Milestone 2

AST5220

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1 Introduction

In this projet we wish to follow in the footsteps of Petter Callin[1] who numerically reproduces the power spectrum obtained by the CMB data. This will be done in several steps, where each step simulates the different physical processes that make up the power spectrum.

The first milestone consisted of calculating the background cosmology of the whole universe. For this milestone, the goal is to simulate the physics behind recombination. This will be done by computing how the optical depth and visibility function evolves in time. In doing so, we will also need to solve the Saha equation and the Peebles equations.

As with the first part of this project, all numerical solutions will be obtained by utilising the C++ code base provided by our lecturer, Hans Winther.

2 Theorethical Background

2.1 Optical depth

As mentioned, the main goal of this project is to compute how the optical depth evolves in time. In short terms, the optical depth explains whether a medium is optically thin, or optically thick. If you send a beam of light through an optically thick medium, the light will be scattered in all directions, and not much will pass through, which of course means that if you do the same through an optically thin medium, most, if not all of the light will pass through.

The intensity I of such a beam is given by $I(x) = I_0 e^{-\tau(x)}$ where I_0 is the initial intensity at the source and $I(x)$ is the intensity measured after some distance x. Here, τ represents the optical depth. If $\tau \ll 1$, we say the medium is optically thin, and if $\tau \gg 1$, the medium is thick. $\tau \approx 1$ is the transition between these two states.

The optical depth can be expressed as an integral

$$\tau(\eta) = \int_{\eta}^{\eta_0} n_e \sigma_T a d\eta' \tag{1}$$

or as an ordinary differential equation

$$\tau' = \frac{d\tau}{dx} = -\frac{n_e \sigma_T}{H}. \tag{2}$$

Here, n_e is the electron density, $\sigma_T = \frac{8\pi}{3}\frac{\alpha^2\hbar^2}{m_e^2 c^2}$ is the Thompson scattering. a and H is of course the scale factor and Hubble parameter. As with milestone 1, η and x are our two time variables of interest, namely the conformal time and the log-scaled scale factor $x = \ln a$ respectively.

The reason for why the optical depth is interesting for us to calculate in regards to recombination because the moment of recombination is really just the moment where the universe goes from being optically thick to optically thin. Before recombination, the universe is hot and dense, too hot for even hydrogen to form, meaning there was a lot of free electrons scattered about for the photons to bounce off of, resulting in an optically thick universe. When the universe cooled down, all the free protons and electrons could form into neutral hydrogen, and the photons could travel freely, making the universe optically thin.

2.2 Electron density

To calculate the optical depth given in eq. (2) we need to know how the electron density $n_e = n_e(\eta)$ behaves in time. To do this, we will calculate the fractional electron density

$$X_e = \frac{n_e}{n_H} \tag{3}$$

where

$$n_H = n_b \approx \frac{\rho_b}{m_H} = \frac{\Omega_b \rho_c}{m_H a^3} \tag{4}$$

is the proton density under the assumption that the only baryons in the universe are protons.

X_e can be solved for in different ways. When the universe is in thermodynamic equilibrium, that is when $X_e \approx 1$, we can use the Saha equation. When the universe begins to cool, during and after recombination, the Saha equation falls short, and we will need to solve the Peebles equation instead. For simplicity we will use the Saha equation in the regime when $X_e > 0.99$ and Peebles equation when $X_e < 0.99$

2.2.1 Saha equation

As mentioned, the Saha equation works perfectly well under the assumption that the universe is in thermodynamic equilibrium. Before recombination, in the dense soup of electrons and protons, we can arguably say that it is.

The Saha equation is defined as

$$\frac{X_e^2}{1 - X_e} = \frac{1}{n_b} \left(\frac{m_e T_b}{2\pi} \right)^{3/2} e^{-\epsilon_0 / T_b}, \tag{5}$$

where m_e is the electron mass and T_b is the baryon temperature. For simplicity, we assume that the baryon temperature follows the photon temperature, that is $T_b = T_r = T_{cmb}/a$.

2.2.2 Peebles equation

When we can no longer trust the solution from the Saha equation, we will use the Peebles equation. The Peebles equation takes on the form

$$\frac{dX_e}{dx} = \frac{C_r(T_b)}{H} \left[\beta(T_b)(1 - X_e) - n_H \alpha^{(2)}(T_b) X_e^2 \right], \tag{6}$$

where

$$
\begin{aligned}
C_r\left(T_b\right) &= \frac{\Lambda_{2s\to 1s}+\Lambda_\alpha}{\Lambda_{2s\to 1s}+\Lambda_\alpha+\beta^{(2)}\left(T_b\right)} \\
\Lambda_{2s\to 1s} &= 8.227\mathrm{s}^{-1} \\
\Lambda_\alpha &= H\frac{\left(3\epsilon_0\right)^3}{(8\pi)^2 n_{1s}} \\
n_{1s} &= \left(1-X_e\right)n_H \\
\beta^{(2)}\left(T_b\right) &= \beta\left(T_b\right)e^{3\epsilon_0/4T_b} \\
\beta\left(T_b\right) &= \alpha^{(2)}\left(T_b\right)\left(\frac{m_e T_b}{2\pi}\right)^{3/2} e^{-\epsilon_0/T_b} \\
\alpha^{(2)}\left(T_b\right) &= \frac{64\pi}{\sqrt{27\pi}}\frac{\alpha^2}{m_e^2}\sqrt{\frac{\epsilon_0}{T_b}}\phi_2\left(T_b\right) \\
\phi_2\left(T_b\right) &= 0.448\ln\left(\epsilon_0/T_b\right).
\end{aligned}
$$

This does indeed look a bit scary. The Peebles equation is a solution to the Boltzmann equation when looking at the reaction $e^- + p \leftrightarrow H + \gamma$, where the Peebles equation take the transition rates between the ground state and the first excited state of hydrogen into account.

2.3 Visibility function

And last but not least, the visibility function, whic reads as

$$
\tilde{g}(x) = -\tau' e^{-\tau}, \quad \int_{-\infty}^{0} \tilde{g}(x)dx = 1. \tag{7}
$$

The visibility function is a probability distribution that gives the probability of a given photon scattering at time x.

3 Method and implementation

3.1 Code structure

For this milestone, all main coding was done in the file `RecombinationHistort.cpp`. We again utilized the Spline- and ODEsolver-methods from the GSL package. All visualization of the data was done using Python, and can be found in `milestone2_plots.py`.

3.2 Reintroduction of constants

As most physicists, we like to keep things simple, meaning that we don't like to drag around constants unless we absolutely have to. This means that in all equations above we have used natural units, meaning that $c = \hbar = k_b = 1$. Now, had we implemented the equations as they stand now, it would lead to some problems. First of all, most of our equations contains an exponential, and the argument of an exponential has to be unitless. Second of all, we're calculating X_e, which is unitless, which means that the equations used to find this quantity will also need to be unitless.

To achieve this we reintroduced the constants $c, \hbar, k_b$ in the equations so that they have the right dimensionality again. This can be done in several clever and rigorous ways. Or it can be done by making educated guesses, throwing some constants at the equations and see what sticks. We, of course, did the latter, anything else would have been silly... *it would also probably have been much quicker.*

The units for the three constants we want to reintroduce are as following:

$$[\hbar] = Js = \frac{kgm^2}{s}$$
$$[c] = \frac{m}{s}$$
$$[k_b] = \frac{J}{K} = \frac{kgm^2}{Ks^2}.$$

The very messy process of fixing the dimensionality will be fully explained with the Saha equation, by then both the reader and the author will probably be tired of reading and writing about how "we tried this and that until it worked", so the process behind the Peebles equation will be kept short and sweet with a focus on the main logic behind all educated guesses.

3.2.1 Saha equation

As a reminder, the Saha equation looks like

$$\frac{X_e^2}{1-X_e} = \frac{1}{n_b}\left(\frac{m_e T_b}{2\pi}\right)^{3/2} e^{-\epsilon_0/T_b}, \tag{8}$$

.

where the left hand side if, of course, unitless. Now, the units for each constant on the right hand side is $[n_b] = 1/m^3$, $[m_e] = kg$, $[T_b] = K$ and $[\epsilon_0] = eV = J$.

First and foremost, we know that every ϵ_0/T_b should be ϵ_0/k_bT_b, as both ϵ_0 and k_bT_b has units energy. The exponential in the expression is thus dealt with.

The remaining units to deal with are then as following

$$\frac{1}{n_b}\left(\frac{m_e T_b}{2\pi}\right)^{3/2} = m^3(kgK)^{3/2}. \tag{9}$$

To make this easier to work with, we squared everything, resulting in

$$m^6K^3kg^3, \tag{10}$$

meaning we have to find a combination of constants with the units $m^{-6}kg^{-3}K^{-3}$.

So, the first obvious choice here is that we need the Boltzmann constant k_b, as that is the only constant with temperature as part of its units. Specifically, we need $[k_b^3] = kg^3m^6/K^3s^6$. This is where a more rigorous approach would have been more appropriate, and would have been easier to replicate on paper, but basically the process from here on out consisted of just observing that we at least need kg^-6 and m^{-12} as a start, and then just staring really hard at what we had to work with until it became obvious that we needed to divide by $\hbar^6$. This yielded

$$\frac{k_b^3}{\hbar^6} = \frac{kg^3 m^6}{K^3 s^6} \frac{s^6}{kg^6 m^{12}} \tag{11}$$

$$\frac{k_b^3}{\hbar^6} = \frac{1}{kg^3 m^6 K^3}, \tag{12}$$

which is what we wanted. Taking the square root of this and inserting it back into eq. (8) gives

$$\frac{X_e^2}{1 - X_e} = \frac{1}{n_b \hbar^3} \left(\frac{m_e T_b k_b}{2\pi} \right)^{3/2} e^{-\epsilon_0 / k_b T_b}. \tag{13}$$

3.2.2 Peebles equation

Now, to say that we followed this exact procedure with the Peebles equation would be an oversimplification, given the more complicated nature of the equation with all it's different products. But in essence, that's what was done with each separate subequation. The important part was to keep track on which subequations are coupled and to work in a clever order from there. This process will be explained as briefly as possible as to not give the reader a headache!

Again, as a reminder, the Peebles equation takes on the form

$$\frac{dX_e}{dx} = \frac{C_r \left(T_b\right)}{H} \left[\beta \left(T_b\right) \left(1 - X_e\right) - n_H \alpha^{(2)} \left(T_b\right) X_e^2 \right], \tag{14}$$

where

$$\begin{aligned}
C_r \left(T_b\right) &= \frac{\Lambda_{2s \to 1s} + \Lambda_\alpha}{\Lambda_{2s \to 1s} + \Lambda_\alpha + \beta^{(2)} \left(T_b\right)} \\
\Lambda_{2s \to 1s} &= 8.227 \mathrm{s}^{-1} \\
\Lambda_\alpha &= H \frac{\left(3\epsilon_0\right)^3}{(8\pi)^2 n_{1s}} \\
n_{1s} &= \left(1 - X_e\right) n_H \\
\beta^{(2)} \left(T_b\right) &= \beta \left(T_b\right) e^{3\epsilon_0 / 4T_b} \\
\beta \left(T_b\right) &= \alpha^{(2)} \left(T_b\right) \left(\frac{m_e T_b}{2\pi} \right)^{3/2} e^{-\epsilon_0 / T_b} \\
\alpha^{(2)} \left(T_b\right) &= \frac{64\pi}{\sqrt{27\pi}} \frac{\alpha^2}{m_e^2} \sqrt{\frac{\epsilon_0}{T_b}} \phi_2 \left(T_b\right) \\
\phi_2 \left(T_b\right) &= 0.448 \ln \left(\epsilon_0 / T_b\right).
\end{aligned}$$

are the aforementioned subequations.

The end goal is to make $\frac{C_r}{H} \beta(T_b)(1 - X_e)$ and $\frac{C_r}{H} n_H \alpha^{(2)}(T_b) X_e^2$ unitless. First of all, all ϵ_0 / T_b are in fact $\epsilon_0 / k_b T_b$ as before.

Now comes the fun part. We started looking at C_r. We know that $[\Lambda_{2s \to 1s}] = s^{-1}$, meaning that the easiest thing to do is to make all other parts of this equation have units s^{-1} as well. Achieving this would yield C_r unitless, making everything down the line easier.

To do this, we first looked at Λ_α. As it stands, this has units $[\Lambda_\alpha] = s^{-1}J^3m^3$. Multiplying this with $(\hbar c)^{-3}$ does the trick. This results in

$$\Lambda_\alpha = H\frac{(3\epsilon_0)^3}{(8\pi)^2 n_{1s}}(\hbar c)^{-3}, [s^{-1}]. \tag{15}$$

Furthermore, $\beta^{(2)}$ should also have units s^{-1}. To achieve this, we added a k_b in the exponential and decided to look at $\beta(T_b)$ immediately, yielding

$$\beta^{(2)}(T_b) = \beta(T_b)e^{3\epsilon_0/4k_bT_b}, [s^{-1}]. \tag{16}$$

This puts a constraint on $\beta(T_b)$, namely that it should also have units s^{-1}. Looking back at the eq. (14), this makes sense, as $\frac{C_r}{H}\beta(T_b)(1-X_e)$ should be unitless, and $[H] = s^{-1}$. This means we're on the right track! But this is also where it's important to pay attention to the end goal. $\beta(T_b)$ contains the function $\alpha^{(2)}(T_b)$, which we need to make sure have the right units because $\frac{C_r}{H}n_H\alpha^{(2)}(T_b)X_e^2$ needs to be unitless. Thus, we dealt with $\alpha^{(2)}$ first.

Now, after inserting all k_b we need in both $\alpha^{(2)}$ and ϕ_2, we have $[\alpha^{(2)}] = kg^{-2}$. Again, we want $\alpha^{(2)}$ to cancel out the units of $[\frac{C_r}{H}n_HX_e^2] = s/m^3$. This means had to find a combination of constants giving $[kg^2m^3/s]$, which $\hbar^2/c$ does. Inserting this into $\alpha^{(2)}$ yields

$$\alpha^{(2)}(T_b) = \frac{64\pi}{\sqrt{27\pi}}\frac{(\hbar\alpha)^2}{cm_e^2}\sqrt{\frac{\epsilon_0}{k_bT_b}}\phi_2\left(T_b\right), [m^3/s] \tag{17}$$

with

$$\phi_2(T_b) = 0.448\ln(\epsilon_0/k_bT_b). \tag{18}$$

Looking at eq. (17), it contains the fine structure constant α which is not part of the list of constants provided in the code base. It is however a part of the Thompson scattering σ_T, which we inserted into the equation, giving

$$\alpha^{(2)}(T_b) = \frac{8}{\sqrt{27\pi}}c\sigma_T\sqrt{\frac{\epsilon_0}{k_bT_b}}\phi_2(T_b). \tag{19}$$

Almost finished! Now all that's left is to get $[\beta(T_b)] = s^{-1}$. With the units for $\alpha^{(2)}$ known, we also know that $[\beta(T_b)] = m^3/s\cdot(kgK)^{3/2}$. This looked awfully familiar, so we just inserted the solution already found from the Saha equation, namely that $k_b^{3/2}/\hbar^3$, which returns

$$\beta(T_b) = \frac{\alpha^{(2)}}{\hbar^3}\left(\frac{m_ek_bT_b}{2\pi}\right)^{3/2}e^{-\epsilon_0/k_bT_b}, [s^{-1}]. \tag{20}$$

3.2.3 Optical depth

The last equation to rewrite is eq. (2). As it stands now, it has units $[s/m]$, meaning we only needed to multiply by c, giving

$$\frac{d\tau}{dx} = -\frac{cn_e\sigma_T}{H}. \tag{21}$$

Now all equations has the proper dimensionality and can be implemented in the code. *Phew. Now that was neither brief, short or sweet, and it might be a bit more headache-inducing than I meant for it to be.*

3.3 Implementation

All equations was solved in the time span $x \in [-18, 0]$, but only the solution in $x \in [-12, 0]$ was saved and plotted. All solutions were found using the same cosmological parameters as in milestone 1, namely

$$\begin{aligned}
\Omega_{b,0} &= 0.046 \\
\Omega_{CDM,0} &= 0.224 \\
\Omega_{r,0} &= 5.04318 \times 10^{-5} \\
\Omega_{\Lambda,0} &= 0.72995 \\
h &= 0.7 \\
T_{cmb} &= 2.725 \\
Y_p &= 0.
\end{aligned}$$

3.3.1 Finding Xe and ne

To find Xe we first solved the Saha equation. We solved this simply as a quadratic equation with some modification in the end points. Rewriting it on a worm that is simpler to work with yields

$$\frac{X_e^2}{1 - X_e} = C, \tag{22}$$

where

$$C = \frac{1}{n_b\hbar^3}\left(\frac{m_eT_bk_b}{2\pi}\right)^{3/2} e^{-\epsilon_0/k_bT_b}. \tag{23}$$

We rewrote eq. (22) as $X_e^2 + CX_e - C = 0$, and solved it as a quadratic equation, giving

$$X_e = -\frac{C}{2} + \frac{\sqrt{C(C+4)}}{2}, \tag{24}$$

where we have used only the positive solution to the equation, as X_e is a ratio that should be positive at all times.

Now, X_e is a ratio that should start at 1 and decrease to 0 with time. Looking at eq. (22), we observed that this could lead to some problems. Taking the limit $X_e \to 1$, the factor $1 - X_e$ becomes zero, meaning $C \to \infty$. This is obviously a problem. To mitigate this we brute forced X_e to be exactly one when C is greater than some big constant. To avoid instabilities in the end points where X_e approaches 0, and to make sure it never actually reaches 0 because we want to spline the logarithm of X_e, we brute force X_e to be some small constant when C is smaller than some small constant. These two constants where found by trial and error to make sure they did not interfere with any interesting parts of the solution. This means the final equation we used to solve the Saha equation reads as

$$X_e = \begin{cases} 0 & C < 10^{-20} \\ 1 & C > 10^{6} \\ -\frac{C}{2} + \frac{\sqrt{C(C+4)}}{2} & \text{else.} \end{cases} \tag{25}$$

We solved the Saha equation twice. Both as part of getting the full solution of X_e, with the Saha solution when $X_e > 0.99$ and the Peebles equation when $X_e < 0.99$, but also for the whole evolution of X_e, This was done to be able to compare the solutions later and see where Saha stops being a good approximation.

Now, onto Peebles, where arguably the hardest part was to not mess up all the different equations. Solving the equation itself was just like solving any other ODE in this code base, namely with the ODEsolver method provided.

With Saha and Peebles solved, we found n_e by $n_e = X_e \cdot n_H$, where n_H is defined in eq. (4). To ensure stability, we splined the logarithm of these values, and saved the exponential of those logarithmic splines.

We were also interested in finding the times x_{rec} and z_{rec} where $X_e = 0.5$. We wanted to find these both for the full Saha+Peebles solution, but also for the Saha only approximation. This was quickly done utilizing `numpy.argmin` in Python.

3.3.2 Optical depth and visibility function

Having found n_e, we could now solve the optical depth. While this is also just another ODE we can easily solve, we needed to do some trickery to make it work. We do not know the initial conditions for τ. The only thing we know is that it should be 0 today, so $\tau(x = 0) = 0$. Utilizing the fact that eq. (21) does not have a τ in the RHS, we set the initial value to some arbitrary, large number, overshooting the solution. Then, we simply scaled it by finding how far off from 0 we were in the last point. The solution for tau and its derivatives where then splined, where the derivatives were found by using the built-in `[spline_name].deriv_x` method.

With τ now obtained, we could find the visibility function $\tilde{g} = -\tau' e^{-\tau}$ easily. Its derivatives was found by again using the built-in method in Spline.

Finally we wanted to find the times x_* an z_* of recombination, defined as the point where $\tau = 1$, or where the visibility function peaks. We chose to find it according to where $\tau = 1$. As with x_{rec}, this was done in Python using numpy.

All results were saved to a file and imported in Python and plotted. To make the plot of the visibility function more readable we scaled $\tilde{g}'$ with 1/10 and $\tilde{g}''$ with 1/100.

4 Results

4.0.1 Fractional electron density

In fig. 1 we see how the fractional electron density X_e evolves as a function of time. Both the full solution and the Saha only solution is plotted in the same figure to clearly show the difference between them. We see, as expected, that when only using Saha, X_e approaches 0, while the full solution flattens out. This flattening of the curve represents the electrons "freezing out" of thermal equilibrium. Comparing this plot with fig. 1 in Callin, we see that X_e flattens out for a bit too high values. Our curve flattens at around $X_e = 10^{-3}$ while Callin's doesn't flatten out until closer to 10^{-4}, so there's something going on here. It might hint at a missing factor in Peebles somewhere, but after staring at the implementation for too long and not finding it, we gave up, for fear of going completely mad.

The time for when recombination is halfway, x_{rec} and z_{rec} where found to be

$$\begin{aligned} x_{rec} &= -7.17 \\ z_{rec} &= 1292 \\ x_{rec}(\text{Saha}) &= -7.23 \\ z_{rec}(\text{Saha}) &= 1239. \end{aligned}$$

where we see that Saha predicts this point to be earlier than Peebles.

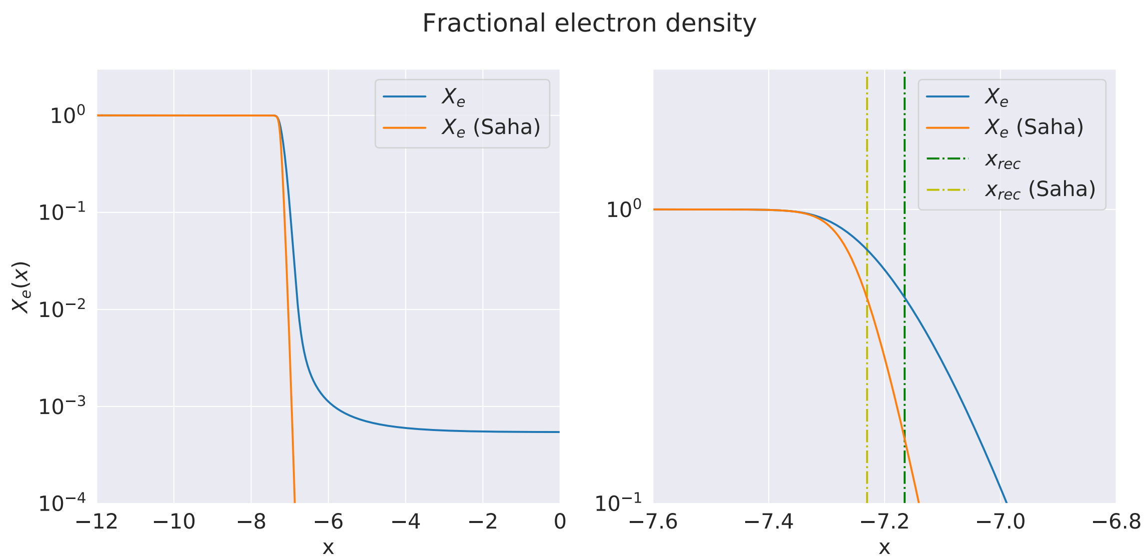

Figure 1: Figures showing how the fractional electron density X_e behaves in time. Both plots show the full solution and the solution obtained using only the Saha equation. The left figure shows the full time evolution, while the right figure is zoomed in to show where the two solutions diverge. The lines represent the time where $X_e = 0.5$, where the green line was obtained from the full solution while the yellow line was obtained from only the Saha approximation.

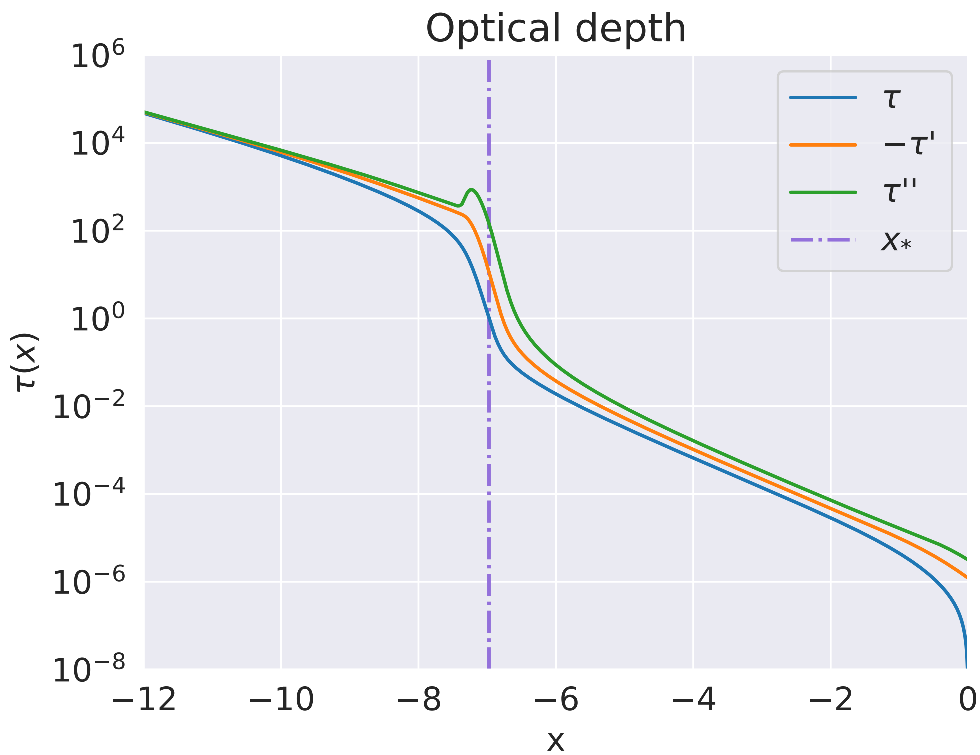

Figure 2: Figure showing the time evolution of the optical depth τ and its first and second derivatives. The time of recombination x_*, where $\tau = 1$ is marked with the purple line.

4.0.2 Optical depth and visibility function

In fig. 2 we see how the optical depth τ and its first and second derivative evolves with time. The point x_* where $\tau = 1$ is marked by the purple line. This is the time for the last scattering surface. It should correspond with where the the visibility function peaks, which will be addressed further down. On each side of this line we clearly see the two eras of the universe, where it starts of as optically thick with $\tau \gg 1$, approaches $\tau = 1$ and ends up as optically thin with $\tau \ll 1$, just as we expected.

The time of last scattering x_* and z_* where found to be

$$x_* = -6.97$$
$$z_* = 1066.$$

Finally, in fig. 3 we see the visibility function and its first and second derivatives. The derivatives are scaled appropriately as to not loose information in the plot. The visibilty function represents the probability density of a photon to scatter at time x. We therefore expect it to peak at recombination for $x = x_*$, which it clearly does! The derivatives show how this peak is not perfectly symmetric.

References

[1] Petter Callin. How to calculate the cmb spectrum, 2006.

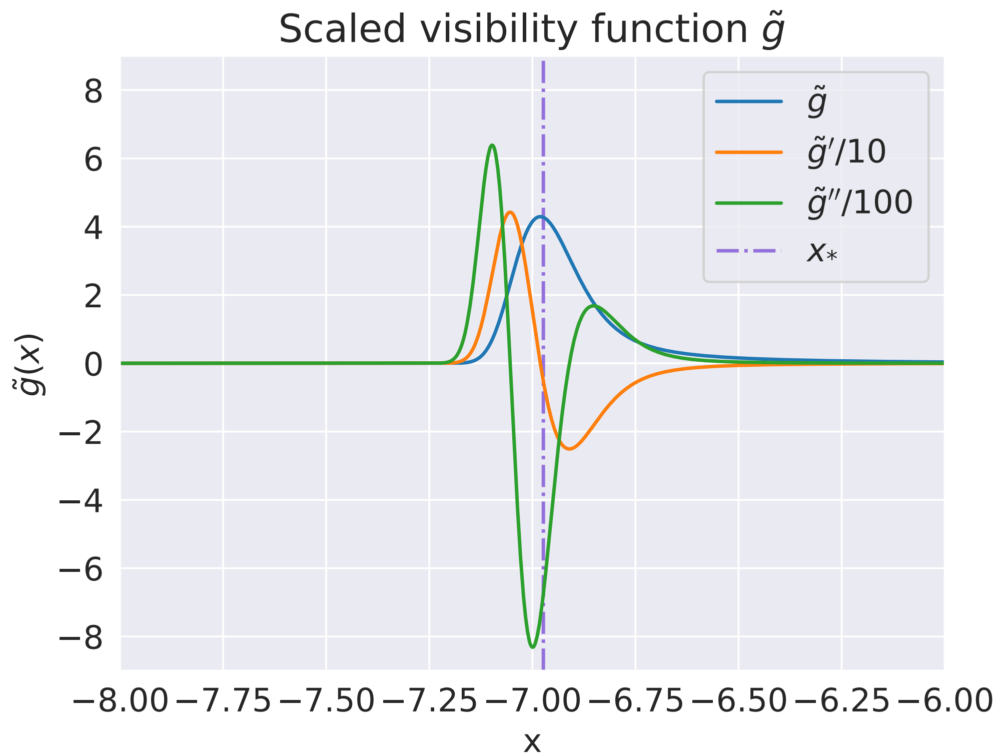

Figure 3: Figure showing the visibility function $\tilde{g}$ and its first and second derivatives. The derivatives have been scaled down by a factor 1/10 and 1/100 respectively, and the plot is zoomed in on the most interesting parts and does not show the whole time interval. The purple line is again x_*, which corresponds nicely with the peak of $\tilde{g}$.