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AST5220-Milestone II: The Recombination History

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Abstract

We have simulated the recombination history of the universe under the assumption of the only (baryonic) matter content of the universe being hydrogen and neglecting the reionization epoch. We have computed the evolution of the optical depth $\tau(x)$ and the visibility function $\tilde{g}(x)$, as well as their first two derivatives, as functions of the log-scale factor x. To do so, we first had to compute the free electron density n_e through finding the free electron fraction X_e by solving the Saha and Peebles equations. Defining recombination to happen when $X_e = 0.5$, we determined the time of recombination to be at $x = -7.16$ corresponding to a redshift $z = 1285.7$. The Saha only solution did as expected undershoot and recombination occurred somewhat earlier in this model at $x = -7.23$ or $z = 1379.25$. The transition from an opaque to a transparent universe defining the surface of last scattering when $\tau = 1$ or at the peak of $\tilde{g}(x)$ both found to be at $x = -6.99$ or at redshift $z = 1080$. Our results were found to be well behaved and were consistent with results by Callin (2006) and Winther (2020).

The codes for this paper can be found at:
https://github.com/SagittariusA-Star/AST5220-Milestones

1. INTRODUCTION

After having simulated the large scale background evolution of the universe in Stutzer (2020), we now want to compute the optical depth and the visibility function of the universe throughout its evolution. The computations made will expand upon the code previously made (Stutzer (2020)). The optical depth and the visibility function are important quantities as, they essentially quantify how far a photon can travel in the universe before getting extinct (when looking back in time). From these quantities one can estimate the time of recombination and last scattering, which are important for CMB cosmology.

We make several assumptions, which amongst other things are that extinction through Thomson scattering provides the only extinction process and that the only baryons is hydrogen atoms. Also the epoch of reionization will be neglected, as a simplification. Computing the optical depth and visibility function is in principle not that hard, however, only if one is provided the density of free electrons. Thus, most of the work will be finding the electron density evolution of the universe and from it the optical depth and visibility function.

2. METHOD

The formulas and equations presented here are provided by Winther (2020) and/or Dodelson (2003), unless otherwise stated.

2.1. *The Optical Depth*

As mentioned in the introduction computing the optical depth of the universe is in theory governed by fairly simple relations. When light travels through a medium, a given amount of photons are removed and added to the beam. The amount of photons that are added depend on the emissivity of the medium. We assume here that the gas the light travels through has a negligible emissivity. Furthermore the amount of attenuation is given by the extinction coefficient

$$\alpha = n_e \sigma_T, \tag{1}$$

where we assume Thomson scattering on electrons to be the only mechanism to attenuate photons. Here $\sigma_T = \frac{8\pi}{3}\frac{\alpha^2\hbar^2}{m_e^2c^2}$ and n_e are the Thomson cross-section and the free electron density respectively. The optical depth is given by

$$\tau(\eta) = \int_\eta^{\eta_0} n_e \sigma_T a d\eta', \tag{2}$$

where a and η are the scale factor and the conformal time of the universe. The optical depth corresponds to the factor of e the radiation is damped by when passing through a medium (gas in the universe). Thus opaque and transparent objects are characterized by $\tau \gg 1$ (optically thick) and $\tau \ll 1$ (optically thin) respectively. We place the threshold for transparency at $\tau = 1$ after which most photons travel freely.

For practical reasons we choose to solve for τ by solving the ordinary differential equation (ODE)

$$\frac{\mathrm{d}\tau}{\mathrm{d}x} = -\frac{n_e \sigma_T}{H} = -\frac{n_e \sigma_T}{H}c, \tag{3}$$

where $x = log(a)$ and $H = \frac{\dot{a}}{a}$ are the log-scale factor and the Hubble parameter respectively. The Hubble parameter is found by the Friedmann equation through the previously developed code in Stutzer (2020). We choose this ansatz instead of the integral, so we can use the `ODEsolver` routine provided by Winther (2020). Note we went from natural units to SI units in the last step in eq. (3). The equations provided by Winther (2020) are given in natural units, however we want them to be in SI units, so as to enable solving in C++ using the constants in `Utils.h` provided by Winther (2020). We will show the dimensional analysis to go from natural units to SI on the example above, and than just provide the equations in SI units with all the constants from now on. As one can see in eq. (3) the l.h.s. of the equation if dimensionless because τ and x both are. Thus the r.h.s. must be dimensionless too. We however see that the r.h.s. has units

$$1 = \frac{[n_e][\sigma_T]}{[H]}[c]^\alpha = \frac{\mathrm{m}^{-3}[\mathrm{m}^2]}{\mathrm{s}^{-1}}[c]^\alpha = \frac{\mathrm{s}}{\mathrm{m}}[c]^\alpha \tag{4}$$

The only physical constant that is reasonable to use here is thus the light speed c, with units m/s, thus $\alpha = 1$ in this case. Similarly, when having units for instance Js or K "too much" on one side in natural units, one can correct with the reduced Planck constant $\hbar$ or Boltzmann constant k_B to go to SI units.

Now, as can be seen from eq. (3), there is one problem however; we need to know the electron density. We will address this problem in the following subsection.

2.2. *The Free Electron Fraction and Density*

In order to compute the optical depth we need to know the free electron density n_e. We can compute this through the free electron fraction X_e and use the baryon, i.e. hydrogen density, as a translational factor. We thus get that the electron density as a function of the electron fraction and the hydrogen density is

$$n_e = X_e n_H, \tag{5}$$

where

$$n_H = n_b \approx \frac{\rho_b}{m_H} = \frac{\Omega_{b0}\rho_{c0}}{m_H a^3}, \tag{6}$$

where we have assumed all baryons to be in hydrogen. This should be a reasonable approximation since the hydrogen atoms are the dominant species of baryons in the universe. Here the baryon density parameter and the critical density today are given as their regular expressions found in and computed in Stutzer (2020). The time dependence of the baryon density is solely in the scale factor dependent $a^{-3} = e^{-3x}$ factor.

The remaining work is to find n_e, through finding X_e. This turns out to be the hardest part of the total work. We can find X_e through solving the Boltzmann equation for a recombination/ionization reaction of the type $e^- + p^+ \rightleftharpoons H + \gamma$. The Boltzmann equation, $df/dt = C$, describes the change of the distribution function f (space×momentum-dimensional distribution) of a given particle species that interacts with other species (with interaction term C). A thorough treatment of the problem shown in Dodelson (2003), and we will merely show a rough overview. At early times the energies of the constituent particles were high enough to keep the (ionization/recombination) reaction in or close to equilibrium. As long at the reaction is close to equilibrium Saha's approximation (Dodelson 2003, p. 70) ensures that

$$\frac{n_e n_p}{n_H} = \frac{n_e^{(0)} n_p^{(0)}}{n_H^{(0)}}, \tag{7}$$

where the $n_i^{(0)}$ denote the equilibrium distribution species i. That is because sufficiently close to the equilibrium the ration between the reactant's densities (on each side of the reaction equation) equals the same ratio at equilibrium. As the universe's net charge is zero, we can safely assume their to be as many free electrons as free protons, i.e. $n_e = n_p = n_H$ (assuming that all baryons are protons/hydrogen). The Saha approximation and the given assumptions can be rewritten to get the Saha equation for recombination given as

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

(Dodelson 2003, p. 70). This equation describes the free electron fraction for a given time, under the assumption of being close to equilibrium. Here m_e and ϵ_0 are the electron mass and the ionization energy of hydrogen respectively (Winther 2020). The temperature T_b is the baryon temperature, which in principle should be found separately, however we can approximate it to the radiation temperature T_r (Winther 2020). It is is thus given as $T_b = T_r = T_{\mathrm{CMB}}/a = 2.7255\mathrm{K}/a$.

Because eq. (8) is a simple quadratic equation its solution is simply $X_e = \frac{1}{2}(-R \pm \sqrt{R^2 + 4R})$, where R stand for the r.h.s. of Saha's equation. Note that only the "+"-solution is physically valid. We will also briefly come back to this solution in sec. 2.3 to discuss some numerical issues with this solution.

We have, however, not yet found a complete solution, since the Saha equation is only valid if X_e is close to unity, i.e. close to equilibrium. To solve for X_e if X_e falls below some tolerance, which we choose to be $X_e = 0.99$, we need to use the better approximation to X_e given by the Peebles' equation

$$\frac{dX_e}{dx} = \frac{C_r(T_b)}{H}\left[\beta(T_b)(1-X_e) - n_H\alpha^{(2)}(T_b)X_e^2\right]. \quad (9)$$

The two terms of the equation represent "creation" and "distribution" of free electrons respective according to the reaction equation stated earlier. Here

$$C_r(T_b) = \frac{\Lambda_{2s\to 1s} + \Lambda_\alpha}{\Lambda_{2s\to 1s} + \Lambda_\alpha + \beta^{(2)}(T_b)}, \quad (10)$$

$$\Lambda_{2s\to 1s} = 8.227\mathrm{s}^{-1} \quad (11)$$

$$\Lambda_\alpha = H\frac{(3\epsilon_0)^3}{(8\pi)^2(\hbar c)^3 n_{1s}} \quad (12)$$

$$n_{1s} = (1-X_e)n_H \quad (13)$$

$$\beta^{(2)}(T_b) = \beta(T_b)e^{3\epsilon_0/4T_b k_B} \quad (14)$$

$$\beta(T_b) = \alpha^{(2)}(T_b)\left(\frac{m_e T_b k_B}{2\pi\hbar^2}\right)^{3/2} e^{-\epsilon_0/T_b k_B} \quad (15)$$

$$\alpha^{(2)}(T_b) = \frac{8}{\sqrt{3\pi}}\sigma_T c\sqrt{\frac{\epsilon_0}{T_b k_B}}\phi_2(T_b) \quad (16)$$

$$\phi_2(T_b) = 0.448\ln(\epsilon_0/T_b k_B), \quad (17)$$

are constants describing simple atomic transitions between the ground state of hydrogen (1s) and the first excited state (2s) (Winther 2020). We need to consider at least the first excited state of hydrogen, because a recombination to the ground state would simply again produce an ionizing photon, which in turn would ionize another atom. Thus there would not be a net effect. Thus we need to consider recombination to the fist excited state, which produces a lower-energy photon that is not able to again ionize further atoms (Dodelson 2003, p. 71). Importantly, Peebles equation is also simply a first order approximation for X_e. A more thorough handling would be to include different atomic species as well as several more transitions. We will however stick with our two level hydrogen model, as it should be sufficiently accurate for our purposes.

For comparison sake we will later compute the full Saha+Peebles solution together with the Saha only solution. Since the Saha only solution is expected to drop exponentially once outside its validity regime, we expect it to predict an earlier recombination time (when $X_e = 0.5$) than the complete solution.

Note that even though Peebles equation is a valid solution of the Boltzmann equation for this reaction, it diverges at early times in our case. One way to see this is that n_{1s} becomes very small (or even zero) when approaching $X_e = 1$ at early times. Since we devide by n_{1s} in Λ_α we get a divergence. Thus we must use both Saha and Peebles equations, in their respective era of validity, in order to solve the complete problem.

The Peebles' equation is simply another linear ODE which we can simply solve using the `ODEsolver`-routine by Winther (2020) as discussed in sec. 2.3. Now that we have an expression for X_e we can as mentioned earlier easily find n_e and again use the `ODEsolver`-routine to find the optical depth tau.

The time at which we place recombination, i.e. when most electrons and protons have formed neutral hydrogen, is defined to be at the time when $X_e = 0.5$. However, recombination is really an epoch rather than a single event in time, as the free electrons and protons recombine gradually as opposed to all at once. The time of recombination thus is merely a definition we have set.

The only remaining quantity we need to compute is the visibility function

$$\tilde{g}(x) = -\frac{\mathrm{d}\tau}{\mathrm{d}x}e^{-\tau}, \quad (18)$$

which quantities the probability density for a photon to last scatter at a given log-scale factor x before decoupling from matter. It is a true probability density function (PDF), meaning it integrates to unity over all of the universe's history. The time of last scattering x_{lss} will thus correspond to the peak of $\tilde{g}$ and marks the last-scattering-surface (lss) where photons decouple (hence also called decoupling). This point is the point of highest probability density of last scattering and corresponds to where $\tau = 1$.

2.3. *Implementation*

As mentioned previously the main goal of this paper is to compute X_e so as to find $\tau(x)$ and $\tilde{g}(x)$. The main strategy is to loop through values of x and at each step compute the solution of Saha's equation. If this solution is at some point below the tolerance $X_e = 0.99$ we switch to Peebles' equation. When in the Peebles regime we set up an ODE with one step for each (outer) loop iteration over x. The electron fraction is than found by step-wise solving the Peebles ODE using the `ODEsolver`-routine by Winther (2020). Simultaneously as computing X_e we compute the electron density n_e as discussed earlier. Splines are made using the `Spline`-routine by Winther (2020), of the logarithm (because they vary by orders of magnitude over the x-range) of X_e and n_e to enable a continuos representation.

Importantly there are two numerical subtleties when solving the Saha and Peebles equations. The first is that when solving the quadratic Saha equation, the

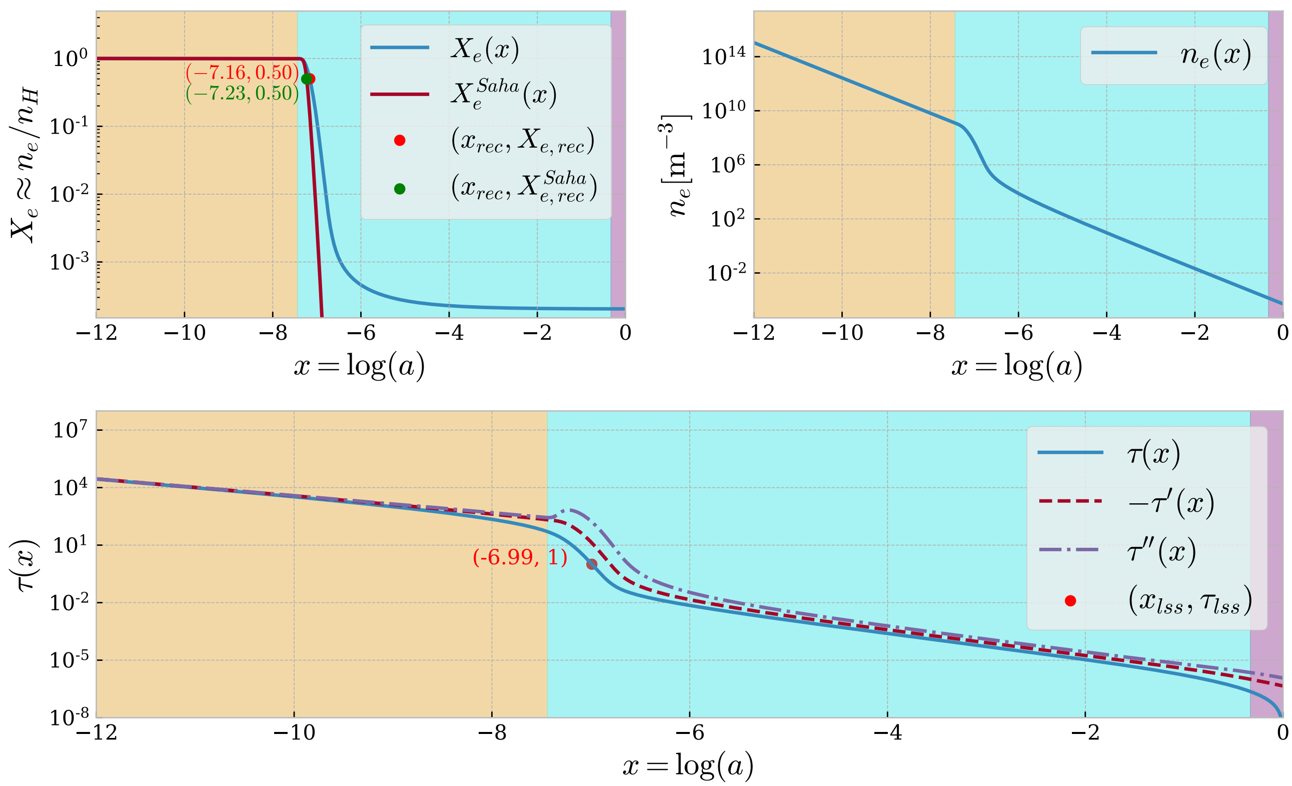

Figure 1. Upper left: Figure showing the free electron fraction X_e as a function of the log-scale factor x for both the general and the Saha only solution. The times of recombination for the two solutions are marked with dots. **Upper right**: Figure showing the free electron density n_e as a function of the log-scale factor x. **Lower panel**: Figure showing the optical depth $\tau(x)$ of the universe due to Thomson scattering on free electrons only, as well as the derivative $\tau'(x)$ and second oder derivative $\tau''(x)$ w.r.t and as functions of the log-scale factor x. The surface of last scattering corresponding to $\tau = 1$ is marked by a red dot. **Note**: The background color in all the plots shows the epoch of dominance for reference. Yellow marks the era of radiation dominance, blue the epoch of matter domination and purple corresponds to the epoch of dark energy. The color domain is found by checking when the corresponding density parameter is dominant, however, in reality the transitions between each epoch should be smoother than shown here.

case when the r.h.s. R of eq. (8) can result in something of the form $-R + R\sqrt{1+4/R} = -R + R = 0$, i.e. "large" - "large" $= 0$, because a computer lets $1 +$ "small" $= 1$. Then $X_e = 0$ even though it should be $X_e = 1$. This happens when R becomes large, i.e. at early times. To solve the problem we consider the solution

$$X_e = \frac{1}{2}(-R + \sqrt{R^2 + 4R}) = \frac{1}{2}(-R + R\sqrt{1+4/R}) \tag{19}$$

$$\approx \frac{1}{2}(-R + R(1 + 2/R)) = 1, \tag{20}$$

using a taylor expansion to first order, since $4/R \ll 1$ when $R \gg 1$. This yields the correct result $X_e = 1$ at early times. We thus simply include an `if`-test to check for this, in which case $X_e = 1$ and else we compute the solution according to the regular formula. We chose to use $4/R = 10^{-9}$ as the tolerance, under which we set $X_e = 1$.

The second subtlety is that in the Peebles equation we have expressions containing exponential functions with positive exponents that can be very large at late times. In particular we have $\exp(3\epsilon_0/4T_b k_B)$ in the expression for $\beta^{(2)}$ which can easily overflow. Fortunately, there is a relatively easy solution; simply combine the expressions for $\beta^{(2)}$ and β directly. This way the exponential factor in $\beta^{(2)}$ becomes $\exp(-\epsilon_0/4T_b k_B)$, which in case of a large fraction $\epsilon_0/T_b k_B$ will simply underflow and give zero, which is alright in our case.

Now, having solved for the free electron density, finding τ and subsequently $\tilde{g}$ is easy. We simply set up an ODE for τ and solve it using the `ODEsolver`-routine (Winther 2020), all in one go. There is, however, one thing we have to handle. The `ODEsolver`-routine cannot integrate the ODE backwards with initial condition $\tau(x = 0) = 0$, and τ at early times is unknown. There is,

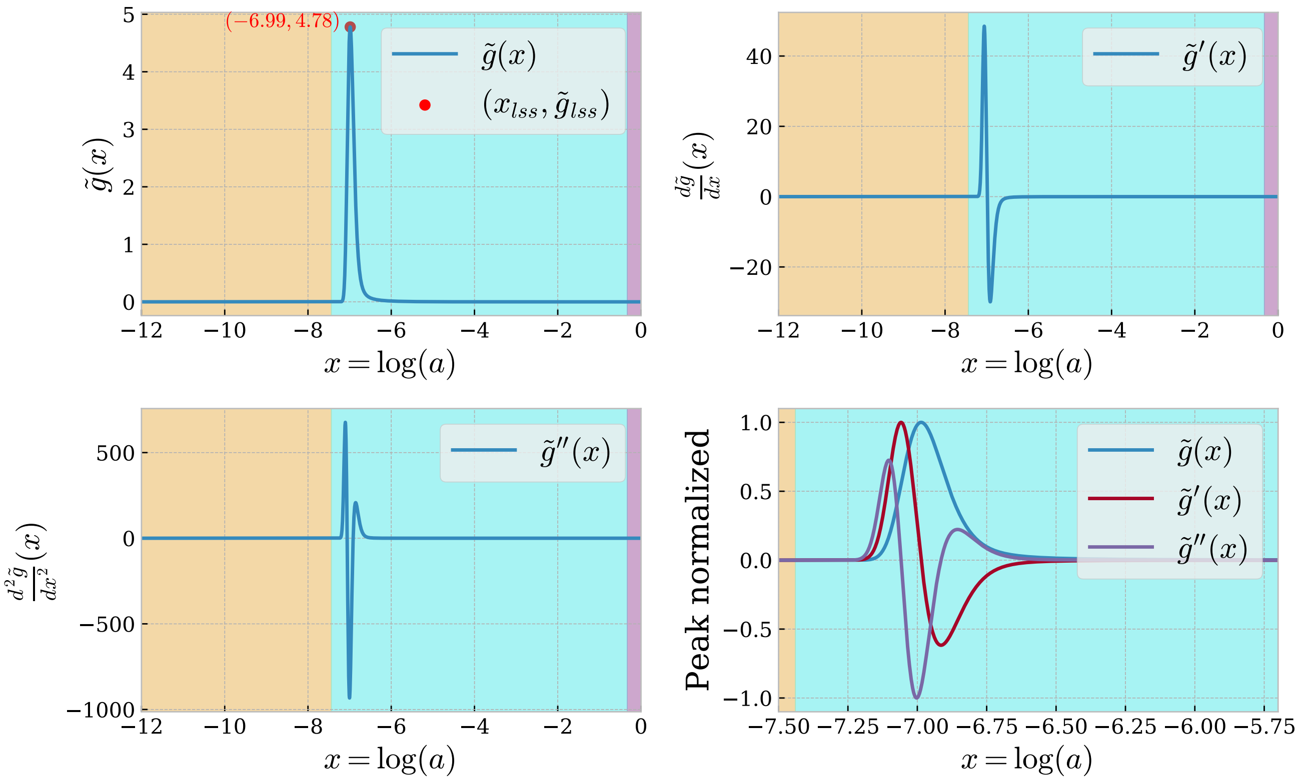

Figure 2. Upper left: Figure showing the un-normalized visibility function $\tilde{g}$ as a function of the log-scale factor x. The red dot marks the peak of $\tilde{g}$ and its x-value corresponds to the log scale factor of the surface of last scattering. **Upper right**: Figure showing the un-normalized first order derivative of $\tilde{g}$ w.r.t. and as a function of the log-scale factor. **Lower left**: Figure showing the un-normalized second order derivative of $\tilde{g}$ w.r.t. and as a function of the log-scale factor. **Lower Right**: Figure showing the visibility function and its first two derivative together in one plot, where all functions are normalized to their respective extremum value (peak or valley). Also we have zoomed in somewhat to show more details.

however, a simple trick; simply use some random initial condition, and find $\tau(x=0)$ (in our case always the last array value of the solution with random initial condition for τ), then subtract $\tau(x=0)$ from all $\tau(x)$ values found by the `ODEsolver`. This way we simply move the origin to correct for the wrong initial condition. We found that using an initial condition of $\tau(x_{\text{start}}) = 1000$ yielded satisfactory results, where $x_{\text{start}} = -13$ and $x_{\text{end}} = 0$. Subsequently splines of τ and of its derivative (to avoid numerical errors in the derivative) were made. The second derivative was extracted from the spline of the fist derivative.

Computing the visibility function $\tilde{g}(x)$ is now just a matter of using the computed splines for τ and $\frac{\mathrm{d}\tau}{\mathrm{d}x}$. A spline is than also made for the visibility function, and the first and second derivatives are found through the spline.

Finally the results are printed to a data file and subsequently plots are produced using a Python script.

3. RESULTS/DISCUSSION

The results produced were computed with the same cosmological parameters used as in Stutzer (2020), originally given by Callin (2006). However, we have used some debug parameters given by Winther (2020); $\Omega_{b0} = 0.05$, $\Omega_{CDM0} = 0.45$, $\Omega_{\Lambda 0} = 0.5$ and $h = 0.7$ in order to cross-check whether our results were consistent with those of Winther (2020). The quantities found were computed from $x_{\text{start}} = -13$ until $x_{\text{end}} = 0$.

In Figure 1 one can see the resulting solution of the electron fraction $X_e(x)$, the electron density $n_e(x)$ and the optical depth $\tau(x)$ as well as its derivatives, all as functions of the log-scale factor x.

When looking at the electron fraction X_e we see that it initially behaves like a constant. This is the phase of the universe's history where the temperatures are so high that almost all hydrogen will be instantly ionized, therefore yielding a electron fraction $X_e = 1$, as there is one electron for each protons. Here we are still very close to equilibrium. Then shortly after matter-radiation equality (see color code in caption) the free electron fraction starts to drop rapidly, eventually passing the point of recombination $X_e = 0.5$ at $x \approx -7.16$ or redshift $z \approx 1285.7$ (see red dot) at which time there is double the amount of hydrogen compared to free electrons. For the Saha only solution this occurred at $x = -7.23$ or $z = 1379.25$ (see green dot). Once too far from equilibrium, the Saha solution will simply drop to zero in an exponential fashion, because we are outside the era where Saha is valid, and will thus predict an earlier recombination time. We see that the complete solution of X_e drops fast too as more and more hydrogen is forming from free electrons and protons. But rather than dropping totally to zero X_e eventually starts flattening out at $X_e \sim 10^{-4}$. When the electron fraction flattens out and becomes roughly constant, the electrons are frozen out, because the spatial distance between the reactants becomes too large for recombination reactions to happen. Being mostly neutral as there are now few free electrons, photons rarely scatter, making the universe mostly transparent. This is also seen in the optical depth, which is low well after recombination has happened.

The free electron density as seen in the left upper panel of Figure 1, also behaves as expected. We see that in the two regimes before and after around recombination, the graph behaves linearly. Since the electron density is proportional to the inverse of the scale factor a cubed, we should see n_e dropping with a linear slope of -3 in a log-log (base 10) plot. This is exactly what we see (keep in mind that the x-axis is in a natural log-scale). The linear regimes of n_e thus correspond to when X_e is stable at $X_e = 1$ and $X_e \sim 10^{-4}$ initially and at the end, and the bend in n_e correspondingly is due to the fall-off of the electron fraction due to an increasing recombination.

The optical depth also behaves as one would expect and is consistent with the findings of Callin (2006). We see that it starts out very large at $\tau(x = -12) \approx 10^4$ initially, i.e. the intensity of radiation received today from that epoch is damped by a factor $exp(-10^4)$ being basically extinguished. Thus initially the universe was very opaque, due to the large free electron density on which photons could (Thomson) scatter. Hence it makes sense that the optical depth decreases linearly similar to n_e as the universe expands (initially). As we approach $x \sim -8$ we start to notice a drop in the optical depth, because of increasing a recombination rate as the universe expands and the temperature drops. As successively more electrons and protons bond to form hydrogen, the photons have no free electrons to scatter on. At the same time there are too few ionizing high-energy photons, as temperature has dropped sufficiently, that can ionize the the newly formed hydrogen. Hence τ drops rapidly.

The transition from an opaque to a transparent universe is defined to be at $\tau = 1$, which happens at $x_{lss} = -6.99$ (see red dot in lower panel of Figure 1). This corresponds to the peak of the visibility function $\tilde{g}$, where the probability density of last scattering is the highest. The transition $\tau = 1$ corresponds to where the photons are one mean free path from the surface, i.e. from the observer (us), of the dampening medium at hand. Thus the mean free path of the photons at x_{lss} corresponds to the proper distance (which is not computed here) from today to lss.

After the period of recombination the optical depth again establishes a linear-like behavior, until the epoch of dark energy begins (close to the current age) were it drops to zero very fast. After recombination optical depth $\tau \ll 1$ and the universe is thus said to be transparent or optically thin.

The shape of the derivatives of τ resemble that of τ quite closely. Note especially that the first order derivative of τ behaves very similar to the electron density due to the direct proportionality. They both are very linear outside the era of recombination, and have a matching behavior in the epoch of reionization. The first derivative of the optical depth can roughly be interpreted as the ratio between the reaction rate of the recombination/ionization reaction to the expansion rate of the universe. Once this ration drops below 1 (slightly after $x_{lss} = -6.99$), there are hardly any reactions happening anymore, due to the expansion of space between the reactants. The second order derivative also seems to behave reasonably well and is consistent with the one found by both Callin (2006) and Winther (2020).

Lastly, in Figure 2 one can see the visibility function and its derivatives both un-normalized and peak-normalized. The visibility function and its derivatives presented here seem to be consistent with those found by Callin (2006). The visibility function, quantifying the probability density of a photon last scattering, is seen to peak sharply at $x = -6.99$ being consistent with our finding of the time of transition between an opaque to a transparent universe at the same value for x (up to some negligible differences due to finit x-grid resolution). The value of $x_{lss} = -6.99$ or redshift $z \approx 1080$ is what we would call (the time of) the surface of last scattering where the photons decouple. This value of x_{lss} corresponds to the peak found by Callin (2006). We can also see in the derivative of the visibility function that its two extrema are different in height, emphasizing the same thing seen in the visibility function itself; its slope is larger on the left than the right side of the peak. The second order derivative also seems to depict the curvature of $\tilde{g}$ correctly and behaves reasonable.

In order to check whether $\tilde{g}$ indeed acts like a true PDF, we integrated it numerically and found it to be within about seven digits of unity, justifying calling it a true PDF.

4. CONCLUSION

We have expanded our simulation of the large scale evolution of the universe to include the recombination history of the universe. Our final goal being the calculation of the optical depth and the visibility function of the universe as a function of time, we first had to compute the electron fraction and density. From the computed quantities we could find the time of recombination and last scattering. All the computed quantities were found to behave according to our expectations and reflect known physics. Thus we can conclude that our simulations successfully depict the recombination history within the limitations of the initial assumptions made.

REFERENCES

Callin, P. 2006, How to calculate the CMB spectrum, , , https://arxiv.org/abs/astro-ph/0606683

Dodelson, S. 2003, Modern Cosmology, Elsevier Science

Stutzer, N.-O. 2020, AST5220-Milestone I: The Background Cosmology, , , https://github.com/SagittariusA-Star/AST5220-Milestones/blob/master/doc/Milestone_I_Report_Nils_Stutzer.pdf, Last visited: 19.03.2020

Winther, H. A. 2020, Milestone II: Recombination History, , , http://folk.uio.no/hansw/AST5220/notes/milestone2.html, Last visited: 19.03.2020