AST3220, spring 2022, project 2

March 29, 2022

1 Moral speech

This project consists of a set of tasks, some analytical, some numerical. It is important that you explain how you think, just writing down a bunch of equations with no explanations will not give you a maximum score. I recommend that you write your answers using LaTeX. Posting handwritten lecture notes and solutions to problems is a privilege that belongs to the lecturer alone.

Your figures should have a clear layout with proper axis labels and units, and with a caption explaining what the figure shows. The figures should be referenced in the main text. You are also required to hand in your source code in a form that can be easily compiled. If you use python, use python 3 as this makes testing your codes easier for us.

VERY IMPORTANT: Use your candidate number, and nothing else, to identify yourself in the report. In previous years we have seen several examples of students handing in reports with their full name and/or e-mail address. The evaluation process is supposed to be anonymous. Therefore, if we find your full name in the report, we will deduct 5 points from your score.

2 General Parameters

Unless stated otherwise, the following values are used for these parameters (which will be defined later in the text):

$$h = 0.7,$$

 $N_{\rm eff} = 3,$
 $\Omega_{b0} = 0.05.$

The Hubble parameter is

$$H_0 = 100h \,\mathrm{km \, s^{-1} Mpc^{-1}},$$

where $Mpc = 3.09 \times 10^{22} m$, and the critical energy density of the universe today is given by

$$\rho_{c0} = \frac{3H_0^2}{8\pi G} \approx 9.2 \times 10^{-27} \,\mathrm{kg}\,\mathrm{m}^{-3}.$$

The paper that this project is based on uses CGS units instead of SI units, i.e. it uses grams and centimeters instead of kilograms and meters. Make sure you use these units in your code, otherwise your reaction rates will be incorrect.

3 Big Bang Nucleosynthesis - Predicting the abundance of light elements

Big Bang Nucleosynthesis (BBN) describes the production of the lightest elements in the first few moments after the Big Bang. At this time the universe was very hot $(T \sim 10^9 K - 10^{10} K)$ and much denser than today, with all the four fundamental forces of nature playing a major role. In this project we will use the Boltzmann equation to compute the abundances of the lightest elements; hydrogen/free proton (H or p),

deuterium (H^2 or D), tritium (H^3 or T), helium-3 (He^3), helium-4 (He^4), lithium (Li^7), and beryllium (Be^7), as well as the free neutron (n).

Before BBN starts, the baryonic matter in the universe is almost entirely in the form of free protons and neutrons (and an equal number of the much lighter electrons, such that the universe is electrically neutral, but we will largely neglect these in this project). These interact via the weak nuclear force, with protons transforming into neutrons and vice verse;

$$n + \nu_e \rightleftharpoons p + e^-,\tag{1}$$

$$n + e^+ \rightleftharpoons p + \bar{\nu_e},\tag{2}$$

$$n \rightleftharpoons p + e^- + \bar{\nu_e}.\tag{3}$$

Here e^- and e^+ are the electron and its antiparticle, the positron, and ν_e and $\bar{\nu_e}$ are the electron neutrino and its antiparticle. Initially, the neutrons and protons are in equilibrium, with a preference for protons because it is slightly lighter,

$$\frac{n_n^{(0)}}{n_p^{(0)}} = \left(\frac{m_p}{m_n}\right)^{3/2} e^{-(m_n - m_p)c^2/k_B T},\tag{4}$$

where $n^{(0)}$ denotes the equilibrium number densities. At very high T we see that $n_n^{(0)} \approx n_p^{(0)}$, whereas for temperatures below the mass difference $k_B T < (m_n - m_p)c^2$, the neutron fraction drops and would in time fall to zero had they followed this equilibrium distribution indefinitely. They do not, however, and at some point the rate at which these particles interact becomes lower than than the rate at which the universe expands, due to both decreasing temperature and densities. When this happens, the protons and neutrons fall out of equilibrium, and the total number of protons and neutrons "freezes out". The free neutrons still spontaneously decay into protons via reaction (3), and the neutron fraction eventually decreases anyway.

To describe the change in proton and neutron number densities via reactions (1), (2), and (3), both in and out of equilibrium, we must use the Boltzmann equation, which for a particle specie "*i*" is of the form

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} + 3Hn_i = J_i. \tag{5}$$

The term $3Hn_i$ is the dilution of number density due to expansion, where $H = a^{-1}da/dt$, while J_i is the rate of change due to all reactions that particle *i* participates in. If there are no reactions, $J_i = 0$, then we simply get $n_i \sim a^{-3}$, i.e. the number density decreases solely due to expansion. The first type of reaction that we must consider are decays,

$$J_i \supset \sum_{j \neq i} [n_j \Gamma_{j \to i} - n_i \Gamma_{i \to j}], \tag{6}$$

where $\Gamma_{i \to j}$ is the decay rate, and is essentially the fraction of particle *i* per unit time that is converted into particle *j*. The " \supset " is the superset symbol, to indicate that the given reaction terms are part of J_i . Note that decays of both *i* into other *j*, and from other *j* into *i*, are included, and that in general $\Gamma_{i\to j} \neq \Gamma_{j\to i}$. The second type of reaction we must include are two-body interactions of the form $i + j \rightleftharpoons k + l$. These contribute to the change in number densities as

$$J_i \supset \sum_{jkl} [n_k n_l \gamma_{kl \to ij} - n_i n_j \gamma_{ij \to kl}], \tag{7}$$

which depends on the interaction rates $\gamma_{kl \to ij}$ and the product of the particle densities $n_k n_l$. Note that both directions of the interaction is included, and again we have in general that $\gamma_{kl \to ij} \neq \gamma_{ij \to kl}$.

In the following we will model all the weak force reactions between p and n as decays, with the effect of the electrons and neutrinos included in the decay rates. We therefore have

$$\frac{\mathrm{d}n_n}{\mathrm{d}t} + 3Hn_n = n_p \Gamma_{p \to n} - n_n \Gamma_{n \to p},\tag{8}$$

$$\frac{\mathrm{d}n_p}{\mathrm{d}t} + 3Hn_p = n_n \Gamma_{n \to p} - n_p \Gamma_{p \to n}.$$
(9)

It is advantageous to define the relative number densities $Y_n = n_n/n_b$ and $Y_p = n_p/n_b$, where $n_b = n_{b0}a^{-3} = \rho_{b0}a^{-3}/m_p$ is the total baryon nucleon number density, and $\rho_{b0} = \Omega_{b0}\rho_{c0}$ the total baryon mass density. It will also be easier to use the logarithm of the temperature $T = T_0a^{-1}$ as our time variable.

a) [5 points]

Show that the equations for $dY_n/d(\ln T)$ and $dY_p/d(\ln T)$, starting from from eqs. (8) and (9), are

$$\frac{\mathrm{d}Y_n}{\mathrm{l}(\ln T)} = -\frac{1}{H} [Y_p \Gamma_{p \to n} - Y_n \Gamma_{n \to p}],\tag{10}$$

$$\frac{\mathrm{d}Y_p}{\mathrm{d}(\ln T)} = -\frac{1}{H} [Y_n \Gamma_{n \to p} - Y_p \Gamma_{p \to n}]. \tag{11}$$

The decay rates $\Gamma_{p\to n}$ and $\Gamma_{n\to p}$ can be computed from quantum field theory, but this is an exercise far outside the scope of this course. Instead we will use the results from Table 2 in ref. [1];

$$\Gamma_{n \to p}(T,q) = \frac{1}{\tau} \Biggl[\int_{1}^{\infty} \frac{(x+q)^2 (x^2-1)^{1/2} x}{[1+e^{-(x+q)Z_{\nu}}]} dx + \int_{1}^{\infty} \frac{(x-q)^2 (x^2-1)^{1/2} x}{[1+e^{-xZ}][1+e^{(x-q)Z_{\nu}}]} dx \Biggr],$$

$$\Gamma_{p \to n}(T,q) = \Gamma_{n \to p}(T,-q),$$
(13)

where $\tau = 1700$ s is the free neutron decay time, $q = (m_n - m_p)/m_e = 2.53$, $Z = m_e c^2/k_B T = 5.93/T_9$, and $Z_{\nu} = m_e c^2/k_B T \nu = 5.93/T_{9\nu}^{-1}$. We have also defined the quantities $T_9 = T/10^9$ and $T_{9\nu} = T_{\nu}/10^9$ for ease.

We must also know what the expansion rate of the universe was at the time of BBN, as well as the temperature of the cosmic plasma T, and of the decoupled neutrinos T_{ν} . The cosmic microwave background has given us precise measurements of $T = T_0/a$ today, $T_0 = 2.725$ K, and the neutrino temperature is related to T as $T_{\nu} = (4/11)^{1/3}T$. Furthermore, at the time of BBN our universe was completely dominated by radiation, and the Friedmann equations is simply

$$H = \frac{1}{a} \frac{\mathrm{d}a}{\mathrm{d}t} = H_0 \sqrt{\Omega_{r0}} a^{-2},\tag{14}$$

where $\Omega_{r0} = \rho_{r0}/\rho_{c0}$ is the fraction of energy in the form of radiation in our universe today.

Bonus question [5 points]

Make an order-of-magnitude estimate of the baryon mass density at the time of BBN, e.g. at $T \sim 10^9$ K. How does this compare to the mean density of the Sun?

Make a similar order-of-magnitude estimate for the ratio ρ_b/ρ_r between the baryon and radiation energy densities at the time of BBN, with $\Omega_{r0} \sim 10^{-4}$.

b) [5 points]

Show why the relation $T_{\nu} = (4/11)^{1/3}T$ holds.

What assumption have we made if we take this relation to be true throughout our treatment of BBN? *Hint: Consider the conservation of total entropy before and after electrons and positrons have become non-relativistic and annihilate.*

¹Note that we have set $\phi_{\nu} = 0$ compared to [1]

c) [5 points]

Assuming that photons and $N_{\rm eff}$ number of neutrino species make up all of the radiation in our universe, show that

$$\Omega_{r0} = \frac{8\pi^3}{45} \frac{G}{H_0^2} \frac{(k_B T_0)^4}{\hbar^3 c^5} \Big[1 + N_{\text{eff}} \frac{7}{8} \Big(\frac{4}{11}\Big)^{4/3} \Big].$$
(15)

d) [5 points]

Integrate the Friedmann eq. (14) to get a(t), as well as t(T). Use the latter to find how old the universe was at $T = 10^{10}$ K, $T = 10^{9}$ K, and $T = 10^{8}$ K.

e) [5 points]

Assuming that all of the baryonic mass ρ_b at the initial temperature T_i is in neutrons and protons, and that they are in thermal equilibrium at this temperature, show that

$$Y_n(T_i) = [1 + e^{(m_n - m_p)c^2/k_B T_i}]^{-1},$$
(16)

and

$$Y_p(T_i) = 1 - Y_n(T_i).$$
(17)

Use that $m_p \approx m_n$ outside of exponentials.

f) [10 points]

Write a code that solves eqs. (10) and (11) from $T_i = 100 \times 10^9 \text{K}$ to $T_f = 0.1 \times 10^9 \text{K}$, with the initial conditions from e). Use this code to reproduce Figure 1.

Hint: In Python, you can use scipy's **quad** integrator for eq. (12), and **solve_ivp** for the the set of differential equations, with method="Radau", rtol=1e-12, atol=1e-12. The code might be a bit slow, using a few minutes per run, at least when we include more elements and reactions later. Increasing rtol and atol will speed things up when testing, but might yield solutions that are not very "nice" looking.



Figure 1: The solution of Y_n and Y_p from eqs. (10) and (11), shown in solid lines, as well as the equilibrium values from eqs. (16) and (17), shown in dotted lines.

We have up to this point given a description of the processes that lead up to where BBN really gets going, i.e. when nuclides heavier than hydrogen is produced. This doesn't happen until the temperature falls to around $T \approx 9 \times 10^8$ K. At temperatures above this there are enough high-energy photons present to instantaneously disintegrate any deuterium that forms. This is called the deuterium bottleneck, since BBN cannot proceed until deuterium survives for long enough to participate in further reactions.

To proceed we will need the general Boltzmann equation for a particle i that interacts with any number of other particles j, both through decays and two-body reactions;

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} + 3Hn_i = \sum_{j\neq i} [n_j \Gamma_{j\to i} - n_i \Gamma_{i\to j}] + \sum_{jkl} [n_k n_l \gamma_{kl\to ij} - n_i n_j \gamma_{ij\to kl}].$$
(18)

g) [5 points]

Show that the equation for $dY_i/d(\ln T)$, starting from eq. (18), is

$$\frac{\mathrm{d}Y_i}{\mathrm{d}(\ln T)} = -\frac{1}{H} \left\{ \sum_{i \neq j} [Y_j \Gamma_{j \to i} - Y_i \Gamma_{i \to j}] + \sum_{jkl} [Y_k Y_l \Gamma_{kl \to ij} - Y_i Y_j \Gamma_{ij \to kl}] \right\},\tag{19}$$

where we have defined $\Gamma_{ij \to kl} = n_b \gamma_{ij \to kl}$.

The reactions we need are given in ref. [1], which uses a slightly different notation compared to what we have used so far. For instance, if we write down the Boltzmann equations for n, p and D with reactions 1)-3) in part a), and 1) in part b) of Table 2, we get

$$\frac{\mathrm{d}Y_n}{\mathrm{d}(\ln T)} = -\frac{1}{H} \Big\{ -\lambda_w(n)Y_n + \lambda_w(p)Y_p + \lambda_\gamma(D)Y_D - [pn]Y_nY_p \Big\},\tag{20}$$

$$\frac{\mathrm{d}Y_p}{\mathrm{d}(\ln T)} = -\frac{1}{H} \Big\{ -\lambda_w(p)Y_p + \lambda_w(n)Y_n + \lambda_\gamma(D)Y_D - [pn]Y_nY_p \Big\},\tag{21}$$

$$\frac{\mathrm{d}Y_D}{\mathrm{d}(\ln T)} = -\frac{1}{H} \Big\{ -\lambda_\gamma(D)Y_D + [pn]Y_nY_p \Big\},\tag{22}$$

where $\lambda_w(n) = \Gamma_{n \to p}$, $\lambda_w(p) = \Gamma_{p \to n}$, $\lambda_\gamma(D) = \Gamma_{D \to n} = \Gamma_{D \to p}$, and $[pn] = \Gamma_{np \to D\gamma}$.

h) [10 points]

Write a code that solves the Boltzmann equations for n, p, D, up to the deuterium bottleneck using reactions 1)-3) from part a), and 1) from part b) of Table 2 in ref. [1], i.e. eqs. (20), (21), and (22). Integrate from $T_i = 100 \times 10^9$ K to $T_f = 0.1 \times 10^9$ K, with the initial conditions from e) for Y_n and Y_p , and $Y_D = 0$. Use this code to reproduce Figure 2, and give a short description of what is happening in the figure as the temperature decreases.



Figure 2: The solution of Y_n , Y_p , and $2Y_D$ from eqs. (20), (21), and (22), shown in solid, as well as the equilibrium values from eqs. (16) and (17), shown in dotted. We have included the mass number A_i of particle *i* (i.e. number of neutrons pluss protons), such that the fraction of the total baryon mass in the different particle species is shown.

We are now in a position to write a code that implements all the reactions necessary for accurately computing the abundance of elements up to Li^7 . The reactions that we must include are 1)-3) from part a), and 1)-11) + 15)-18) + 20) + 21) from part b) of Table 2 in ref. [1]. Adding all of these can, understandably, result in an unwieldy set of equations if written out in full. From a coding point of view, it might be easier to add the contribution of each reaction one at a time. In Python, the first few reactions might therefore be written as

```
# Code snippet from a function that computes the ODE for BBN elements.
# dYi corresponds to d(Yi)/d(lnT), and the contributions are
# added one reaction at a time.
# Lets add contribution from the various reactions
# From "ON THE SYNTHESIS OF ELEMENTS AT VERY HIGH TEMPERATURES"
# by R.V.Wagoner et al, 1967
```

```
### Table 2:
### a) Weak interactions
# 1) n + nu <-> p + e-
# 2) n + e- <-> p + nu_bar
# 3) n <-> p + e- + nu_bar
rate_lambda_w_n, rate_lambda_w_p = cmpt_n_to_p(T9, Tnu9, rhob)
dYp = dYp - 1/H*(-Yp*rate_lambda_w_p + Yn*rate_lambda_w_n)
dYn = dYn - 1/H*( Yp*rate_lambda_w_p - Yn*rate_lambda_w_n)
### b) Strong and electromagnetic interactions
# 1) p + n <-> D + gamma
rate_pn, rate_lambda_gamma_D = cmpt_pn_to_Dgamma(T9, Tnu9, rhob)
dYp = dYp - 1/H*(-Yp*Yn*rate_pn + YD*rate_lambda_gamma_D)
dYn = dYn - 1/H*(-Yp*Yn*rate_pn + YD*rate_lambda_gamma_D)
dYD = dYD - 1/H*( Yp*Yn*rate_pn - YD*rate_lambda_gamma_D)
# 2) p + D <-> He3 + gamma
rate_pD, rate_lambda_gamma_He3 = cmpt_pD_to_He3gamma(T9, Tnu9, rhob)
             - 1/H*(-Yp*YD*rate_pD + YHe3*rate_lambda_gamma_He3)
     = dYp
dYp
      = dYD - 1/H*(-Yp*YD*rate_pD + YHe3*rate_lambda_gamma_He3)
dYD
dYHe3 = dYHe3 - 1/H*( Yp*YD*rate_pD - YHe3*rate_lambda_gamma_He3)
```

The two-body reactions in the Boltzmann equations actually include some extra factors when there are two particles of the same type, which has not been included in eq. (18) for notational ease. We state here what these factors are: For reactions that produce two particles of the same type, such as $k + l \rightarrow i + i$, an extra factor 2 must be included in the production of i in the equation for i, and a factor 1/2 must be added in the production of k and l in the equations for k and l, i.e. for the opposite reaction $k + l \leftarrow i + i$. For example, for reaction 20) in part b) of Table 2 in ref. [1], $p + Li^7 \rightleftharpoons He^4 + He^4$, we would get

```
# 20) p + Li7 <-> He4 + He4
rate_pLi7_He4, rate_He4He4_p = cmpt_pLi7_to_He4He4(T9, Tnu9, rhob)
dYp = dYp - 1/H*( -Yp*YLi7*rate_pLi7_He4 + 0.5*YHe4*YHe4*rate_He4He4_p)
dYLi7 = dYLi7 - 1/H*( -Yp*YLi7*rate_pLi7_He4 + 0.5*YHe4*YHe4*rate_He4He4_p)
dYHe4 = dYHe4 - 1/H*(2*Yp*YLi7*rate_pLi7_He4 - YHe4*YHe4*rate_He4He4_p)
```

i) [20 points]

Write a code that solves the Boltzmann equations for n, p, D, T, He³, He⁴, Li⁷, and Be⁷, using reactions 1)-3) from part a), and 1)-11) + 15)-18) + 20) + 21) from part b) of Table 2 in ref. [1]. Integrate from $T_i = 100 \times 10^9$ K to $T_f = 0.01 \times 10^9$ K, with the initial conditions from e) for Y_n and Y_p , and $Y_i = 0$ for the remaining elements. Use this code to reproduce Figure 3. *Hint:* A very simple test that might help you catch some errors when writing out all the reactions is to check if $\sum A_i Y_i = 1$, i.e. that the total number of nucleons is conserved throughout your BBN simulation. A_i is the particle mass number.



Figure 3: The mass fractions $A_i Y_i$, where A_i is the mass number of particle *i* (i.e. number of neutrons pluss protons).

Lets pause for a moment to appreciate what we have achieved so far: We have accurately computed the production of elements through nuclear reactions involving all the fundamental forces of nature, which happens in the first few seconds after the Big Bang and the life of our universe. This is quite a feat, and we can now use BBN to learn more about the content of our universe by comparing our theoretical predictions to observations. The observables that we will use are the abundance fractions of D and Li⁷ relative to hydrogen, Y_D/Y_p and Y_{Li^7}/Y_p , and the mass fraction of He⁴, $4Y_{\text{He}^4}$. The half-life of tritium and beryllium is sufficiently short that nothing of these survive until today, but they decay to He³ and Li⁷, respectively. The final values of Y_{T} and Y_{Be^7} that we get from our calculations must therefore be added to the final number fractions of He³ and Li⁷ to get what we would observe today; $Y_{\text{He}^3}(\text{today}) = Y_{\text{He}^3} + Y_{\text{T}}$, and $Y_{\text{Li}^7}(\text{today}) = Y_{\text{Li}^7} + Y_{\text{Be}^7}$. Note, however, that we do not use He³, since inferring the primordial abundance of He³ from observations has proven to be problematic, and is therefore not a good probe for BBN. The observed values that we will use are

$$Y_D/Y_p = (2.57 \pm 0.03) \times 10^{-5},$$
 (23)

$$4Y_{\rm He^4} = 0.254 \pm 0.003,\tag{24}$$

$$Y_{\rm Li^7}/Y_p = (1.6 \pm 0.3) \times 10^{-10}.$$
 (25)

Given a choice of parameters, such as the baryon fraction Ω_{b0} and the effective number of neutrino species N_{eff} , we would like to know the probability of the model given the data. There is no unique recipe for calculating this probability, but a result known as Bayes' theorem says that

$$P(\text{model}|\text{data}) = \frac{P(\text{data}|\text{model})P(\text{model})}{P(\text{data})}.$$
(26)

The second factor in the numerator is the probability we would assign to the model before obtaining the data, and it is called the *prior*. The factor in the denominator is known as the *evidence*. We will, as is quite common, consider both of these factors to be constants, and we then have the result

$$P(\text{model}|\text{data}) \propto P(\text{data}|\text{model}).$$
 (27)

The probability on the right-hand side is known as the likelihood, and the point is that it is possible to work out how to calculate it. For example, we will assume that the observations are drawn from a Gaussian distribution, and that the measurements are uncorrelated. This means we assume that if we measure some set of observables d_i with measurement error σ_i , then we can write

$$P(\text{data}|\text{model}) = \frac{1}{\sqrt{2\prod_{i}\sigma_{i}^{2}}} \exp\left[-\sum_{i} \frac{(d_{i}(\vec{p}) - d_{i})^{2}}{\sigma_{i}^{2}}\right],$$
(28)

where $d_i(\vec{p})$ are the predicted values for the observables given the model parameters \vec{p} . We can infer the most probable values for the model parameters by maximizing eq. (28) as a function of the model parameters, or equivalently, by minimizing

$$\chi^2(\vec{p}) = \sum_i \frac{(d_i(\vec{p}) - d_i)^2}{\sigma_i^2}.$$
(29)

In principle we could try to fit all the parameters of the model at the same time in this way, but in this project we will only do one at a time.

j) [15 points]

Compute the relic abundances in the range $\Omega_{b0} = [0.01, 1]$, and compare against the measurements (23), (24), and (25). Reproduce Figure 4, and find the most probable value for Ω_{b0} , i.e. the best fit given the data.

The total matter content of the universe is around $\Omega_{m0} = 0.3$, where a significant fraction of this is in the form of some unknown and unseen (dark) matter. What does the value for Ω_{b0} that we infer from BBN tell us about what this dark matter can, or cannot, be?

Hint: The code is probably quite slow, so we can use a trick to speed things up. Since the functions are quite smooth in log-space, we can use scipy's **interp1d** with kind="cubic" on $\ln Y_i(\ln T)$ to interpolate from around 10 to 20 computed points to as many as we need to make a smooth plot and find a reasonably accurate value for the best-fit value of Ω_{b0} . To avoid possible numerical errors when taking the log of Y_i , we can put a lower bound on Y_i , e.g. 10^{-20} .



Figure 4: The relic abundance of elements are shown as a function of the baryon density Ω_{b0} , along with measurements (23), (24), and (25) (horizontal shaded regions). In the lower plot the normalized probability eq. (28) is shown. The best-fit value of Ω_{b0} is indicated by the dotted line.

k) [15 points]

Compute the relic abundances in the range $N_{\text{eff}} = [1, 5]$, and compare against the measurements (23), (24), and (25). Reproduce Figure 5, and find the most probable value for N_{eff} , i.e. the best fit given the data.

How does the best-fit value for the effective number of neutrino species $N_{\rm eff}$ compare to your expectations?



Figure 5: The relic abundance of elements are shown as a function of the effective number of neutrino species N_{eff} , along with measurements (23), (24), and (25) (horizontal shaded regions). In the lower plot the normalized probability eq. (28) is shown. The best-fit value of N_{eff} is indicated by the dotted line.

References

 Robert V. Wagoner, William A. Fowler, and F. Hoyle. On the synthesis of elements at very high temperatures. 148:3. ADS Bibcode: 1967ApJ...148....3W.