://lambda.gsfc.nasa.gov

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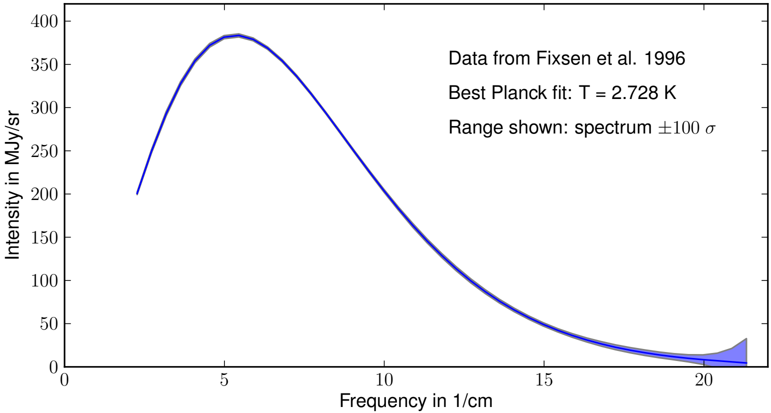

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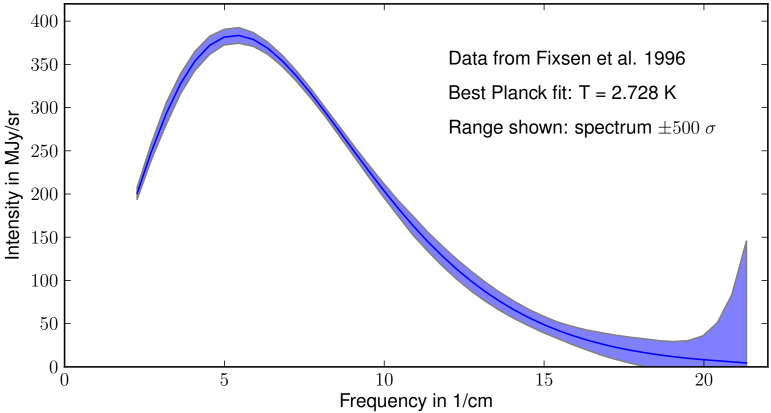

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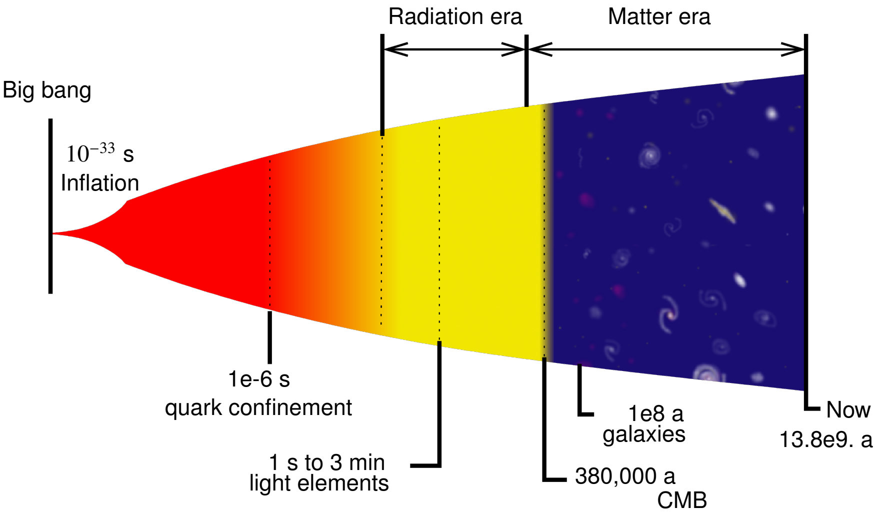
The big picture



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