Simulations of Cosmic Reionization
Simulations of Cosmic Reionization

Shapes & Sizes of H II regions around Galaxies and Quasars

by

Martina M. Friedrich
Coverimage:
Photomontage showing me standing on a computer harddisk painting the
temperature map from test4 from PAPER II looking at the code algorithm.
The background shows a photo of Stockholm with the City hall on the left
hand side.

The design element used in the chapter headings is a position-redshift slice
provided by Garrelt Mellema. It should be noted that the redshift direction is
stretched in this representation.
Abstract

After the era of recombination, roughly 360000 years after the big bang (redshift 1100), the universe was neutral, continued to expand and eventually the first gravitationally collapsed structures capable of forming stars, formed. Observations show that approximately 1 billion years later (redshift 6), the Universe had become highly ionized. The transition from a neutral intergalactic medium to a highly ionized one, is called the epoch of Reionization (EoR). Although quasar spectra and polarization power-spectra from cosmic microwave background experiments set some time-constrains on this epoch, the details of this process are currently not known.

New radio telescopes operating at low frequencies aim at measuring directly the neutral hydrogen content between redshifts 6 - 10 via the HI spin-flip line at 21cm. The interpretation of these first measurements is not going to be trivial. Therefore, simulations of the EoR are useful to test the many ill-constrained parameters such as the properties of the sources responsible for reionization. This thesis contributes to such simulations.

It addresses different source models and discusses different measures to quantify their effect on the shapes and sizes of the emerging H II regions. It also presents a new version of the widely used radiative transfer code C2RAY which is capable of handling the ionizing radiation produced by energetic sources such as quasars. Using this new version we study whether 21cm experiments could detect the signature of a quasar.

We find that different size measures of ionized regions can distinguish between different source models in the simulations and that a topological measure of the ionized fraction field confirms the inside-out (i.e. overdense regions ionize first) reionization scenario. We find that the HII regions from luminous quasars may be detectable in 21cm, but that it might not be possible to distinguish them from the largest HII regions produced by clustered galaxies.
ENJOY...
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This thesis is based on the following publications, which are referred to in the text by their Roman numerals.


The reprints of this publications can be found at the end of this thesis. My contribution to these publications is as follows:

PAPER I: I performed the analysis presented, produced all the figures and wrote the initial paper draft which was revised by the co-authors and me.

PAPER II: I developed the code-extensions subject to this publication, performed the test simulations presented in the paper (except the cosmological simulation test 3 without helium and the hydrogen only simulation of test 4), produced all figures and wrote the initial draft which was revised by the co-authors and me.

PAPER III: I performed the radiative transfer simulations including helium (i.e. not the hydrogen only simulations), made the analysis presented in Section 3 and in the conclusions. I wrote the first draft of Sections 1-3, the abstract and most of the conclusions. I participated in the discussion and editing but not in the analysis and writing of Sections 4–7. The whole draft was revised by the co-authors and me.

Publications not included in this thesis:

## List of acronyms and abbreviations

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<td>21CMA</td>
<td>21 Centimeter Array</td>
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<td>CDM</td>
<td>flat, cold dark matter model including dark energy</td>
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<td>AGN</td>
<td>active galactic nucleus</td>
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<tr>
<td>bb</td>
<td>big bang</td>
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<td>BB</td>
<td>black body</td>
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<td>BH</td>
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<tr>
<td>CDM</td>
<td>cold dark matter</td>
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<td>CMB</td>
<td>cosmic microwave background radiation</td>
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<td>DM</td>
<td>dark matter</td>
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<tr>
<td>EDGES</td>
<td>Experiment to detect the global Epoch of Reionization signature</td>
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<td>EE</td>
<td>E-mode polarization power spectrum</td>
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<td>EM</td>
<td>electro magnetic radiation</td>
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<td>EoR</td>
<td>Epoch of Reionization</td>
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<td>GMRT</td>
<td>Giant Metrewave Telescope</td>
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<td>GP</td>
<td>Gunn-Peterson</td>
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<td>GRB</td>
<td>gamma ray bursts</td>
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<td>HST</td>
<td>Hubble Space Telescope</td>
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<td>IGM</td>
<td>intergalactic medium</td>
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<td>IMF</td>
<td>initial mass function</td>
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<td>JWST</td>
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<td>OTS</td>
<td>on the spot</td>
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<td>LOFAR</td>
<td>Low Frequency Array</td>
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<td>Acronym</td>
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<tr>
<td>mfp</td>
<td>mean free path</td>
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<td>MWA</td>
<td>Murchison Widefield Array</td>
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<td>PAPER</td>
<td>Precision Array to Probe the Epoch of Reionization</td>
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<td>POP II</td>
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<td>POP III</td>
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<td>PS</td>
<td>power spectrum</td>
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<td>QSO</td>
<td>quasi stellar object</td>
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<td>RJ</td>
<td>Rayleigh-Jeans</td>
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<tr>
<td>SDSS</td>
<td>Sloan Digital Sky Survey</td>
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<tr>
<td>SED</td>
<td>spectral energy distribution</td>
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<td>SKA</td>
<td>Square Kilometre Array</td>
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<tr>
<td>TE</td>
<td>temperature-E-mode cross correlation power spectrum</td>
<td></td>
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<tr>
<td>UV</td>
<td>ultraviolet</td>
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<tr>
<td>WMAP</td>
<td>Wilkinson Microwave Anisotropy Probe</td>
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<tr>
<td>i.e.</td>
<td>id est (Latin: that is)</td>
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<tr>
<td>e.g.</td>
<td>exempli gratia (Latin: For Example)</td>
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<td>l.h.s.</td>
<td>left hand side</td>
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The topic of this thesis is the *Epoch of Reionization* (EoR). More specific, it deals with different aspects of modelling this epoch. Little is known to date about the details of this time interval: After recombination, the universe was neutral and continued to expand, the density perturbations grew to form dark matter (DM) halos, first stars and galaxies formed therein and eventually the intergalactic medium (IGM) became ionized (again). The latter we know from quasar spectra and the polarization power spectrum of the cosmic microwave background radiation (CMB).

Chapter 1 places the EoR into a cosmological context and gives an overview of the current observational constrains on the EoR. It also gives some basic background to the planned 21 cm experiments to which the results of EoR simulations can be hopefully compared in the near future.

In Chapter 2, I illustrate how we are modelling the EoR with simulations. Here I also point out at which stage the three publications which form the basis for this thesis contribute to the process of modelling. Chapter 3 serves as an introduction to the methodology PAPER II that describes the changes made in the radiative transfer code C$^2$RAY. In Chapter 4, I give some useful background and justifications for the quasar model used in the simulations of PAPER III. I give a summary of the papers in Chapter 5.

The results from the appended publications (PAPER I – III) are not repeated in the introductory part of this thesis. However, the last chapter comprises a summary of the appended papers. Some of the figures in PAPER I and PAPER II are originally in colour but appear here in black/white.
INTRODUCTION TO COSMIC REIONIZATION

The *Epoch of Reionization* (EoR) usually refers to the timespan in between the following two events: (1) The formation of the first sources of light forming in the first halos that collapse in a neutral Universe under the influence of self-gravity and decouple from the Hubble expansion. (2) The time when most of the intergalactic hydrogen has become ionized by the ionizing radiation emitted from these sources of light and escaping into the IGM. Very roughly, in terms of the age of the universe since the big bang (bb), this corresponds to 0.1 Gyr (1) and 1 Gyr (2). These times dependent on the definition of the “beginning” and “end” of the EoR and the cosmology.

Before going into more details about this epoch and the observational constrains we have about it, we need to define some cosmological foundations. In this thesis, I assume a flat $\Lambda$ cold dark matter ($\Lambda$CDM) model, $\Lambda$CDM to be the underlying cosmological model. Here, flat indicates that the curvature is 0, $\Lambda$ indicates that the model includes dark energy and cold refers to the non-relativistic speed of the dark matter particles at the time of matter decoupling from radiation.

There are good reasons to trust this so called standard model of cosmology: structure formation simulations based on this model agree well with the observed large scale structure of the universe (e.g. Springel et al. 2005), the anisotropies in the CMB observed with *WMAP*\(^1\) can be explained with this model (e.g. Spergel et al. 2003, 2007; Page et al. 2007; Jarosik et al. 2011; Larson et al. 2011), the acceleration of the expansion of the universe caused by $\Lambda$ is actually observed (Riess et al. 1998; Perlmutter et al. 1999; Perlmutter & Riess 1999)\(^2\) and measurements of the deuterium fraction at redshifts $z \sim 3$ are in agreement with the predicted ones from bb nucleosynthesis (Burles & Tytler 1998a,b).

\(^1\)http://map.gsfc.nasa.gov/
\(^2\)Both Saul Perlmutter and Adam G. Riess together with Brian P. Schmidt received the Nobel Prize in physics 2011 for this discovery.
However, there are also potential problems with the model, for example the missing satellite problem\(^3\) and unsolved questions (e.g. what is the nature of dark matter and dark energy? ). This thesis is not about the underlying cosmology but deals with the transport of ionizing radiation through a matter (dominated) universe evolving by means of a fixed cosmology, the flat, cold dark matter model including dark energy (ΛCDM) cosmology. Therefore, I will not provide an introduction to cosmology but follow a more descriptive approach and explain notations when needed, concentrating on the parameters directly related to the study of the EoR.

1.1 Background and observational constrains

The ΛCDM model is a model whose current day energy content is dominated by some yet unknown form of energy Λ. In the model, Λ contributes roughly 70\% to the total energy content in the universe today. In the following, the energy content will be given in units of the critical density \(\rho_{c,0}\) (where the subscript 0 indicates here and henceforth, time \(t = \text{today}\)), which in a flat universe model is equal the total energy content. So we write \(\Omega_\Lambda \approx 0.7\). In analogy, \(\Omega_m\) and \(\Omega_b\) are the total and baryonic mass contents of the universe, respectively. The currently best estimates are \((\Omega_\Lambda, \Omega_m, \Omega_b) = (0.728, 0.272, 0.0455)\) (Komatsu et al. 2011).\(^4\) Although these values are only valid at \(t = \text{today}\), we skip the subscript 0.

The ΛCDM model is a model in which the universe emerges from a singularity and has been expanding since a bb model. The most direct evidences\(^5\) for a bb are Hubble expansion diagrams that locally (i.e. for a small redshift \(z\)) show a linear relation between the distance \(d\) of objects and their recession speed \(v\) (e.g. Hubble 1929; Freedman et al. 2001; Freedman & Madore 2010). However, due to the rather large uncertainties connected to the distance measurements, current estimates of the Hubble parameter \(H_0 = v/d\) using this method have rather large errors (Freedman & Madore 2010, give \(H_0 = 73 \pm \text{random } 2 \pm \text{systematics } 4 \text{ km s}^{-1} \text{ Mpc}^{-1}\)). In general, \(H\) is not a constant,

\(^3\)According to numerical ΛCDM, DM only, simulations, there should be many more dwarf galaxies than are observed (e.g. Moore et al. 1999; Klypin et al. 1999), which might or might not be explained by including detailed gas and radiation physics in the simulations.

\(^4\)The values given above are the maximum likelihood values from considering WMAP and baryonic acoustic osczillations. The mean and 1\(\sigma\) errors are \((\Omega_\Lambda, \Omega_m h^2, \Omega_b) = (0.725 \pm 0.016, 0.1352 \pm 0.0036, 0.0458 \pm 0.0016)\), here \(h\) is the hubble parameter in units of 100 km/s/Mpc, see below and \(h = 0.702 \pm 0.014\).

\(^5\)however not a proof since other models are not excluded by this.
and defined as the ratio of the rate of change of the scale factor \( \dot{a} \) over the scale factor \( a \) where the scale factor today \( a_0 \) is define as 1. This relationship makes it possible to use the Doppler shift of photons emitted from a source at a certain distance as a measure of distance, named the redshift

\[
\lambda = \frac{\lambda_{\text{observed}} - \lambda_{\text{emitted}}}{\lambda_{\text{emitted}}}
\]

Since the speed of light is finite, redshift also serves as a measure of look-back time.

A more accurate estimate of \( H_0 \) (or \( h := H_0/[100 \text{ km s}^{-1} \text{Mpc}^{-1}] \), which I will use from now on for convenience) can be derived from the six primary \( \Lambda \)CDM model parameters (for details, see any of the references following in this paragraph) fitted to the different statistics of the measurements of the anisotropies of the CMB. The best estimate today is \( h = 0.702 \pm 0.014 \) (Komatsu et al. 2011). The bare existence of the CMB is another evidence for a bb: it emerges from the time when the temperature of the universe cooled down to a value where the number of photons energetic enough to ionize hydrogen fell short of the number of protons. This process of (re-)combination is not an instantaneous change but occurred during a finite redshift interval (\( \Delta z \) about several hundreds) and ended at \( z \sim 1100 \) when the temperature was roughly 3000 K. The matter inhomogeneities present at that time can be observed today in the temperature fluctuations (due to gravitational redshift from this time of last scattering, Sachs & Wolfe 1967) in the CMB. However, fluctuations on scales smaller than the scales corresponding to \( \Delta z \) are suppressed due to the finite width of the last scattering. Thanks to the accurate measurements of temperature and polarization anisotropies of the CMB (Spergel et al. 2003, 2007; Page et al. 2007; Jarosik et al. 2011; Larson et al. 2011) and their statistics, there is not only qualitative confirmation of the \( \Lambda \)CDM model, but the model parameters can be fitted to great accuracy (Komatsu et al. 2011).

One of the model parameters that are directly fitted to the CMB data is the so called reionization optical depth

\[
\tau = c \sigma_T \int_0^{t(z_{\text{rec}})} n_e(z(t)) dt.
\]

Here, \( c = 2.998 \times 10^8 \text{ m/s} \) is the speed of light, \( \sigma_T = 6.65 \times 10^{-29} \text{ m}^2 \) is the Thomson scattering cross-section and \( n_e(z(t)) \) is the mean number density of free electrons at redshift \( z \) (e.g. Page et al. 2007). This parameter is derived

\[6\] As well known, given the different energy contents of the universe, the first Friedman equation describes the change of scale factor:

\[
\left( \frac{\dot{a}(t)}{a(t)} \right)^2 = \frac{8\pi G \rho_{\text{matter}}}{3a(t)^2} + \frac{8\pi G \rho_{\text{rad}}}{3a(t)^4} + \frac{\Lambda c^2}{3}.
\]

Here, the curvature term is omitted since in the standard model \( k = 0 \). It should be noted that in most representations, the radiation energy content is omitted due to the fact that it becomes negligible for \( z \gg 3400 \).
primarily from the E-mode polarization power spectrum (EE)\textsuperscript{7}: The scattering off of photons of free electrons at redshift \( z \) introduces additional polarization at the scale of horizon at \( z \), so a bump at low multipole moments \( l \) (for not too small \( l \), \( l = \pi/\theta \), where \( \theta \) is the angular scale) in the EE power spectrum is the result. In theory, from the shape of the bump, more information than just an integrated optical depth can be extracted. However, the measurement errors are too large wherefore the power spectrum is integrated over a range of \( l \) values, see Larson et al. (2011). The currently best estimate for the optical depth is \( \tau = 0.088 \pm 0.014 \) (Komatsu et al. 2011). Assuming an instantaneous reionization (\( \text{HI} \rightarrow \text{HII} \) and \( \text{HeI} \rightarrow \text{HeII} \)) and assuming helium became doubly ionized at \( z \sim 3.5 \), this results in an ionization redshift of \( z_{\text{reion}} = 10.5 \pm 1.2 \) (Komatsu et al. 2011; Larson et al. 2011). The inclusion of electrons from \( \text{HeII} \rightarrow \text{HeIII} \) ionization is a new feature in the code used to make model fits, CAMB (Lewis et al. 2000; Lewis 2008), this resulted in slightly lower \( z_{\text{reion}} \) for the WMAP\textsuperscript{7} results than those published for the WMAP5 results (Spergel et al. 2007; Page et al. 2007).

To summarize EoR results from the CMB: By statistics of the CMB measurements, one can acquire information about the time-integrated electron density and therefore, assuming an instantaneous reionization, a redshift of reionization \( z_{\text{reion}} \). The rather large change in the best fit for \( \tau \) from WMAP1 to WMAP3 is partly due to a change in strategy (using mainly the EE power spectrum instead of the TE power spectrum). The change in best fit \( z_{\text{reion}} \) between WMAP5 and WMAP7 are mainly due to the inclusion of helium ionization electrons. Therefore, sceptics arguing that WMAP results have not been consistent through the years regarding the EoR do not have a strong point.

The CMB results constitute one of two main constraints for the EoR available today. The other comes from spectra of high redshift quasars. Gunn & Peterson (1965) found the Ly\( \alpha \) line of a quasar at \( z \sim 2.01 \) to show “no obvious asymmetry” and a maximum depression on the blue side of the line, of 40\%. They converted this into a number density for neutral hydrogen of \( 6 \times 10^{-11} \text{ cm}^{-3} \) in proper (i.e. not comoving) physical units at that redshift. This meant either that the total mass density of hydrogen is much smaller than expected or that the IGM at those redshifts must be very highly ionized. They ruled out a collisionally ionized IGM since the timescales (collisional ionization time scale and necessary ionization time scale) do not match for realistic IGM temperatures (which should not violate the X-ray background from free-free emission). They also ruled out quasi stellar object (QSO) and normal galax-

\textsuperscript{7}As Spergel et al. (2007) mention, the Wilkinson Microwave Anisotropy Probe (WMAP) 1st year results were mainly based on the temperature-E-mode cross correlation power spectrum (TE) and \( \tau \) was degenerate with the power law spectral index of primordial density fluctuations \( n_s \), where the likelihood for \( \tau \) varied over a large range [0.05 – 0.3] only slightly, which resulted in a rather high value for \( \tau \) as the best fit parameter
ies as sources of reionization. Their best bet was black body (BB) radiation from the IGM itself, assuming a temperature of $T_{\text{IGM}} \sim 2.5 \times 10^5$ K. While the latter is excluded today, the question of the main sources of reionization still remains.

As time went by, QSO spectra at higher and higher redshifts were taken and the spectra blueward of the Ly$\alpha$ emission line were examined for the existence of complete absorption, called the Gunn-Peterson (GP) trough, expected from a moderately neutral IGM, as shown by Gunn & Peterson (1965). The spectra of QSOs around redshift 6 found in the Sloan Digital Sky Survey (SDSS)$^8$ were the first to indicate a low, but rapidly rising neutral fraction (Fan et al. 2006; Willott et al. 2007), see Fig.1.1 for a reproduction of a plot showing the calculated effective GP optical depth $\tau_{\text{eff}}$. This suggests that the EoR ended around a redshift $z \sim 6$.

There are other observations which set more indirect limits on the EoR, such as the measurement of the ultraviolet (UV) background photoionization rate $\Gamma$ from $2 \leq z \leq 6$ (see for example Faucher-Giguère et al. 2009., who confirm by integrating the luminosity functions of galaxies and quasars the values measured by HI Ly$\alpha$ forest$^{10}$ data of $\Gamma \sim (5-10) \times 10^{-13}$ /s/neutral atom) or direct observations of high redshift galaxies constraining the luminosity function at high redshifts. The problem with the former is that the UV background is observed at a time where reionization is (almost) completed and therefore the information on the sources that ionized the universe some redshift units earlier, is not clear. The problem with the latter is that only the brightest galaxies can be observed at redshifts relevant for reionization. Those galaxies are very rare and most likely not the main contributor to cosmic reionization. However, gravitational lensing might help, as Hall et al. (2011) point out: as is well known, the area probed by gravitational lensing decreases with increasing magnification. This means that the probed area in space decreases with the minimum intrinsic luminosity of background galaxies to be still observable. (Galaxies with lower intrinsic luminosity need to be magnified more and therefore, the area of investigation is smaller) However, the luminosity function, which describes the number of galaxies in a certain volume of space as a function of luminosity, is believed to be very steep at the faint end and therefore the number of small galaxies increases rapidly with decreasing intrinsic luminosity. Hall et al. (2011) found that the probed area (as function of

$^8$http://www.sdss.org/

$^9$Fan et al. (2006) define the effective GP optical depth as the natural logarithm of the average of the ratio observed flux over intrinsic flux, $\tau_{\text{eff}} = \ln\left(\frac{f_{\text{obs}}}{f_{\text{int}}}\right)$.

$^{10}$The Ly$\alpha$ forest is the part in a spectrum of a distant quasar/galaxy (bluewards of its Ly$\alpha$ emission line) where many thin absorption lines, originating from neutral hydrogen clouds in the IGM between us and the quasar/galaxy, are visible.
Figure 1.1: Reproduction of figure 4 from Goto et al. (2011) by permission of John Wiley and Sons (original in colour). Effective GP optical depth $\tau_{\text{eff}}$ from several high redshift quasars. The limits from the spectrum of CFHQS J2329-0301, a $z=6.4$ quasar are from Ly$\alpha$, Ly$\beta$ and Ly$\gamma$, as indicated in the legend, the black triangles are from Fan et al. (2006) and the small squares are from Songaila (2004). The solid line is the best power-law fit to the data at $z < 5.5$ by Fan et al. (2006) $\tau_{\text{eff}} = 0.85 ((1 + z)/5)^{4.3}$ (their equation 5) including more low-redshift quasars from Songaila (2004). The lower limits on the effective optical depth come from no-flux-detections.

magnification and hence minimum intrinsic luminosity) decreases slower than the expected number of galaxies with a certain minimum luminosity. Therefore, number counts should still be possible. Measurements of the soft X-ray background can be used to limit the contribution from quasars to the EoR (Dijkstra et al. 2004, 2011).

1.2 Future observations

Although there are other promising future observations such as new constrains on the anisotropies in the CMB from Planck\textsuperscript{11} (smaller errors on $\tau$, see e.g. Zaldarriaga et al. 2009), probing intergalactic Ly$\alpha$ absorption with gamma ray bursts (GRB) afterglow spectra or observing Ly$\alpha$ emitters during the EoR (see

\textsuperscript{11}This is not an acronym, it is named after Max Planck. www.rssd.esa.int/planck/
for example Dijkstra 2010) with the James Webb Space Telescope (JWST)\textsuperscript{12}, I concentrate in this section on the future 21cm observations. See McQuinn (2010) for a more detailed overview of current and future observational constrains.

A complementary probe of the state of the IGM can be obtained by observing neutral hydrogen directly via the hyperfine structure line of ground state neutral hydrogen at a wavelength of $\lambda_{21} = 21$ cm ($v_{21} = 1.45$ GHz). This corresponds to an energy difference between the two states (parallel and anti-parallel spins of the electron and the proton, where the parallel state is more energetic) of $\Delta E = 5.9 \times 10^{-6}$ eV or in terms of a temperature $T_e = \Delta E/k_B = 0.068$ K (see e.g. Furlanetto et al. 2006; Pritchard & Loeb 2011, for reviews on physics of and with the 21cm line), where $k_B = 1.38 \times 10^{-23}$ m$^2$ kg s$^{-2}$K$^{-1}$ is the Boltzmann constant. Although this spin-flip has a very low transition probability (for a single atom, spontaneous emission occurs about once every 10 Myr), it can be observed because hydrogen is so abundant in the universe. In thermal equilibrium, Kirchhoff’s law applies and there is a fixed relation between absorption and emission coefficients dependent on the temperature of the emitting/absorbing medium and the frequency, see e.g. Spitzer (1978). Since the wavelength of the peak of the BB radiation (today at 1.9 mm, but smaller by $(1 + z)^{-1}$ at higher redshifts) is much smaller than the wavelength of the spin-flip line, the Planck law for the radiation field intensity of the CMB (and the BB of the emitting/absorbing medium) can be approximated by the low energy Rayleigh-Jeans (RJ) limit, $I_v = 2v^2k_B T/c^2$. This is used to convert all intensities into temperatures and the resulting brightness temperature $T_B$ of the 21cm radiation is then

$$T_B = T_{CMB} e^{-\tau} + T_S (1 - e^{-\tau}) \quad (1.1)$$

Here, $T_S$ is the equivalent temperature of the emitting/absorbing medium (at that frequency) and $\tau$ the optical depth at the frequency in question. What is measured by a (single-dish) radio telescope is the differential brightness temperature\textsuperscript{13}. For a given frequency (for a specific line this corresponds to a certain redshift), this is

$$\delta T_B := \frac{T_B - T_{CMB}}{1+z} = \frac{T_S(1 - e^{-\tau}) + T_{CMB} e^{-\tau} - T_{CMB}}{(1+z)} \approx \frac{T_S - T_{CMB}}{1+z} \tau. \quad (1.2)$$

\textsuperscript{12}http://www.jwst.nasa.gov/

\textsuperscript{13}Interferometers miss an absolute scaling and measure therefore the fluctuations against a background radiation $\delta T$. In PAPER III, we subtracted the mean of $\delta T$ to simulate this effect. The background radiation for the IGM is the CMB

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CHAPTER 1. INTRODUCTION TO COSMIC REIONIZATION

The approximation made in the last step is valid for small $\tau$. This is a very good assumption for the 21cm radiation.

For the 21cm line of neutral hydrogen, $T_S$ is defined through the ratio of the number of atoms in excited state $N_1$ over ground state $N_0$ which is given by the Boltzmann equation $N_1/N_0 = 3e^{-T_*/T_S}$ (3 is the ratio of the statistical weights between the excited triplet state and the singlet ground state). Since $T_*$ is so small, the ratio of excited states over ground state is almost independent of $T_S$ and equals 3. This is used below to obtain the factor $1/4$ (one out of 4 hydrogen atoms is in the ground state and contributes to the optical depth).

Since $h\nu \ll k_B T_S$, the optical depth can be expressed as

$$\tau(\nu) = \frac{N_{\text{HI}}}{4} \frac{h\nu}{c} B_{jk} \frac{h\nu}{kT_S} \phi(\nu)$$

(Spitzer 1978). To relate the absorption coefficient $B_{jk}$ to the spontaneous emission coefficient $A_{kj}$, thermodynamic equilibrium can be assumed to yield $B_{jk} = 3\frac{c^3}{8\pi h\nu^4} A_{kj}$. $N_{\text{HI}}$ is the column density of neutral hydrogen and $\phi(\nu)$ is the line shape. In the cosmological context (Furlanetto et al. 2006) one can approximate $\phi N_{\text{HI}}(z)$ by $(cn_{\text{HI}})/(H(z)\nu)^{14}$. In a matter dominated universe ($3400 \gg z \gg 0.3$), $H(z) = H_0\sqrt{\Omega_m (1+z)^{3/2}}$ and therefore (using the definition of $T_*$)

$$\tau(\nu) = \frac{n_{\text{HI}}(z)}{H_0\sqrt{\Omega_{m,0}}} \frac{3\lambda_{21} T_*}{32\pi T_S} (1+z)^{-3/2} A_{kj}$$

Whether this line is measured in absorption ($\delta T_B$ negative) or in (stimulated) emission ($\delta T_B$ positive), depends on the spin temperature $T_S$ and the temperature of the cosmic microwave background $T_{\text{CMB}}$. In the redshift range interesting for reionization, the spin temperature is believed to be coupled to the gas temperature $T_g$ by Ly$\alpha$ coupling through the so called Wouthuysen-Field effect (e.g. Wouthuysen 1952; Field 1959; Furlanetto et al. 2006) or in very high density regions also through collisions. Therefore, it depends on the temperature of the gas if the line is seen in absorption or emission. However, in case the coupling processes (Wouthuysen-Field effect and collisional coupling) are not sufficient, the spin temperature would be radiationally coupled to the CMB and the neutral hydrogen would not be observable.

Taking Eq.1.2 and Eq.1.4 together, the differential brightness temperature can be expressed as

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14Here we neglect the peculiar velocity contribution.
\[ \delta T_b = \frac{T_S - T_{\text{CMB}}}{T_S} \approx \frac{3 \lambda_0^3 A_{10} T_*}{32 \pi H_0 \sqrt{\Omega_m}} (1 + z)^{-5/2} n_{HI}(z) \]  \hspace{1cm} (1.5)

Under the assumptions that the spin temperature is coupled to the gas temperature and not to the CMB temperature and that the gas temperature is much larger than the spin temperature, the first factor in Eq.1.5 is 1. The second factor is a constant which can be evaluated to approximately \( \mathcal{K} = 4.6 \times 10^4 \) K cm\(^3\). Further, considering the comoving density \( n_{\text{comoving}} = n_{\text{physical}}/(1 + z)^3 \) instead of the physical density, Eq.1.5 reads

\[ \delta T_b = \mathcal{K} n_{HI}(z, \text{comoving}) \sqrt{z + 1} \]  \hspace{1cm} (1.6)

This approximation was used in PAPER III to convert the ionization fraction and density fields into a differential brightness temperature field\(^{15}\). However, we note that the signal could be much stronger if the gas would be cooler than the CMB temperature, since the first term in Eq.1.5 could then reach large negative values with absolute values much larger than 1.

Given the above constrains on the redshift range on reionization from WMAP measurements and QSO spectra, the interesting frequency range for observing this transition is roughly \( v = v_{21} \times \left[ \frac{1}{(1 + 6)} - 1/(1 + 14) \right] \approx [200-100] \) MHz (which corresponds roughly to \( \lambda = 1.5 - 3 \) m). Existing and future radio telescopes capable of measuring at such low frequencies (Giant Metrewave Telescope (GMRT)\(^{16}\), 21 Centimeter Array (21CMA)\(^{17}\), Low Frequency Array (LOFAR)\(^{18}\), Murchison Widefield Array (MWA)\(^{19}\), Precision Array to Probe the Epoch of Reionization (PAPER)\(^{20}\) Square Kilometre Array (SKA)\(^{21}\)) should be able to detect the signal of the neutral hydrogen during the EoR. Luckily, the atmosphere is transparent for electromagnetic radiation (EM) of wavelength between several cm to tens of meters (radio window). However, at these frequencies, the contribution from galactic and extragalactic foregrounds (e.g. radio galaxies) is much stronger than the signal from the EoR itself. Therefore, a careful modelling of the foregrounds is needed in order to extract the signal (e.g. Jelic 2010). Since we are dealing

\(^{15}\)We are aware that some groups (e.g. Baek et al. 2010) follow the heating and inclusion of X-rays and find non global heating. However, we note that they lack low mass sources.
\(^{16}\)http://gmrt.ncra.tifr.res.in
\(^{17}\)http://21cma.bao.ac.cn
\(^{18}\)http://www.lofar.org
\(^{19}\)Murchison Widefield Array, http://www.mwatelescope.org
\(^{20}\)http://astro.berkeley.edu/~dbacker/eor
\(^{21}\)http://www.skatelescope.org/
with line radiation, one could in theory map the spatial time-dependent
distribution of neutral hydrogen in the Universe, but the line of sight direction
and time-information are mixed. Such measurements would require a higher
sensitivity than can be achieved with e.g. LOFAR. Instead, what will be
measured first are power spectra.

Two such experiments using the 21cm line already gave first results: Bow-
man & Rogers (2010) used a broadband radio spectrometer, *Experiment to
detect the global Epoch of Reionization signature* (EDGES) (Rogers & Bow-
man 2008; Bowman et al. 2008) designed to measure the global signal in
the above mentioned frequency range. They did not detect any signature that
would be introduced (an edge) by a rapid reionization, they were able to set a
lower limit on the duration of reionization of \( \Delta z > 0.06 \). Paciga et al. (2011)
use the GMRT to constrain the morphology of the ionized fraction for the
case of a cold IGM\(^{22}\) at \( z \sim 8 - 9 \) by a non detection of features in the power
spectrum (PS) of 21cm radiation.

\(^{22}\)as mentioned above, the absorption signal can be much higher than the emission signal
In this section I describe a generic way of modelling the EoR numerically. There are other approaches, such as semi-numerical modelling (e.g. Mesinger & Furlanetto 2007; Santos et al. 2010), on which I will not expand here. Instead, I concentrate on the path we took in the publications this thesis is based on. A pictorial description of this path is given in Fig. 2.1. While describing, I will refer to the individual steps by the Latin upper case letters as indicated in that figure.

We start by performing large scale cosmological DM only simulations (A). For this, we use the CUBE³M code (Particle-Particle, P-Mesh) (see Iliev et al. 2008, for a short description of the code) which was developed from the
CHAPTER 2. MODELLING THE EOR

PMFAST (Particle-Mesh) code (Merz et al. 2005). This particle distribution representing the density field, say, at time $t_1$, is used to extract halos at that time $t_1$ (B). The particle data is converted into a density field on a grid by smoothing the DM particle distribution using a kernel and integrating in each cell of the grid the parts of the kernel that intersect with it. In fact, what I show in (A) is already the density field on the grid. However, the halos are extracted from the particle data. We assume the gas to follow closely the DM density distribution and we assume a constant DM/baryonic matter fraction everywhere. For the scales of interest, this is a good approximation\textsuperscript{23}. So, after (A) and (B) we have the gas density fields and halo lists at times $t_i$.  

Next, we need to illuminate the halos (C). In the simulations of PAPER I, this is solely done by assuming stellar sources: We assume some fraction of the gas in each halo is being converted into stars (a star formation efficiency). Multiplied with the total baryonic halo mass, this gives a total stellar mass (or number of baryons in stars) in the halo. Next, we set the number of ionizing photons produced per baryon in a star. For a single star, this depends on two things: How effective is the nuclear fusion to convert rest-mass energy into EM energy (about 0.7\% of the rest mass energy)? And: How much of this EM energy is in form of photons more energetic than 13.6 eV? The latter depends on the spectrum, that is, on the effective temperature of the star and therefore on the mass of the star. The former depends on the details of the nuclear reactions and the amount of energy carried away by neutrinos. Both are connected to the metallicity. For galaxies, Iliiev et al. (2005) give the following numbers: Adopting a Salpeter initial mass function (IMF) and Population II (POP II) stars\textsuperscript{24}, yields around 3000 ionizing photons/stellar baryon and for POP III stars (first stars, no metals, massive and hot) values above 25000 would be appropriate. Of course, this has to be seen as an average over the population lifetime, approximately 10 Myr.\textsuperscript{25} Some groups working in the

\textsuperscript{23}During reionization, where the ionization fronts move supersonically through the IGM, the mechanical feedback to the gas by pressure forces can be neglected (Shapiro & Giroux 1987). Therefore, doing the radiative transfer (RT) as post-processing on the N-body density field is a valid approximation.

\textsuperscript{24}Low metallicity stars, less massive than Population III (POP III). Today, the only remainings of this population of stars are the lightest long-lived ones in the population. Therefore, POP II stars today are older, lower luminosity stars, typically found in the nucleus of galaxies. However, if I refer to POP II stars this is to indicate that they are not metal free and not extremely massive.

\textsuperscript{25}Sparke & Gallagher (2007) give as an estimate for stellar lifetimes $\tau_l$ as function of their mass $\tau_l \sim 10^{10} \left( \frac{M}{M_\odot} \right)^{-2.5}$ yr, so a 15 $M_\odot$ corresponds to a lifetime of roughly 10 Myr. The effective temperature of such a star is about 30000 K. Sternberg et al. (2003) give for such a star an ionizing photon output $Q_H \sim 10^{48}$s$^{-1}$ which translates into roughly 10000 ionizing photons per 10 Myr per baryon.
field include a chemical enrichment model and therefore have time-dependent photons/stellar-baryon rates (e.g. Trac & Cen 2007).

Not all the produced photons escape from the galaxy into the IGM. To take this into account, one introduces an escape fraction. In principle, this escape fraction can be dependent both on the direction and on the source distribution and density distribution inside the galaxy (see for example galaxy sized (semi-) numerical studies of Ciardi et al. 2002; Fujita et al. 2003). It may also be redshift dependent and differ for galaxies of different mass (see Razoumov & Sommer-Larsen 2006; Gnedin et al. 2008, for large scale cosmological numerical studies that investigate among other things the dependence of the escape fraction on galaxy-mass). Observational estimates of the escape fraction of lower redshift galaxies give mostly upper limits due to non detections (e.g. Deharveng et al. 2001; Leitherer et al. 1995; Malkan et al. 2003), but Bergvall et al. (2006) reported a detection and estimate the escape fraction to be around 4 – 10 %. Since this thesis is not about escape fractions, I will not expand on this but note that the escape fraction is a rather unconstrained parameter.

By including the escape fraction, we already account for the ionization of the gas in the galaxy. Therefore we subtract it from the density field before doing the radiative transfer. For reasonable values of (1) the star formation efficiency (2) the number of ionizing photons produced per stellar baryon (3) the escape fraction, the resulting conversion factor between halo mass and emitted ionizing photons in 10 Myr is some tens to hundreds of photons per halo baryon. These three ingredients are degenerate for reionization and the only important number for our simulations is the product of these, not the individual multiplicands. This is quantified in PAPER I\textsuperscript{26}. In Section 4, I outline the line of thinking for converting halo mass into quasar luminosity, this is quantified in PAPER III.

In the next step (D), we transfer the ionizing radiation through the IGM until the next \( t_i \) (next N-body/source list output). How we do the radiative transfer is outlined in Section 3 and described in Mellema et al. (2006) and PAPER II. Here, one has the possibility of including sub-grid physics, for example, one can introduce a clumping factor, \( C \) which will affect the recombinations: the recombination rate depends on the square of the number density, \( n^2 \). However, the density value in the cell is in fact an average over the cell. Therefore, the recombination in the cell is calculated on the basis of the square of the average density, \( \langle n \rangle^2 \). If the density varies much on scales smaller than the cell, the recombination varies much, and its average in the cell would be proportional to

\textsuperscript{26}Note however that Eq.1 in PAPER I contains an error and an inconsistency in the naming: The mean molecular weight in the denominator should not be there since we are considering total number of baryons. \( \Omega_0 \) should really be named \( \Omega_m \), the total current mass content in units of critical density. See PAPER II, Eq. 21 for the correct equation.
the average of the squares of the density, $\langle n^2 \rangle$. To correct for this, one can include a factor $C = \langle n^2 \rangle / \langle n \rangle^2$ in the recombination (and collisional ionization) calculations. $C$ as a function of density can be fitted to the N-body simulation and can be included in the RT simulation. However, this clumping is based on the dark matter density field since the underlying N-body simulations are dark matter only. Due to the heating of the gas, the gas clumping is expected to be smaller than the clumping of dark matter and therefore, the gas recombination is expected to be somewhere between the cases without inclusion of a clumping factor and the cases with including a clumping factor based on the N-body results. McQuinn et al. (2007) investigate several different clumping models and find that the effect on the large scale structure of H II regions is small but that it adds small scale structure at the edges of H II regions.

The result of such a simulation (A-D) is a time dependent ionization fraction field (E) which can be statistically analysed (G), as we did in PAPER I to test the effect of different source models (C). However, the important quantity related to observations is actually not the ionization fraction but the neutral density. Therefore, we multiply the neutral fraction of each cell (i.e. 1-ionization fraction) with the density of each cell (at each time $t_i$) to receive the neutral density field (F). This can be transformed into a differential brightness temperature (assuming a global heating) as outlined at the end of Section 1.2 which in theory is measurable at the interesting redshifts. In PAPER III, we present the prospects of detecting quasar H II regions in redshifted 21cm maps by using a method developed by Datta et al. (2007) and Datta et al. (2008) (H).

It should be mentioned that in all practical cases we have been studying, the mean free path for the vast majority of the photons is smaller than the light-travel distance during one timestep. Therefore, we do not need to deal with remaining photons in timestep $i + 1$ that were not absorbed in timestep $i$. 

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The equation of radiative transfer in an expanding universe in comoving coordinates is (e.g. Norman et al. 1998; Abel et al. 1999; Gnedin & Abel 2001)

\[
\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \frac{n \cdot \nabla I_\nu}{\bar{a}} - \frac{H(t)}{c} \left( \nu \frac{\partial I_\nu}{\partial \nu} - 3I_\nu \right) = j_\nu - \kappa_\nu I_\nu,
\]

(3.1)

where \(I_\nu\) is the specific intensity at frequency \(\nu\), \(n\) is the unit vector in the direction of light ray propagation, \(H(t) = \dot{a}(t)/a(t)\) is the Hubble constant at time \(t\), \(c\) is the speed of light, \(\bar{a} = \frac{1+z_{\text{em}}}{1+z(t)}\) is the ratio of cosmic scale factors at emission and present time \(t\), \(j_\nu\) is the emission coefficient and \(\kappa_\nu\) is the absorption coefficient.

Norman et al. (1998) show that in the case of local sources, i.e. the mean free path (mfp) of photons, \(\lambda_{\text{mfp}}\), is small against the simulation box scale \(L\) (the scale of interest), and if \(L\) is small against the horizon scale, \(c/H(t)\), the third term on the l.h.s. of Eq. 3.1 is negligible\(^{27}\). This means that the cosmological redshift of the photons between emission and absorption and the dilution due to the expansion of the universe is negligible.

Furthermore, since \(z_{\text{em}} = z(t + \lambda_{\text{mfp}}/c) \sim z(t)\), \(^{28}\) it follows that \(\bar{a} \sim 1\). This implies that the change of path length along a ray due to cosmic expansion is negligible. Consequently Eq. 3.1 reduces to the classical transfer equation (e.g. Peraiah 2001)

\[
\frac{1}{c} \frac{\partial I_\nu}{\partial t} + n \cdot \nabla I_\nu = j_\nu - \kappa_\nu I_\nu.
\]

(3.2)

\(^{27}\)However, as Abel et al. (1999) point out, this is strictly only valid if the radiation has a rather smooth spectrum, see there for details on fixes for line radiation.

\(^{28}\)For very high energetic photons, this might not hold since \(\lambda_{\text{mfp}}\) can be very large, Furlanetto (2009) give the comoving mean free path of X-rays with energy \(E\) as \(\lambda_{\text{mfp}} = 4.9 \langle x_{\text{HI}} \rangle^{-1/3} ((1+z)/15)^{-2}(E/300\text{eV})^{3/2}\) Mpc. However, we currently do not follow photons for distances longer than the simulation box size \(L\). Also, as noted at the end of Chapter 2, long mean free paths might force to implement explicitly the limited speed of light which in turn means that not absorbed photons have to be stored with their current position. This is not implemented in the code at the moment.
In a further approximation one neglects the time dependence in the absorption and emission coefficients, which is equivalent to assuming that the light travel time through the box is much shorter than the time scale on which the absorption and emission coefficients change. This reduces the equation to:

\[ \mathbf{n} \cdot \nabla I_\nu = j_\nu - \kappa_\nu I_\nu \] (3.3)

A common way of reducing the dimensionality of the equation further is to separate the anisotropic (local point sources) from the isotropic (diffuse radiation due to recombination) contribution of \( I_\nu = I_{\nu{\text{diff}}} + I_{\nu{\text{ps}}} \). This results in two equations that are coupled to each other via the absorption coefficient \( \kappa_\nu \), (see e.g. Abel et al. 1999, for details).

Since we assume that \( \lambda_{\text{mfp}} \) is small, we ignore the contribution from sources outside the box. Furthermore, we treat the diffuse photons from recombinations in an on-the-spot (OTS, see below) manner and incorporate their effect on \( \kappa_\nu \) in this way in the equation for the local point sources. Therefore, we are only left with one equation. In one dimension (i.e. in the spherically symmetric case) it can be written as (dropping the super-script \( \text{ps} \) and the subscript \( \nu \))

\[ \frac{\partial I}{\partial r}(r) = -\kappa(r)I(r) \] (3.4)

A formal solution to Eq. 3.4 is then

\[ I(r) = I_0 \exp \left( -\int_0^r \kappa(s) ds \right), \] (3.5)

where \( I_0 \) is the intrinsic intensity of the source assuming a point source such that \( L = 4\pi I_0 \). Introducing as usual the optical depth as the integral, \( \tau(r) = \int_0^r \kappa(s) ds \), gives

\[ I(r) = I_0 \exp (-\tau(r)) \] (3.6)

For ionizing radiation, \( \tau \) (at each frequency \( \nu \)) is given by the sum of the products of the column densities \( N_i \) and ionization cross section \( \sigma_i(\nu) \) of species \( i \): \( \tau(\nu) = \sum_i N_i \sigma_i(\nu) \). \( I(r) \) can be related to the flux \( F(r) \) going through a unit surface at distance \( r \) by \( F = I/r^2 \) (assuming a point like emission source). Instead of evaluating the flux, in the case of ionizing radiation, one is interested in the ionization rate which can be locally written as (e.g. Osterbrock 1989)

\[ \Gamma(r) = \frac{1}{4\pi r^2} \int_\nu L(\nu)\sigma(\nu)e^{-\tau(\nu,r)} \frac{e^{-\tau(\nu,r)} \nu}{h\nu} d\nu. \] (3.7)

This ionization rate alters the ionization fraction at any instance in space and changes therefore the column density and therefore the optical depth. How
to solve simultaneously for the ionization rate and the ionization fraction is explained in the next section.

3.1 Solving radiative transfer in one dimension

Mellema et al. (2006) described how to solve the ionizing radiation transport problem (i.e. to solve Eq. 3.4 combined with the change of $\kappa$ due to photoionisation) in a photon conserving fashion. In the following, I will sketch the basic ideas since it is this code that I extended to include helium (see PAPER II). For details on the original $C^2R$AY code, I refer the reader to Mellema et al. (2006). For details on the inclusion of helium, I refer the reader to PAPER II. This section serves solely as a conceptual introduction.

The basic idea of $C^2R$AY is to equal the number of ionizations in a given cell to the number of absorptions in that cell. The latter is given by the difference between photons entering the cell and photons leaving the cell per unit time. The number of photons entering the cell per unit time is dependent on the optical depth $\tau_{in}$ to the cell. The number of photons leaving the cell is a function of this $\tau_{in}$ and the optical depth over the cell $\Delta \tau$. The $\Delta \tau$ changes due to the effect of ionizing radiation (assuming that the incoming ionizing radiation/ optical depth has been solved for already). The iteration procedure can be schematically represented as in Fig. 3.1.

\[ \Gamma_{in} (\tau_{in}) \]
\[ n^i = n \]
\[ \Delta \tau^i = n^i \Delta x \sigma \]
\[ n^{i+1} = \frac{n - (\Gamma_{in} - \Gamma_{out}^i)}{\Delta x^3} \]
\[ n^{i+2} = \frac{n - (\Gamma_{in} - \Gamma_{out}^{i+1})}{\Delta x^3} \]

Figure 3.1: Schematic iteration for finding the photon conserving outgoing ionization rate and optical depth of a single cell $\Delta \tau$. The index $i$ counts the iteration. $n$ without any index is the neutral number density from the last timestep. $\Gamma_{in(out)}$ is the ingoing (outgoing) photoionisation rate.
In any practical application, time and space are discretised in finite timesteps $\Delta t$ and widths of cells $\Delta x$. These discretisations introduce two problems: (a) During one timestep, the neutral fraction in a given cell can change substantially (with respect to time). (b) the optical depth over a cell can vary substantially because the neutral fraction can vary substantially within a cell (with respect to space) and because of the intrinsic dependence of $\tau$ on the path length. Since we are only interested in the ionization rate that comes out of the cell, (b) is not a problem since any algorithm following the sketch above would give immediately a spatial average of the neutral fraction and therefore a correct $\Delta \tau$ for the cell. Analogously, (a) is not a problem (we are only interested in the ionization rate at the end of the timestep) if we use a time averaged neutral fraction in the cell to calculate the outgoing optical depth.

Assuming a constant electron density, and knowing the ionizing flux, the set of rate equations for the hydrogen only case can be represented as in Fig. 3.2. These are ordinary linear differential equations that can be solved analytically. Therefore, a time averaged fraction over a timestep can be calculated easily.

Figure 3.2: Left: Schematic ionization diagram of hydrogen only. $\triangle$ symbolize recombination, $\bigcirc$ symbolizes ionizations (photo- and collisional ionizations) and $\triangledown$ symbolizes recombination photons which are taken into account by using $\alpha_B$ recombination (sum of all recombination rates to all states but the ground state, symbolized by the white frame around the triangle) rates; Right: Symbolic rate equations with the same meaning of the symbols. $\bigtriangledown$ means negative contribution from recombination.

The arrow in the left hand panel of Fig. 3.2 pointing back from the recombinations to the ionizations represent the recombinations to the ground level. Here, a photon is emitted that itself again is able to ionize a hydrogen atom. As mentioned above, those are treated on-the-spot, assuming that they ionize close to their origin. This means in practice that the recombinations to the ground state are not counted, instead one uses the so called B-recombination rate, $\alpha_B$. Therefore, in the symbolic notation of the rate equation, these recombination photons are not explicitly included since they have been already subtracted from the recombination rate.

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29This is the sum of the recombination rates to all levels but the first, see for example Osterbrock & Ferland (2006).
Figure 3.3: Left: Schematic ionization diagram of hydrogen and hydrogen coupling. \(\triangle\) symbolize recombinations, \(\bigcirc\) symbolizes ionizations (photo- and collisional ionizations) and \(\triangle\gamma\) symbolizes recombination photons; Right: Symbolic rate equation with the same meaning of symbols, \(\nabla\) means negative contribution from recombination photons. Note the symmetry.

When helium is included, dealing with the recombination photons gets slightly more complicated. Using a similar symbolic representation of the processes involved, we illustrate the situation with helium in Fig. 3.3.

The photons from helium recombination that are energetic enough to at least ionize hydrogen now have to be included explicitly. Those that are energetic enough to ionize at least two species have to be split between the species in question depending on their relative optical depths. This is explained in detail in PAPER II. The set of equations for coupled helium and hydrogen (helium only) can be reduced to 3 (2) equations by taking into account that the ionization fractions for each of the two species individually add up to 1.
3.2 Ray-tracing

In two or three dimensions one needs a method to compute the optical depths to all the cells in every direction from the source as well as over every cell. In one dimension, the latter is trivial and the former is simply the sum over the optical depth in all cells between the source and the cell. For multiple dimensions, there are two so-called ray-tracing approaches, which can also be combined: the long-characteristic approach and the short-characteristic approach.

In the long-characteristic approach, a ray from the source is cast through every cell. The optical depth to the cell is the sum of the optical depths through the cells that the rays crosses on the way, weighted by the path length of the ray through each cell. Several steps have to be taken in this approach: 1) Choosing direction angles for casted rays. 2) Determining which cells are crossed by each ray and 3) finding the path lengths in each cell (e.g. Abel et al. 1999). The advantage of this method is that each ray is independent of the others. Therefore, they can be calculated in parallel. Obviously the density of rays decreases with the distance to the source. Since every cell has to be reached by at least one ray, this results in an oversampling of the cells near to the source if the accuracy at larger distances should be maintained. To solve this problem, Abel & Wandelt (2002) split rays into child-rays as a function of distance to the source.

Another way of avoiding the redundant calculations near the source is the method of short characteristics. Rays are cast from the source to the centre of each cell, but only the ray-segment in the last cell is retained. The actual way to the source, i.e. the optical depth between the source and each cell, is approximated by the cells which are nearest to the point where the ray enters the cell in question. Mellema et al. (2006) describe in Appendix A the ray-casting method used for C²RAY and motivate the choice of the weighting functions for the cells contributing to the optical depth to the cell. The optical depth over the cell is just twice the optical depth from the point where the ray enters the cell to the cell centre.

The disadvantage of the short characteristics approach is that the optical depths from the neighbouring cells have to be known, setting constraints on the domain decomposition in the case of a parallel computation. Also, since the optical depth to a given source cell is calculated via interpolation, there is some diffusion of radiation.

Rijkhorst et al. (2006) use a combination of long- and short-characteristic ray-tracing schemes, where the simulation volume is divided into patches containing a number of cells. Inside every patch, the method of
short-characteristics is used, but long-characteristics is used for the patches, which enables parallel calculation for the patches.

When more than one source is present, the problem arises that a ray from one source (“a”) may alter the neutral hydrogen fraction in a cell on the way of a ray from another source (“b”). The calculation of the ionization fractions in cells of the ray from source (“b”) that are located behind the crossing point of the cells now depends on the order of calculation if the contributions would be calculated independently. To circumvent this problem, the iteration loop displayed in Fig. 3.1 should not be done for every source independently. Instead, in each cell, the ionization rates from all sources have to be added before the ionization fractions in the cells are updated. In the picture of Fig. 3.1, this means that \((\Gamma_{\text{in}} - \Gamma_{\text{out}})\) has to be replaced by \((\sum_{i=\text{sources}} (\Gamma_{\text{in}}^i - \Gamma_{\text{out}}^i))\). First after all sources have contributed to the ionization rate in each cell (calculated on the basis of the optical depth from the last iteration), this ionization rate is applied to the cell to calculate a new ionization fraction in each cell. See figure 2 of PAPER II for an iteration flow chart for the case of three dimensions. Ray-tracing methods typically scale as the product of number of grid cells and number of sources.

Alternatives to ray-tracing methods are Monte Carlo approaches (e.g. Cia-rdi et al. 2001; Maselli et al. 2003) and Moment methods (e.g. Gnedin & Abel 2001; Norman et al. 1998). The latter have the advantage of not scaling with the number of sources. However, they are less accurate for very anisotropic and heterogeneous intensity distributions and tend to be rather diffusive. Several codes used for reionization simulations participated in a comparison project, see Iliev et al. (2006) for a description of the results.
This chapter serves as an introduction to PAPER III were we investigate the detectability of a quasar H II region during the EoR. It provides the motivation and more background for the parameter choices of the quasar properties in that paper.

Quasars (quasi stellar radio source) were first observed in radio (e.g. Bolton et al. 1949) and matched with their optical counter parts later when more precise position measurements at radio wavelength became possible (e.g. Schmidt 1963; Matthews & Sandage 1963). Due to their point-like appearance (angular extends of less than an arcsecond), they were also named quasi stellar object (QSO). The prefix quasi- was added because of their unusual spectrum consisting of many emission lines. From the redshift of these emission lines it became clear that these sources were in fact extragalactic, which meant that they must be extremely luminous given their rather low apparent magnitudes. Time-variability in the emission (e.g. Matthews & Sandage 1963; Boller et al. 1997) set constrains on the spatial extent of the sources. These observations together (high luminosity from a very small region) put constrains on the source of energy for these objects.

In the following, I use the terms quasars, active galactic nucleus (AGN) and QSO interchangeable. In the standard model of AGN today, the main ingredient of a quasar is an accreting black hole (BH) in the centre of a galaxy surrounded by a hot accretion disk. Gravitational energy is partly converted (via friction) into electromagnetic energy.\textsuperscript{30} The accretion is limited by radiation pressure. Assuming isotropic radiation and spherically symmetric accretion, the limiting so called Eddington luminosity can be calculated by equating the inward and outward forces. The Eddington luminosity only depends on the mass of the accreting object since both the radiation pressure and the gravita-

\textsuperscript{30}The accretion disk has increasing temperatures towards the centre. Due to the different peaks of the BB-curves, the spectrum looks very different from a typical BB spectrum. Parts of the emitted photons are reprocessed in the hot electron corona around the disk and boosted to higher energies via inverse Compton scattering.
tional attraction decrease with distance squared, hence

\[ L_{\text{Edd}} = \frac{4\pi M_{\text{BH}} m_p c}{\sigma_T} \approx 1.3 \times 10^{31} \frac{M}{M_\odot} \text{W}, \]  

(4.1)

(e.g. Robson 1996). Here, \( G \) is the gravitational constant, \( M_{\text{BH}} \) the mass of the BH, \( m_p \) the proton mass, \( c \) the speed of light and \( \sigma_T \) the Thompson scattering cross section. One introduces an Eddington efficiency parameter, commonly named \( \lambda \), where

\[ L_{\text{QSO}} = \lambda L_{\text{Edd}}(M_{\text{BH}}). \]  

(4.2)

An AGN with \( \lambda = 1 \) accretes therefore at its Eddington limit. As mentioned, the above equating of the inward and outward forces assumes spherically symmetric accretion and isotropic radiation. Heinzeller et al. (2007) show by numerical simulations that for the case of a thin accretion disc, super-Eddington luminosities with up to \( \lambda = 20 \) are possible\(^31\). However, as Steinhardt & Elvis (2010) and Steinhardt & Elvis (2011) show by examining over 60000 SDSS quasars, most quasars emit below their Eddington limit. I reproduce here figure 1 from Steinhardt & Elvis (2010), see Fig. 4.1. It shows the loci of the SDSS quasars in the mass-luminosity plane. The dashed line shows the Eddington luminosity. It can be seen that there is a large spread in \( \lambda \) but most quasars are below the Eddington luminosity\(^32\).

As mentioned above, the energy that is radiated away is basically gravitational energy. The amount of energy obtainable for radiation depends on the lowest state of potential energy that can be reached before the accreted matter falls into the BH: Matter of mass \( m \) at infinity, has potential energy 0 (with respect to the BH) and a rest mass energy \( mc^2 \). It can be shown (e.g. Misner et al. 1973; Kembhavi & Narlikar 1999) that the last stable orbit of a non-rotating BH is at \( 3R_S \) where \( R_S = 2GM_{\text{BH}}/c^2 \) is the Schwarzschild radius where the escape velocity is equal to the speed of light. The total energy of the matter at this distance to the BH is lower than the rest mass energy (since the potential energy is negative) and has to be calculated relativistically, Misner et al. (1973) give \( E(\text{last stable orbit}) = \frac{1}{2} \sqrt{2mc^2} \). Therefore it follows that the difference between the rest mass energy and the last stable orbit energy (the

\(^{31}\)Loeb (2009) mention that theoretical models predict that radiation pressure puffs up the inner edge of the accretion disc and therefore the inner geometry is more spherical and the concept of an Eddington limited accretion holds. This is also more in line with observations

\(^{32}\)The mass of a BH can be measured my a technique called reverberation mapping. It is based on the geometrical model of the quasar according to which the continuum radiation from the quasar originates from very close to the BH while the line radiation originates from gas further out at a distance \( d \). Any luminosity change in the continuum radiation will eventually (with a time delay \( \Delta t = cd \)) show up in the line radiation. Measuring the time delay and the line width, the virial theorem can be used to calculate \( M_{\text{BH}} \).
difference is the binding energy) is lost from the BH system. It is radiated away as

\[ \int_t L_{QSO} \, dt = \varepsilon m c^2. \quad (4.3) \]

Here \( t \) is the time for accreting the mass \( m \). In the case of a non-rotating BH, the upper limit for the efficiency is \( \varepsilon = 1 - 2\sqrt{2}/3 \approx 0.053 \). But one can show (e.g. Misner et al. 1973) that for an extreme rotating BH, \( \varepsilon \approx 0.42 \), the last stable orbit is closer to the BH. By accreting the matter, the non-rotating BH grows its mass by \( 2\sqrt{2}/3m \), or more generally by \( (1 - \varepsilon)m \). Therefore,

\[ L_{QSO} = \varepsilon \dot{m} c^2 \quad \text{and} \quad \dot{M}_{BH} = (1 - \varepsilon)\dot{m} \quad (4.4) \]

where \( \dot{M}_{BH} \) is the BH mass growth rate. So a higher \( \varepsilon \) means that the actual mass accretion rate \( \dot{m} \) for reaching a certain luminosity \( L_{QSO} \) can be smaller than for a lower value of \( \varepsilon \). However, equating Eq. (4.4) and Eq. (4.2) gives

\[ \dot{M}_{BH} = \frac{\lambda(1 - \varepsilon)}{\varepsilon c^2} L_{Edd}. \quad (4.5) \]

This shows that a higher value of \( \varepsilon \) also implies a lower mass growth rate of the black hole. Therefore, to grow quickly very massive black holes, the efficiency \( \varepsilon \) to convert rest-mass energy into EM should be small. But to reach
observed luminosities of quasars and to avoid unrealistically high mass accretion rates, the accretion efficiency should be high. If the mass supply is limited, the accretion efficiency has an effect on the quasar’s luminous lifetime. Reasonable values for the accretion efficiency are thought to be several to several tens of percent, $\epsilon \sim 0.05 - 0.2$ (Haiman & Hui 2001; Shankar et al. 2010; Martini & Weinberg 2001). As Volonteri & Gnedin (2009) point out, a black hole with no rotation will accumulate angular momentum and in this way increase $\epsilon$. This could be a natural way for the BHs to grow relatively fast in mass at early times and to reach high radiation efficiencies later. However, it is still not clear how super-massive BH (such as the one in ULAS J1120+0641 which was approximated to have a mass $2 \times 10^9 M_\odot$ see Bolton et al. 2011, at $z \sim 7.1$, so only roughly 750 Myr after the bb ) can grow so massive in such short times. See for example Volonteri (2010) for a recent review on this topic.

To include quasars as sources in our reionization simulations, we need to identify the location of the quasar (i.e. which halos host active quasars), the total luminosity of the quasar, the lifetime of the quasar and we need a spectrum of the quasar.

In Sect. 4.1, I outline how we connect the quasar luminosity to the host-halo mass and discuss the limitations of this relation. In Sect.4.2, I summarize observational results that are used to estimate the lifetime of quasars. Sect.4.3 gives an overview of the observations of quasar spectra. Finally, Sect.4.4 summarizes our rather crude recipes to include quasars in our simulations.

4.1 Quasar luminosity – Halo mass relation

The general idea of this section is to connect the host halo mass to the quasar luminosity. This can be done in three steps: (1) The quasar luminosity $L_{\text{QSO}}$ can be connected to the black hole mass $M_{\text{BH}}$. $^{33}$ (2) $M_{\text{BH}}$ can be connected to the mass of galaxy bulges $M_B$. (3) $M_B$ can be connected to the total mass of the halo $M_{\text{halo}}$. First, I will give details to each of those steps. Afterwards I will give an overview of observations which give rise to doubts to the existence of such a relation.

Assuming an Eddington limited accretion, what is needed for connecting the quasar luminosity to the host halo mass, is a relation between black hole mass and host halo mass. For low (here, $z \leq 3$, or so) redshifts, Magorrian et al. (1998) observed a relation between the masses of the central massive

$^{33}$In the introductory section to this chapter, see Fig. 4.1, it was shown that there is a correlation between $M_{\text{BH}}$ and $L_{\text{QSO}}$, however with a large scatter.
dark object (BH) and bulge (B) (this corresponds to step 2 from above):

\[ \frac{M_{BH}}{M_B} = 0.006 \]  

(4.6)

This relation is known as the Magorrian relation, or as the M-\( \sigma \) relation, where \( \sigma \) refers to the central velocity dispersion, the velocity dispersion of the bulge. This is the actual measured quantity.

Newer formulations of this are \( M_{BH} \approx 0.002M_B \) (Marconi & Hunt 2003, their measurements also use bulge luminosities\(^{34}\) in addition to the velocity dispersion) or slightly non-linear relations such as \( \frac{M_{BH}}{M_\odot} \approx 7.6 \times 10^{-5} \left( \frac{M_B}{M_\odot} \right)^{1.12} \) (Häring & Rix 2004) and from Tundo et al. (2007) (equation A5)\(^{35}\):

\[ \frac{M_{BH}}{M_\odot} = 10^{8.21} \frac{\sigma}{200 \text{ km/s}}^{3.83} \]  

(4.7)

Further, a correlation between the outer circular velocity \( v_c \) of galaxies to this central velocity dispersion \( \sigma \) of the following form is observed (Ferrarese 2002, equation (2))\(^{36}\):

\[ \frac{v_c}{[\text{km s}^{-1}]} = 10^{0.55} (\sigma/[\text{km s}^{-1}])^{0.84} \]  

(4.8)

For virialized systems, the outer circular velocity \( v_c \) is related to the halo velocity \( v_{vir} \) at the virial radius \( r_{vir} \) which is determined by the mass enclosed in the virial radius \( M_{vir} \) of the halo, \( v_{vir} = \sqrt{\frac{GM_{vir}}{r_{vir}}} \) (These two relations, the connection between the velocity dispersion of the bulge to the circular velocity of the galaxy; and the connection between the circular velocity of the galaxy to the virial velocity of the halo comprise step 3 from above). The details depend on the assumed halo mass profile and the stellar and gaseous content, see Mo et al. (1998). In the following I set \( v_c = v_{vir} \). Using equation 2 from Bullock et al. (2001), the set of cosmological parameters (\( h=0.702, \Omega_b=0.0455, \Omega_m=0.272 \)) and a required overdensity of 200 for the virial radius (from the spherical collapse model), the resulting equation relating halo mass and virial velocity reads\(^{37}\):

\[ M_{vir} = \frac{4\pi}{3} \frac{200 \rho_c}{3} \left( \frac{GM_{vir}}{v_{vir}^2} \right)^3 = \frac{v_{vir}^3}{10H\Omega} \approx 3 \times 10^5 M_\odot \left( \frac{v_{vir}}{\text{km s}^{-1}} \right)^3 \]  

(4.9)

\(^{34}\)Applying some constant mass-to-light ratio, the bulge luminosity can be converted to a bulge mass.

\(^{35}\)in all cases, the values are based on averages. For information about the spread around those averages, I refer the reader to the original publications

\(^{36}\)Kormendy & Bender (2011) combine the data points from Ferrarese (2002) with several other measurements in their figure 1 and conclude that there is no such relation. I will however continue based on the relation found by Ferrarese (2002).

\(^{37}\)in the second step \( \rho_c = \frac{3H^2}{8\pi G} \) was used.
These relations together (using Equation 4.7 to 4.9) give a relation between (virial) halo mass $M_{\text{vir}}$ and the mass of the central black hole $M_{\text{BH}}$:

$$M_{\text{BH}} = 10^{8.21} \left( \frac{\sigma}{200} \right)^{3.83}$$

$$= 10^{8.21} \times 200^{-3.83} \left( \frac{v_c}{10^{0.55}} \right)^{1/0.84}^{3.83}$$

$$= 10^{8.21} \times 200^{-3.83} \times 10^{0.55}^{-3.83/0.84} \left( \left( \frac{M_{\text{vir}}}{3 \times 10^5} \right)^{1/3} \right)^{1/0.84}^{3.83}$$

$$\approx 3.7 \times 10^{-12} M_{\text{vir}}^{1.52} \quad (4.10)$$

Here, all velocities are in units of km/s and masses are in solar masses $M_\odot$. Shankar et al. (2010) and Ferrarese (2002) perform an analysis along the same lines and come to similar results. The former include a redshift dependence and the latter test for several assumptions about the density profile, among other things. I include some of their models in Fig. 4.2. Haiman & Hui (2001) give an upper limit for the black hole mass by using the $M-\sigma$ as originally by Magorrian et al. (1998) and setting $\Omega_b/\Omega_m M_{\text{halo}}$ as an upper limit for the bulge mass. This results in: $M_{\text{BH}} \approx 0.006 M_B \leq 0.006 M_{\text{halo}} \Omega_b/\Omega_m \approx 0.001 M_{\text{halo}}$.

Zaroubi et al. (2007) use an estimate along the same lines, however they assume a factor 6 lower proportionality factor in the Maggorian relation (which is closer to the slightly newer result from Marconi & Hunt 2003). I summarize selected results in Fig. 4.2 to give a feeling for the spread in $M_B - M_{\text{BH}}$ space.

As indicated at different parts in this section, there are problems with this approach to connect halo mass to QSO luminosity: Merloni et al. (2010) find observationally a larger scatter in the Maggorian-type relation (step 2 from above)38 with increasing redshift. As mentioned earlier, Kormendy & Bender (2011) find no connection between the bulge mass of galaxies and the total host halo mass (step 3 from above). Clustering analysis shows that QSOs are strongly clustered at all redshifts and that the clustering increases with redshift (Shankar et al. 2010; Shen et al. 2008). While this alone is not in contradiction to a relation between halo mass and QSO luminosity, Croom et al. (2005) and Shanks et al. (2011) find no strong luminosity dependence of the quasar clustering. Shanks et al. (2011) argue (supported also by numerical simulations) that this can be interpreted as all quasars residing in similar mass halos, but being observed at different evolutionary stages. This is indicated as the grey box spanning a wide range of BH masses, representing a wide range of quasar luminosities. However, Porciani & Norberg (2006) report to find a luminosity

---

38 However, they look at rather low redshifts $z<2.2$. 
Figure 4.2: Different analytic estimates for the halo mass - black hole mass relation. Note the rather large spread. Shanks et al. (2011) and Croom et al. (2005) suggest a narrow host halo mass range, this is indicated in the figure by a grey rectangle. Also included in this plot are the quasars we included in our simulations of PAPER III.

Since for us, the important parameter is the total luminosity and not the BH mass, I included two possible BH masses for each quasar implementation, one assuming $\lambda = 1$ and one assuming $\lambda = 0.333$. The halo mass corresponds to the mass of the most massive halo in our $164^3$ comoving Mpc$^3$ simulation.

dependence in the clustering and Shen et al. (2008) do find a slight redshift dependence on the minimum halo mass (larger for higher redshifts) which they argue is a selection effect due to the need of higher intrinsic luminosities for objects further away to be observable, which means that there is a luminosity-mass relation. Also White et al. (2008) find from combining quasar clustering and quasar space-density data, that the scatter in quasar luminosity to host halo mass-relation is small.

To conclude this section: Quasars are highly biased objects which reside only in the most massive halos which are very rare objects. If there is a typical mass for halos in which all active quasars reside (and what we see as different luminosities just corresponds to different evolutionary stages) or if there is a relation between quasar luminosity and halo mass, is not clear.
4.2 Quasar lifetime

As mentioned above, the lifetime of a luminous quasar is in practice constrained by the amount of material it can accrete. However, without knowing how much material is available, we cannot, on theoretical grounds, limit its lifetime. As a characteristic timescale \( t_c \) however, one can calculate the time scale after which the mass increases by a factor of \( \exp(1) \) (Haiman & Hui 2001). Inserting the value for the Eddington luminosity (Eq. 4.2) into the expression for the BH mass growth rate (Eq. 4.5) gives

\[
\dot{M}_{\text{BH}}(t) \approx \frac{(1-\varepsilon)\lambda}{\varepsilon} \times 10^{-9} \frac{M_{\text{BH}}(t)}{\text{yr}}
\]

(4.11)

And therefore

\[
M(t) \approx M_0 \exp \left( \frac{2.3\times 10^{-9} \frac{t}{\text{yr}} \lambda (1-\varepsilon)}{\varepsilon} \right)
\]

(4.12)

and

\[
t_c/\text{yr} \approx 4.3 \times 10^8 \frac{\varepsilon}{\lambda (1-\varepsilon)}
\]

(4.13)

Choosing the typical values for \( \lambda \) (\( \sim 1 \)) and \( \varepsilon \) (\( \sim 0.1 \)) gives 50 Myr.

To find observational limits on the lifetime of quasars, one can compare the comoving quasar space density \( \Phi(z) \) with the space density of their potential hosts \( n_{\text{host}}(z) \) and in this way try to match \( n_{\text{host}}(z) \), since \( \Phi(z) \propto n_{\text{host}}(z)t_Q \).

However, the uncertainties are rather large (e.g. Haehnelt et al. 1998, find \( t_Q \sim 10^6 - 10^8 \) yr). Haiman & Hui (2001) and Martini & Weinberg (2001) propose to use the bias of the quasar distribution instead, this has the advantage that the assumptions about the mass of host halos are less constraining. The approach of the latter can be outlined as follows: Use the observed quasar space density to find a minimum mass for a halo hosting a quasar as a function of quasar lifetime over halo lifetime (that is in a way going the other way around as Haehnelt et al. 1998), so \( \Phi(z) \rightarrow M_{\text{min}}(z,t_Q) \). Next, use an analytical estimate relating the halo mass to the halo bias (Mo & White 1996), \( b(M_{\text{halo}}) \), to find an effective bias for halos hosting quasars, so \( M_{\text{min}} \rightarrow b(M_{\text{host}}) \). Since \( M_{\text{min}} \) can be expressed as a function of quasar lifetime, the bias can be expressed as a function of quasar lifetime. This function can be compared with the measured bias of quasars. The advantage here is that one does not make a priori assumptions about the masses of halos hosting quasars. However, this method gives information about the quasar lifetime over the halo lifetime which is equal to the quantity called duty cycle, usually defined as the number of quasars over objects potentially hosting quasars. Haiman & Hui (2001) take a slightly different path and find their results also to be consistent with quasar lifetimes \( t_Q \sim 10^6 - 10^8 \) yr.
A very different way of constraining the lifetime of quasars comes from measurements of their proximity zones\(^{39}\) (e.g. Lu & Yu 2011; Worseck & Wisotzki 2006; Croft 2004). While this does not directly measure the lifetime but the time for which the quasar has been shining, it sets a lower limit on the quasar lifetime. Here, both the proximity zone measured by the quasar light itself (so line of sight proximity zone) as well as the transverse proximity zone measured through the background light from a nearby quasar behind the foreground quasar, are in principle useful to set limits on the lifetime of quasars. Croft (2004) simulate the effect of quasars with lifetimes as short as \(10^7\) yr on the Ly\(\alpha\) forest and compare this to observations (SDSS) and conclude that the best solution to match observations are total quasar lifetimes \(\sim 10^7\) yr but with single burst phases lasting \(\leq 10^6\) yr. Worseck & Wisotzki (2006) report the detection of the transverse proximity effect (however in He II not in HI) and estimate the minimum quasar lifetime to be \(1 - 3 \times 10^7\) yr. They argue that there is no need for anisotropic UV radiation from the foreground quasar (this is how Lu & Yu 2011, try to explain contradicting estimates for quasar lifetimes) but instead that large scale density structure masked the transverse proximity effect. This is based on comparing the He II and HI absorption.

4.3 The spectrum of quasars

Somewhat confusingly there are several different ways in use to express the spectrum of astrophysical sources. While it is not uncommon in the X-ray community to show a spectrum in terms of photons/m\(^2\)/s/keV (over frequency \(\nu\)), in the optical it is more common to view it as spectral flux density \(F_\lambda\) measured in W/m\(^2\)/nm (over wavelength \(\lambda\)) and at radio frequencies as spectral flux density \(F_\nu\) in W/m\(^2\)/Hz (over frequency \(\nu\)). Alternatively it is expressed as \(\lambda F_\lambda = \nu F_\nu\) in W/m\(^2\). Sometimes the latter is referred to as spectral energy distribution (SED)\(^{40}\). However, this concept is not consistently used in the literature since sometimes \(F_\nu\) or \(F_\lambda\) are called SED. To complicate things even more, when approximating the quasar spectrum with a power law, sometimes the power law index is defined as \(F(\nu) \propto \nu^{-\alpha}\) and sometimes without the mi-

\(^{39}\)Originally, proximity zones are only defined for quasars in an already ionized IGM with an existing ionizing background flux. The quasar produces many more ionizing photons so that the ionizing flux density in the vicinity of the quasar is enhanced and therefore the remaining neutral fraction is lower then elsewhere, even in the high density filaments of the cosmic web that go through this region, the neutral fraction is reduced. Therefore, the Ly\(\alpha\)-forest originating from this region is weakned

\(^{40}\)not to be confused with the meaning of SED outside astronomy: Sozialistische Einheitspartei Deutschlands (Socialist Unity Party of Germany)
nus in the exponent. This can lead to serious confusion. In the following, I use the power law index $\alpha$ defined by: energy flux per unit area, per unit time between frequency $\nu$ and $\nu + d\nu$ is proportional to $\nu^{-\alpha}$, so $F_\nu \propto \nu^{-\alpha}$. That means that the output number of ionizing photons in the same frequency interval is proportional to $\nu^{-1-\alpha}$. This index is sometimes called spectral photon index $\Gamma$ (e.g. Yuan et al. 1998). I will not use $\Gamma$ in this context since I use it for denoting the ionization rate, see Sect. 3.

With this definition, Zheng et al. (1997) find $\alpha \approx 1$ for the far ultraviolet radiation of quasars (105 – 220 nm or 5.6 eV – 12 eV) using Hubble Space Telescope (HST)\(^{41}\) data. For the extreme ultraviolet radiation (35 – 105 nm or 12 eV – 35 eV), they find $\alpha \approx 2$, see also their figure 5, reproduced here in Fig.4.3 upper curve. Earlier studies also found a double power law to be a good fit, however, as Zheng et al. (1997) show (for the far UV), there is a rather large spread for the fitted power law indices (see their figure 3). In a newer measurement, Telfer et al. (2002) find $\alpha \approx 1.76$ for (50 – 120 nm or 10 eV – 24 eV) using an enhanced set of quasar spectra, see also their figure 4 reproduced here in Fig.4.3 lower curve. A similar slope is measured for the soft X-ray region (0.6 – 6 nm or 200 eV – 2000 eV) by Laor et al. (1997) who find $\alpha \approx 1.72$.

To conclude this section, we summarize that in the frequency range interesting for reionization simulations (above 13.6 eV [below 91.2 nm]), an average spectral index of $\alpha \sim 1.75$ seems to be a good estimate.

### 4.4 Summary: Quasars in our simulation

In our study, we do not follow the mass growth of even individual halos. Instead, we assume that the accretion is Eddington limited, $\lambda = 1$ in Eq. 4.2 and that there is enough material to accrete for several Myr to several tens of Myr, so $t_{QSO} \sim [5 – 25]$ Myr.

Due to the rather large uncertainty in the measured relation between $v_c$ and $\sigma$ (if there is at all such a relation, see footnote in Section 4.1 and caption of Fig. 4.2) as well as between the halo mass and $v_c$ (which is model dependent), for simplicity we use a linear relation to convert halo mass to QSO luminosity and orientate us towards the upper limit. Our model QSOs are included in Fig. 4.2. For the spectrum, we use a single power law as defined in Sect. 4.3 with $\alpha = 1.5$. This value is slightly lower than the value found by Telfer et al. (2002) for the complete set of quasars, but corresponds to the average of the radio-quiet sub-set. It is this value that was used by e.g. Bolton et al. (2011) for wavelengths below 105 nm.

\(^{41}\)http://hubble.nasa.gov/
Figure 4.3: Mean composite QSO spectra. Upper curve: reproduced by permission of the authors and AAS from Zheng et al. (1997), figure 5, 101 quasars binned to 0.2 nm. Lower curve: reproduced by permission of the authors and AAS from Telfer et al. (2002) figure 4, 184 quasars binned to 0.1 nm. Here, the relative Flux $F_{\lambda}$ is shown over $\lambda$. To convert the power law index into a power law index for $F_\nu$, use $F_\nu \propto F_{\lambda}(\nu)/\nu^2$, so the flat part in the upper spectrum transforms into $\alpha \sim 2$. Telfer et al. (2002) exclude the region below 50 nm in the shown fit, since only 10 QSO contribute to this part of the spectrum, the horizontal black line segments indicate the continuum windows used for their fit. The line segments of Zheng et al. (1997) are omitted in this reproduction to avoid confusion in the already busy plot.
This thesis is based on three publications. While all publications contribute to the large field of simulating the EoR, they are very different in their nature: while PAPER I deals with different methods for analysing ionization fraction results from radiative transfer EoR simulations and testing the effects of different source models on the ionization fraction fields, PAPER II describes an extension of the radiative transfer code C²RAY. PAPER III in turn uses this method to investigate the effect of a quasar on the ionized fraction field during the EoR and investigates prospects of the observability of such a quasar H II region. In Chapter 2, the three publications were put into context. In this chapter, I give a short summary of the appended papers.

5.1 Summary of “Topology and sizes of H II regions during cosmic reionization” (PAPER I)

We analyse the ionization fraction results of several large-scale (54 and 163 comoving Mpc) simulations with different methods. The aim of this paper is two fold: On the one hand, we investigate the usefulness of the methods; on the other hand we use the methods to find discriminating effects on the resulting ionization fraction fields from different source properties.

The four independent methods used to characterize the sizes of ionized regions are the friends-of-friends (FOF) method, the spherical average method (SPA), the power spectrum (PS) and a method based on finding the total surface area and volume of all ionized bubbles (3V/A). The first three size measures mentioned above (FOF, SPA, PS) result in a distribution function of sizes while the 3V/A results in a single size per redshift. Additionally we consider another method to measure the size of H II regions that is similar to the one used by Mesinger & Furlanetto (2007) in the appendix. Since we find that it is less useful due to the dependence on several free parameters, we do not consider this method in the main body of the paper.
CHAPTER 5. SUMMARY OF PUBLICATIONS

The FOF method captures the size distribution of the small scale H II regions which contribute only a small amount to the total ionization fraction. The spherical average method provides a smoothed measure for the average size of the H II regions constituting the main contribution to the ionized fraction. The power spectrum is more similar to the SPA but retaining more details on the size distribution.

To characterize the topology of the ionization fraction field, we calculate the evolution of the Euler Characteristic to which we give a basic introduction. We also point out some flaws introduced by single-cell scale structure in the appendix. The evolution of the topology of the ionization fraction field during the first half of reionization is consistent with inside-out reionization of a Gaussian density field: The Euler Characteristic of the ionization fraction field as a function of time behaves the same way as the Euler Characteristic of the logarithm of the density field as a function of density. The inside-out reionization is further supported by correlating density and ionized fraction on large scales.

5.2 Summary of “Radiative transfer of energetic photons: X-rays and helium ionization in C²-RAY” (PAPER II)

We present an extension to the radiative transfer and photo-ionization code C²-RAY. The qualitative background was introduced in this thesis in Section 3.1.

We review the basic concept of C²-RAY, introduce the extensions to the algorithm in great detail and validate our implementation by a set of tests by comparing to results from the photo-ionization equilibrium code CLOUDY as well as comparisons to the hydrogen only solutions. We validated the time-dependent solutions through convergence studies. Although these tests were mainly for validating the code, we could also confirm the validity of a shortcut often taken in EoR simulations, namely that it is valid to assume that for stellar-type sources, the helium ionization follows that of hydrogen.

The extension consists of the introduction of helium as a second component using the full on the spot (OTS) approximation, multi-frequency ionization/heating and inclusion of secondary ionizations. We described the new elements to C²-RAY, such as the linearised solution of the set of hydrogen and helium rate equations introduced here graphically in Fig.3.3 using the coupled OTS treatment, and the calculation of the multi-frequency ionization and heating rates for both hydrogen and helium. We also show that the often used,
simpler uncoupled OTS (i.e. treating each species isolated) give substantially different results from the here implemented fully coupled OTS approximation.

We further performed the cosmological test from the earlier mentioned Cosmological Radiative Transfer Comparison Project (Iliev et al. 2006) with the inclusion of helium. This test includes the calculation of the IGM temperature. We find that the inclusion of helium significantly affects the temperature distribution as the heating front is found to be steeper than in the hydrogen only case. Helium is an important absorber of extreme UV and soft X-ray photons and should therefore be taken into account when studying hard ionizing spectra.

5.3 Summary of “Prospects of observing a quasar H II region during the EoR with redshifted 21cm” (PAPER III)

We use the extended version of $\text{C}^2\text{RAY}$ (see PAPER II) to simulate quasar H II regions during the EoR. We consider three different cases: an early quasar turn on at $z \sim 8.6$ and a late$^{42}$ quasar turn on at $z \sim 7.7$ in a simulation box with side length of 164 comoving Mpc and a late quasar turn on (also $z \sim 7.7$) in the much larger simulation volume of (607 comoving Mpc)$^3$. The motivation for the quasar model used in this paper is described in more detail in this thesis in Chapter 4. We produce 21cm maps making the assumption of an IGM heated well above the CMB temperature, as outlined here in Chapter 1.2.

The method we use to measure the quasar H II region size is a technique that works directly with the visibilities produced by radio interferometers. It can also subtract the strong foreground emission which affect the redshifted 21cm observations. The method was developed by Datta et al. (2007).

The main aim of this paper is to answer the questions: (1) Is it in principle possible to use LOFAR in combination with the matched filter approach to identify single H II regions during the EoR? (2) Is it possible to tell a quasar H II region apart from H II regions made by galaxies in 21cm maps? (3) If we know prior to investigating the 21cm maps the position of a quasar, can we gain more information about the quasar properties by investigating the quasar H II region by means of analysing the “hole” in the 21cm map?

The answer to the first question is yes, but only if the H II region is large enough. The answer to the second question is no. Even under rather extreme conditions, low efficiency stellar sources, high efficiency quasar, the H II region blown by the quasar seems neither much larger nor much more spherical.

$^{42}$“late” refers here to late compared to very early quasar turn on at redshift above 8, not late in a general sense since a quasar turn on at redshift above 7 should still be considered as an early quasar turn on.
than the largest H II regions made by clustered stellar sources. The answer to the third question is yes if the quasar contribution to the joint H II region made by the quasar and the stellar sources is substantial.
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Acknowledgements

As you can see in the lower right corner, I have not managed to reach the end of the EoR in this thesis. I reached a global volume averaged ionization fraction of almost 95 %\(^{43}\) However, you reached the end of my thesis, or, at least the end of the introductory part. And I reached the end of my stay at the astronomy department at Stockholm University.

Many people walked beside and in front of me during this time and walking like that, it sometimes happens that one steps on the foot of each other. That is almost unavoidable.

While observing the reactions of people reading other peoples acknowledgements, I realized that it is very easy to again step on other peoples foots by not properly acknowledging everybody in the desired way. Since I am sometimes a very forgetful person, I am convinced that, still by the time of printing, I will have forgotten to write here the names of a large percentage of the people I should acknowledge. Yes, I would even say, it is dangerous for me to write such an (incomplete) list of names. Therefore, I go the saver way and just say: Thanks to all who feel like they have directly or indirectly contributed to my work.

Alternatively, I could write a list with names (of persons I know and who know me) who have definitely not contributed in any no matter how minor way, to my work: – If you do not find yourself on this list and you are sure that I know you, then you may feel acknowledged by this acknowledgments.

However, it is easy to name the two persons who contributed in the most direct way to my work. Thank you Garrelt & Kanan!

Y también es muy fácil identificar a la persona que más me ha apoyado durante los últimos años. Muchíssimas gracias Cris!

\(^{43}\)Shown here is simulation S6 from Iliev et al. (2011): It suppresses luminous galaxies in halos below \(10^9 M_\odot\) in regions more ionized than 90%. It has the good (for this purpose here) feature of having few small-scale bubbles. The side length corresponds to 54 comoving Mpc.