LARGE-SCALE SIMULATIONS OF REIONIZATION

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ABSTRACT

We use cosmological simulations to explore the large-scale effects of reionization. Since reionization is a process that involves a large dynamic range—from galaxies to rare bright quasars—we need to be able to cover a significant volume of the universe in our simulation without losing the important small-scale effects from galaxies. Here we have taken an approach that uses clumping factors derived from small-scale simulations to approximate the radiative transfer on subcell scales. Using this technique, we can cover a simulation size up to 1280 $h^{-1}$ Mpc with 10 $h^{-1}$ Mpc cells. This allows us to construct synthetic spectra of quasars similar to observed spectra of Sloan Digital Sky Survey (SDSS) quasars at high redshifts and compare them to the observational data. These spectra can then be analyzed for HI region sizes, the presence of the Gunn-Peterson trough, and the Lyα forest.

Subject headings: cosmology: theory — large-scale structure of universe

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1. INTRODUCTION

The term “reionization” is used to describe the process that turned the once-neutral universe into the universe we observe today, in which the neutral fraction of the gas is less than $10^{-5}$. Around $z \sim 1100$, the expansion of the universe cooled the cosmic microwave background (CMB) to the point where it could no longer keep the gas ionized, and hydrogen recombined to a neutral fraction of $\sim 0.9999$. At this point, fluctuations in density, stemming from quantum fluctuations in the early universe, were imprinted on the CMB in the form of temperature fluctuations. These density variations continued to collapse after recombination and started forming the first gravitationally bound objects, such as galaxies and quasars. Radiation from these first objects later began to reionize the universe. A lot of work has been done on reionization, starting with Giroux & Shapiro (1996) and continuing in many papers, including but not limited to Tegmark et al. (1997), Gnedin & Ostriker (1997), Haiman & Loeb (1999), Gnedin (2000), Chiu & Ostriker (2000), Miralda-Escudé et al. (2000), Loeb & Barkana (2001), Bruscoli et al. (2002), Haiman (2002), Lidz et al. (2002), Hui & Haiman (2003), and Wyithe & Loeb (2003).

Before reionization, bubbles of ionized material formed around objects emitting ionizing radiation in high-density regions. These regions of ionized gas were still separated from each other by neutral high-density gas, because a large number of photons are needed to keep high-density regions ionized. The abundance of ionizing photons increased with time as more objects formed, consequently creating more ionized bubbles. The result was a universe containing high-density regions that were ionized close to ionizing sources and neutral high-density regions farther away from sources, embedded in lower density gas that was becoming increasingly ionized.

Eventually, the ionized regions expanded more and started to overlap. During the overlap period the mean free path of ionizing photons increased drastically, because more sources were visible in each “bubble,” so that all the low- and average-density gas was ionized quickly. The overlap period was brief and left small, high-density pockets of neutral gas. The regions around quasars, however, usually assumed to be of high density, were highly ionized. The ionizing intensity still continued to rise and the neutral regions slowly decreased. This period is called post-overlap (Miralda-Escudé et al. 2000).

Reionization can be probed effectively with high-redshift quasar absorption spectra. In particular, a Gunn-Peterson trough (Gunn & Peterson 1965) should appear at redshifts near and above the epoch of reionization, because of the higher neutral fraction of distributed gas. Several quasars have now been observed at high enough redshifts ($z > 6$) to probe the epoch of reionization (Fan et al. 2002; Songaila & Cowie 2002; White et al. 2003; Songaila 2004).

The Lyα forest observed in the spectra of these high-$z$ quasars is remarkably dissimilar to the classical Lyα forest at $z$ between 2 and 4, or, for that matter, to any other type of astrophysical spectra. The Lyα forest at $z > 5$ becomes so dense that flux manages to penetrate only within individual gaps between blends of absorption lines (Maselli & Ferrara 2005). At present it is not clear whether the standard cosmological theory of the Lyα forest can be applied to this kind of spectra, because of the severe blending of lines. So at the moment, detailed numerical simulations appear to offer one of the only methods to create realistic-looking synthetic spectra of the $z > 5$ forest and test the models for analysis.

To be observable, high-redshift quasars must be very bright. Because such quasars can ionize an appreciable region around them, the line of sight to them may not be typical. This bias can be hard to assess from observations alone, but can be analyzed using cosmological simulations (Mesinger & Haiman 2004; Mesinger et al. 2004).

To compare the synthetic spectra to observational data, we need to include high-luminosity quasars in our simulation. This means that we need to create a model of a significant volume of the universe, so that enough objects with low volume density, such as high-luminosity quasars, are included. Such a task is not trivial, since we have to cover a large range of scale, from stars, which are thought to be vital in the process of reionization, to extremely rare quasars of luminosities in excess of $10^{12} L_\odot$. The simulation has to follow many matter components (e.g., dark matter, gas, stars, and quasars) and also follow the radiative
transfer in order to model such a complicated process (Gnedin 2000; Ciardi et al. 2003a, 2003b; Sokasian et al. 2001, 2003).

In this paper we create a physical model of reionization in large volumes. For these large-scale simulations, we have to develop a method to include the small-scale structure. Here this is done with a formalism of “clumping factors” to approximate radiative transfer at scales smaller than the resolution of our simulation. Thus, a clumping factor model allows us to drastically expand the dynamical range of our simulations and thus create a physical model of reionization on scales unreachable by other approaches.

First, we will describe the simulations and the method used to obtain the models for the clumping factors (§ 2.1 and 2.2). Then we will demonstrate how we obtained the synthetic spectra and show some applications they can be used for (§ 3.1 and 4). In § 5 we will show the results obtained so far and finish with a discussion of future work.

2. APPROACH

2.1. Simulations

We use the softened Lagrangian hydrodynamics (SLH; Gnedin 1995) code as our main simulation tool. While the detailed methods for following gas dynamics and the dark matter dynamics are not important in this work, since we are dealing with quasi-linear scales, the main advantage of the SLH code for this project is its ability to follow time-dependent and spatially resolved radiative transfer using the optically thin Eddington tensor approximation (OTVET) of Gnedin & Abel (2001). We have modified the code to include the clumping factors in the ionization and thermal balance equations.

In simulating large volumes, such as our 256 to 128 $h^{-1}$ Mpc boxes, it is important to include various sources of ionizing radiation correctly. In this paper we split the total term in the radiative transfer equation $S$ into two components: a “smoothly distributed” component $S_S$ that includes sources that cluster on scales below our resolution, and an “isolated sources” component $S_I$ that accounts for sources that cluster on scales above our resolution length. For the smoothly distributed component we assume that the source density is directly related to the matter density $\rho$ with a power-law relation,

$$S_S(\mathbf{x}, \nu, t) = g_S(t) \rho^b_S(\mathbf{x}, t),$$

where $b_S$ is the “bias factor” and $g_S$ is the spectral shape of the smoothly distributed sources (which can be time-dependent). The isolated sources component consists of individual sources that follow the predefined luminosity function and are biased with respect to the matter density with a bias factor $b_I$.

In this paper we assume that the only type of isolated sources present in the universe are quasars. We adopt the parameterization of the quasar luminosity function from Schirber & Bullock (2003) (see Fig. 1),

$$\phi(L) = \phi_\star / L^\gamma_S (L/L_\star)^{\gamma_B},$$

where $\phi_\star$ and $L_\star$ are parameters and the faint and bright slopes of the luminosity function are $\gamma_S = 1.6$ and $\gamma_B = 2.6$, respectively. Following Schirber & Bullock (2003), we parameterize the time dependence of $\phi_\star$ and $L_\star$ as

$$\phi_\star = e^{1.72} \times 10^{2.30 - 0.81(\epsilon - 3)} \text{ Gpc}^{-3},$$

$$L_\star = e^{-1.72} \times 10^{12.1 - 0.81(\epsilon - 3)} L_\odot.$$  

The advantage of this parameterization is that it satisfies all known observational constraints on the quasar luminosity function and the only freedom remaining is encapsulated into the “effective emissivity parameter” $\epsilon(z)$. Schirber & Bullock (2003) argued that from the measurements of the proximity effect and the Ly$\alpha$ forest flux decrement the value of $\epsilon(z)$ at $z \sim 3$ should be about 1. In order to extrapolate $\epsilon(z)$ to higher redshifts, we assume that it approximately follows the star formation rate from the small-box simulations described in Gnedin (2000), and we adopt the following analytical fit to this dependence,

$$\epsilon(z) = C \exp \left( -\frac{1}{3} \right),$$

where the constant $C$ is chosen so that $\epsilon(3) = 1$.

Thus, our procedure for computing the total source function is the following. At each time step we compute the value for the critical quasar luminosity for which there is at most one quasar in one resolution element. All dimmer quasars are counted as smoothly distributed sources, while all brighter quasars are counted as isolated sources. We then compute the spectral shape of the smoothly distributed sources, $g_S$, as the sum of the stellar contribution and the contribution from the low-luminosity quasars. Then individual point sources of ionizing radiation are distributed in the computational box with the luminosity function given by equation (2). The sources are distributed randomly throughout the computational box with a probability of being located at a given point that is proportional to the local mass density to the $b_I$ power. For the simulations described in this paper we adopt bias factors of $b_S = 2$ for the unresolved smoothly distributed sources, and $b_I = 3$ for the resolved individual quasars. This value $b_I$ is somewhat lower than the one quoted in Croom et al. (2005), but appropriate considering that the quasars in our simulation are overall fainter than the quasars observed.

This choice of linear bias factor corresponds to $M_{DM} \sim 3 \times 10^{11} M_\odot$ or a luminosity around $2 \times 10^{10} L_\odot$ (Kashikawa et al. 2006; Ferrarese 2002). This means that the brightest quasars, which can be compared to observations, will be more biased. However, our adopted value of $b_I = 3$ should give a good estimate for the bias on the complete quasar population.

The isolated sources continue to emit ionizing radiation for a predefined period of time, the quasar “lifetime.” In this paper we assume that all quasars have the same lifetime, independent
of their luminosity, although a luminosity-dependent lifetime would be straightforward to incorporate into our method.

2.2. Clumping Factors

Currently, simulations of box sizes larger than about \(10 \ h^{-1} \) Mpc do not have enough spatial resolution to adequately resolve the structure in the gas down to the smallest scale (the so-called filtering scale; Gnedin & Hui 1998). Our simulation has a resolution of \(2 \ h^{-1} \) Mpc, for example, which does not allow us to resolve features in the \( \text{Ly} \alpha \) forest. Thus, the evolution of gas on spatial scales below the resolution limit must be described approximately with a phenomenological model. Such a model is often called “subcell physics.” In the case of ionization evolution of low-density gas in the intergalactic medium (IGM), a subcell model can be fully described by a set of “clumping factors” (Gnedin & Ostriker 1997; Madau et al. 1999; Ciardi et al. 2000; Miralda-Escudé et al. 2000).

Let us consider the ionization balance equation for hydrogen:

\[
d\frac{d}{dt} n_{\text{H}i} = -3H n_{\text{H}i} - n_{\text{H}1} \Gamma + R(T)n_{e}n_{\text{H}11},
\]

where \( n_{\text{H}1} \), \( n_{\text{H}i} \), and \( n_{e} \) are number densities of neutral hydrogen, ionized hydrogen, and free electrons, respectively; \( \Gamma \) is the photoionization rate, \( R(T) \) is the hydrogen recombination coefficient, and \( H \) is the Hubble parameter. Equation (5) holds at every point in the IGM. Let us now impose a finite spatial scale on the true distribution of cosmic gas; in our case, the finite resolution scale of a simulation will be such a scale. Averaging equation (5) over such a scale (let us call it a “cell”), we obtain

\[
d\frac{d}{dt} \bar{n}_{\text{H}i} = -3H \bar{n}_{\text{H}i} - \bar{n}_{\text{H}1} \bar{\Gamma} + R(T)\bar{n}_{e}\bar{n}_{\text{H}11}.
\]

Since numerical simulation can only deal with quantities defined within one cell, we must express the right-hand side of equation (6) as a function of physical quantities averaged over one cell, namely

\[
d\frac{d}{dt} \bar{n}_{\text{H}i} = -3H \bar{n}_{\text{H}i} - \bar{n}_{\text{H}1} \bar{\Gamma} + C_{I} \bar{R} \bar{n}_{e} \bar{n}_{\text{H}11},
\]

where we use the notation such that for any physical quantity \( f \) the tilde represents the average over one cell, \( \bar{f} \equiv \langle f \rangle_{\text{cell}} \), and \( C_{I} \) and \( C_{R} \) are “clumping factors” defined as

\[
C_{I} = \frac{\langle n_{\text{H}11} \bar{\Gamma} \rangle}{\langle n_{\text{H}11} \rangle \langle \bar{\Gamma} \rangle},
\]

\[
C_{R} = \frac{\langle R(T) \bar{n}_{e} \bar{n}_{\text{H}11} \rangle}{\langle R(T) \rangle \langle \bar{n}_{e} \rangle \langle \bar{n}_{\text{H}11} \rangle}.
\]

Analogously, the radiative transfer equation for the spatially variable ionization intensity \( \bar{J}_{\nu} \) averaged over one cell can be written as

\[
\frac{\partial \bar{J}_{\nu}}{\partial t} + \frac{c}{a} \frac{\partial \bar{J}_{\nu}}{\partial x} + H \left( \nu \frac{\partial \bar{J}_{\nu}}{\partial \nu} - 3 \bar{J}_{\nu} \right) = -C_{I} k_{\nu} \bar{J}_{\nu} + \bar{S}_{\nu},
\]

where \( k_{\nu} \) is the absorption coefficient and \( \bar{S}_{\nu} \) is the source function given by

\[
\bar{S}_{\nu} = \bar{S}_{\nu, I} + \bar{S}_{\nu, S}.
\]

Here \( \bar{S}_{\nu, I} \) is the source function component from individual resolved quasars and \( \bar{S}_{\nu, S} \) is the component from the smooth background.

In particular, it is worth noting that we have two clumping factors, one in the recombination term, \( C_{R} \), and another one in the ionization term, \( C_{I} \). Both clumping factors are necessary to properly account for the evolution in the ionization state of the cell-averaged hydrogen number density.

Clumping factors cannot be derived from the large-scale simulations that only resolve structures on scales above one cell. Thus, additional information must be used to specify the clumping factors and close equation (7).

To determine the clumping factors, we use a simulation of reionization with the small size of the computational box (4 \( h^{-1} \) Mpc) with the softened Lagrangian hydrodynamics (SLH) code (Gnedin 1995, 2000). While this simulation has too small a box size to be useful for modeling effects of bright rare quasars, it has enough spatial resolution to follow the structure of the IGM down to the filtering scale, and thus can be used for computing the clumping factors on scales of interest. Specifically, we split the 4 \( h^{-1} \) Mpc box into eight cubes 2 \( h^{-1} \) Mpc on a side and averaged \( n_{\text{H}1}, n_{\text{H}i}, n_{e}, R(T), \Gamma \), and their appropriate products over the volume of each of eight cubes. We have done this for a range of redshifts from \( z \sim 5 \) to \( z \sim 12 \), obtaining eight data points for each of the two clumping factors for each redshift value. Each cube gives us a different value, depending on the ionization and the density in its volume. This method yields clumping factors that are not dependent on redshift, but only on properties of the gas. We then fitted both clumping factors as functions of two variables, the neutral hydrogen fraction \( x = \bar{n}_{\text{H}1}/\bar{n}_{\text{H}i} \), and the gas density \( \rho \).

Formally, averaging in equation (6) is performed over the volume of one cell. However, different weightings can be used in making the averages. For example, if we take a simple volume-weighted average in equation (6), we will be including ionizations and recombinations not only in the low-density IGM, but also in the high-density regions within the virialized halos. Thus, both clumping factors will be large, but a significant fraction of ionizing photons will be absorbed locally, within the parent halo of an ionizing source, so the ionization and recombination terms in equation (7) will nearly cancel each other. This behavior results in numerical loss of precision, and is not desirable.

Alternatively, we can weight the low-density gas more than the high-density regions, reducing both clumping factors, but still keeping them consistent with each other. In that case we would exclude some of the ionizations and recombinations that take place in high-density regions from equation (7). Such an exclusion is equivalent to counting only a fraction of ionizing photons in the ionization balance equation, and assuming that the rest of ionizing photons are absorbed locally, within the immediate vicinity of the ionizing source. This fraction is commonly known as the “escape fraction,” although the specific mathematical definition of the escape fraction depends on the specific prescription of how averaging is done in equation (6).

In this paper, we consider three different cases for performing averaging in equation (6). If the clumping factors are computed self-consistently and the escape fraction is chosen appropriately, then the results of a simulation should be independent of the way averaging is performed. Thus, comparing results of simulations with different types of averaging used allows us to estimate the uncertainties due to our final spatial resolution and inaccuracies in parameterizing clumping factors.

The first case (case A) we consider is that the averaging in equation (6) is volume-weighted; i.e., all local absorption counts,
including the photons that are absorbed close to the source. In this case all ionizations and recombinations are counted equally, no matter how high the density in a cell is. The clumping factors for case A are large, since all photons are taken into account, and the high-density regions are included. The relations between the clumping factors for case A can be seen in Figure 2. The recombination clumping factor is not a strong function of neutral fraction, because it is dominated by high-density regions. It is well approximated by a power law in density, \( C_R \propto \rho^{2.5} \). The same power law holds for the photoionization clumping factor, but here we additionally have a dependence on neutral fraction. The photoionization clumping factor decreases with increasing neutral fraction, showing that the photoionization rate and neutral fraction are anticorrelated.

The next two cases reduce the importance of high density and so exclude some of the ionizations and recombinations in high-density regions.

The second model (case B) weights the volume by the inverse density, therefore removing some local absorption. This increases the relative weight of the low-density regions, so that high-density regions do not contribute as much to the volume considered for the clumping factors. The clumping factors are much smaller in this case, eliminating a lot of the numerical problems that arise in case A. Figure 3 shows that they are of order unity, compared to order of 10 for case A. In addition, the exponent in the power-law dependence of the clumping factors on \( \rho \) is lower compared to case A. Both factors depend on the neutral fraction in a more complicated way. The scatter is relatively small for the recombination clumping factor and in the low-neutral fraction regime of the photoionization clumping factor. Figure 3 shows that \( C_R \) increases with increasing neutral fraction, meaning that the regions with lower temperature, and therefore higher recombination rate, are more neutral, as is expected. This effect only appears when the neutral fraction is high enough, corresponding to time outputs before reionization. \( C_R \) does not depend on the neutral fraction below \( x_{\text{HI}} \approx 0.1 \), because the high-density regions dominate again at high ionization fractions.

Similarly to case A, \( C_I \) shows a decrease toward higher neutral fraction, but shows no dependence on \( x_{\text{HI}} \) at low neutral fraction. This change in the slope of the data implies that the anticorrelation of the photoionization and the neutral fraction disappears when the \( \text{H} \text{II} \) regions are overlapping.

In the third model (case C), all volume elements with gas density higher than the density at the virial radius were removed from the calculations of the clumping factors. Consequently, in the modeling of case C only photons that escape the high-density halos are used to reionize the IGM. This removes all local ionization and absorption from the simulation. Similarly to case B, the clumping factors are small compared to case A. Also, most features in Figure 4 are similar to case B in the distribution of data for case C. In particular, the recombination clumping factor distribution has the same shape as \( C_R \) for case B, even though its amplitude lies at about 6 instead of 2 in case B.
2.3. Escape Fraction

Generally the phrase “escape fraction” is understood as the fraction of ionizing photons that leave a high-density region surrounding a source without being absorbed locally (Madau et al. 1999). We define an effective escape fraction $f_{\text{esc}}$ that measures the amount of ionizing photons emitted from homogeneously distributed sources (see eq. [11]). Dropping the subscript $\nu$, the smooth component of the source function for each frequency can be described with

$$\tilde{S}_S = f_{\text{esc}} \tilde{S}_{S,0} + \tilde{S}_{S,U},$$

with

$$\tilde{S}_{S,0} \propto \dot{\rho}_e,$$

and

$$\dot{\rho}_e = 0.1 \epsilon(z) \frac{M_\odot}{\text{yr Mpc}^3} \frac{\rho_{\text{gas}}\,\bar{\rho}_{\text{gas}}}{\rho_{\text{gas}}},$$

where $\tilde{S}_{S,0}$ is the contribution from stars in galaxies, $\tilde{S}_{S,U}$ is the contribution to the source function from unresolved quasars, and $f_{\text{esc}}$ is the effective escape fraction. Also, $\dot{\rho}_e$ is the star formation rate described by the gas density $\rho_{\text{gas}}$, the bias factor $b_S$, and the efficiency $\epsilon$ (eq. [4]). $\tilde{S}_{S,U}$ is usually small compared to the stellar component. Both components are given by the star formation rate, and thus are the same in all simulations, making $f_{\text{esc}}$ the only free parameter.

Equation (12) shows that any change in $f_{\text{esc}}$ will change the number of photons present outside the high-density regions and thus the average ionizing flux transmitted through the box. This in turn changes the amount of neutral hydrogen present. Thus, increasing the escape fraction results in a higher number of photons available for ionizing the IGM and influences the time of reionization. In our simulations, we treat the escape fraction as a phenomenological free parameter, which we adjust to fit the mean transmitted flux observed in the spectra of Sloan Digital Sky Survey (SDSS) quasars (see § 5).

For each of the three cases of clumping factors mentioned above, we have to adjust the effective escape fraction, since each case treats the photons emitted and absorbed in high-density regions differently. First we have case A, in which we include all the local absorption in calculating the clumping factors, and second case B, in which we weight the volume by the inverse density, increasing the influence of the lower density regions. Thus, both cases include the high-density regions and the photons absorbed there. On the other hand, case C does not include the high-density regions, and therefore fewer photons are used in the reionization process.

In general, when escape fractions are calculated, only photons that actually escape from the source are counted. Considering that these sources are commonly positioned in high-density regions in the IGM, the conventional definition of escape fraction best corresponds to case C.

Since the effective escape fraction describes the number of photons that escape compared to the number of photons produced, $f_{\text{esc}}$ should be unity for case A if the star formation rate used for the simulation is correct, since all photons are counted. Our model given by equation (4), however, does not calculate the star formation rate perfectly realistically. If the star formation rate is underestimated, it is expected that the effective escape...
fraction will be larger, to correct for the lack of photons. In addition, errors in the calculation of \( C_l \) and \( C_R \) due to scatter in the simulated data (see \( \S \) 2.2) change the value that is required for \( f_{\text{esc}} \) to yield data in agreement with observations. This problem is compounded by the limited resolution of the small-box simulation used to develop the fit for the clumping factors.

3. SPECTRA

3.1. Lines of Sight

The main purpose of our large-scale simulations is to produce synthetic absorption spectra, which can be compared directly to actual spectra. First, we determine the positions of the brightest quasars present in the simulation box at the chosen redshift to get starting points for the lines of sight. Beginning the spectrum at precisely the source’s position is important, because only then does the \( \text{H} \) \( \text{II} \) region surrounding it appear in the spectrum. This will allow us to compare our synthetic spectra to absorption spectra of high-redshift quasars in which the source is used as the background lighting and derive properties of the \( \text{H} \) \( \text{II} \) regions surrounding the bright quasars. The spectrum will not display the increase in transmitted flux expected for an \( \text{H} \) \( \text{II} \) region at the high-\( z \) end of the spectrum if it starts at a different position.

After determining the starting point, we cast a ray from the quasar position through the box by setting a random direction and following it on a straight line through the box. To get additional resolution and a smoother spectrum, we cast the ray with a step size one-quarter of the cell size. The values of density, neutral fraction, and temperature are output at each step by using a weighted average of their values at the eight closest grid points. Because many spectra sampling different directions are necessary for statistical analysis of the \( \text{H} \) \( \text{II} \) regions and IGM properties, we created three to five spectra for each of the 50 brightest objects in the simulation box.

Because of the large distances along the ray, the universe expands measurably while an imaginary photon of our ray of light crosses the computational box. Thus, we have to take into account the expansion of the universe along the spectrum. Accordingly, we not only have to cast the line of sight in space, but also have to consider the time evolution, using consecutive output files of the simulation.

The spectra so obtained represent random samples of the universe between \( z = 6.5 \), corresponding to 9120 Å for Ly\( \alpha \) emission, and \( z = 4.0 \). The starting points for the different sets of spectra were picked to be the redshifts of the most distant SDSS quasars observed, and also included some lower redshifts to determine the evolution of \( \text{H} \) \( \text{II} \) region sizes (starting points between \( z = 6.5 \) and \( z = 5.9 \)). The comoving distance between \( z = 6.5 \) and \( z = 4.0 \) is 891 \( h^{-1} \) Mpc, so depending on the direction of the line of sight and the position of the quasar, a spectrum can cover a distance too long for one box size. In this case, the spectrum wraps around the periodic box to cover the wavelength range from before to after reionization. The direction of the ray is chosen randomly to get around the problem of the ray passing repeatedly through exactly the same region of the simulation. This stacking of boxes is similar to the method used by Mesinger et al. (2004) and Cen et al. (1994).

3.2. Small-Scale Structure

From the simulation output alone we can only extract information about large-scale variations in \( \rho, n_{\text{HI}}, n_{\text{HII}}, \) and \( T, \) because the resolution of the simulation is limited. High-resolution spectra from instruments such as Keck can reveal information about more neutral gas in between the quasar and the observer on small scales, using the Ly\( \alpha \) forest lines. For example, the spectrum (Fig. 5) of quasar SDSS J1030 at \( z = 6.28 \) has a resolution of \( \delta \lambda = 1.63 \) Å, whereas our resolution from the simulation is about \( \delta \lambda = 9 \) Å.

Typically, normal-sized galaxies or Lyman limit systems show Ly\( \alpha \) features on a scale of a few angstroms, smaller than the resolution of the simulation. To allow comparison to real observations, we add, a posteriori, small-scale structure due to density fluctuations below the resolution limit.

In order to generate the small-scale structure along the simulated line of sight, we compute the one-dimensional matter power spectrum as

\[
P_{1D}(k) = \pi \int_{k}^{\infty} q P_{3D}(q) dq,
\]

where \( P_{1D}(k) \) and \( P_{3D}(q) \) are one-dimensional and three-dimensional power spectra, respectively. A similar equation can be written for the velocity fluctuations, which are needed to take into account the effects of Doppler shifts from peculiar motion. To get a resolution in wavelength space fine enough to be able to compare the flux to observational spectra, the number of steps \( n \) were chosen to be 2\( 15 \). We then apply a fast Fourier transform to generate a real-space representation of linear overdensity \( \delta_L \) and velocity \( v_L \) along a line of sight on a uniform spatial mesh with mesh spacing \( \Delta x = 10 \ h^{-1} \) kpc, smaller than the thermal broadening of the synthetic spectra, to alleviate the dependence on this parameter.

We need to modulate the small-scale structure using the large-scale variations directly obtained from the simulation in density \( \rho_{\text{sim}}, \) temperature \( T_{\text{sim}}, \) and neutral hydrogen density \( n_{\text{HII,sim}} \) along the simulated line of sight to obtain the small-scale distributions. This combines the data obtained from the simulation with a resolution on scales of a few \( h^{-1} \) Mpc with the fluctuations implied by the power spectrum on much smaller scales.

We transform the small-scale linear fluctuations \( \delta_L \) along a line of sight using the lognormal model (Shandarin et al. 1995; Bi & Davidsen 1997) to get

\[
\rho_{\text{los}}(l) = \rho_{\text{sim}} e^{\delta_L - \sigma^2/2},
\]
and then use this $\rho_{\text{los}}(l)$ to obtain the distributions for temperature and neutral hydrogen density:

$$T_{\text{los}}(l) = T_{\text{sim}} \left( \frac{\rho_{\text{los}}}{\rho_{\text{sim}}} \right)^{0.2},$$

$$n_{\text{H}}_{\text{los}}(l) = n_{\text{H}}_{\text{sim}} \left( \frac{T_{\text{los}}}{T_{\text{sim}}} \right)^{0.7} \left( \frac{\rho_{\text{los}}}{\rho_{\text{sim}}} \right),$$

where $\rho$ is the mass density, $T$ is the temperature, $n_{\text{H}}$ is the neutral fraction of hydrogen, and $\delta$ is a small-scale overdensity. The subscript “los” refers to small-scale structure along the line of sight and the subscript “sim” again refers to values obtained directly from the simulation (low spatial resolution).

The last two equations assume ionization equilibrium, which is a relatively good approximation after the overlap of $\text{H} \text{II}$ regions (Gnedin 2000), and a density-temperature relation in the form $T \sim \rho^{0.2}$, which is a reasonable approximation for the $5 < z < 6$ redshift interval (Hui & Gnedin 1998; Gnedin 2000).

The resulting distributions of density, neutral fraction, temperature, and velocity yield a synthetic absorption flux along the line of sight that includes the small-scale fluctuations resulting in a synthetic spectrum that represents both large- and small-scale structure.

4. QUASARS AND $\text{H} \text{II}$ REGIONS

Quasars are the brightest objects known at many wavelengths, and thus they can be observed at high redshifts. The brightest quasars have a bolometric luminosity at $z = 6$ of around $10^{12.5} L_{\odot}$. Much of the emitted radiation is mainly in the UV and can ionize a large region of gas surrounding the quasar, called the $\text{H} \text{II}$ region.

In general, the size of the $\text{H} \text{II}$ region depends on both density and clumpiness of the gas and also the abundance of ionizing photons. This means that in addition to density and clumpiness, the age and luminosity of the source play an important role in the process of forming the $\text{H} \text{II}$ region and determining its spatial growth.

Analyzing the distribution of the $\text{H} \text{II}$ region sizes and how they evolve with time can give us information about the characteristics of quasars and the properties of the gas surrounding them. In this paper we use the lines of sight described in § 3.1 to determine the size of the $\text{H} \text{II}$ regions. The edge of the $\text{H} \text{II}$ region around a quasar should be detectable as a clear increase in $\text{Ly} \alpha$ absorption just redward of the quasar’s $\text{Ly} \alpha$ emission line.

The fact that the neutral fraction increases farther away from the quasar due to the dilution of photons can be used to determine the size of the $\text{H} \text{II}$ region. It means that there will be more neutral gas farther away from the quasar, so the ionizing radiation cannot escape and there is a decrease in transmitted flux.

We define the edge of the $\text{H} \text{II}$ region to be the minimum of the flux, before it increases again due to general reionization of the universe. To be able to measure this $\text{H} \text{II}$ region in the simulation, the quasar needs to be bright enough to ionize an area larger than a resolution element of the simulation.

Additional problems in detecting the $\text{H} \text{II}$ regions and determining their sizes are caused by the fact that the $\text{H} \text{II}$ regions are not necessarily spherical and also that the quasars do not have to be positioned at their center. The irregular shape of the $\text{H} \text{II}$ regions is mainly due to the “lumpiness” of the gas, which means that less dense parts of the IGM are ionized faster than other more dense ones.

There are, of course, many different parameters that can influence the size distribution, only some of which can be understood and modeled. For example, larger regions can be caused either by lower density in a relatively uniform IGM, or by higher luminosity of the quasars or by lifetimes long enough for the quasars to reach equilibrium.

The synthetic spectra can serve as the basis of our analysis of the effects of the different clumping-factor models and the simulations of reionization. The following sections will show how we used these lines of sight to obtain distributions of $\text{H} \text{II}$ region sizes and other characteristics of the spectra.

5. RESULTS

5.1. The Mean Transmitted Flux

Our primary goal is to reproduce the spectra of high-redshift SDSS quasars as closely as possible. To accomplish this, the first step was to create a simulation of reionization covering a large volume and compare it to observations taken at high redshifts, using SDSS data to better reproduce the mean transmitted flux.

We ran a large number of simulations with varying $f_{\text{esc}}$ and clumping-factor models to obtain the best fit to the SDSS data possible. These trial runs constrained $f_{\text{esc}}$ for each clumping-factor model. Then this set of runs was used to test our approach and to determine whether our analysis with synthesized spectra was appropriate. Thus, we obtained several 64$^3$ cell test runs with either 10 or 2 $h^{-1}$ Mpc cell size.

The production runs have 128$^3$ cells, again with either 10 or 2 $h^{-1}$ Mpc cell size for all three clump-factor models. In addition, we also have runs for varying quasar lifetime with 128$^3$ cells and 2 $h^{-1}$ Mpc cell size, since this combination of simulation parameters gives us good resolution and a large enough volume to contain some bright quasars.

Table 1 summarizes a few of the best-fit runs with all their initial parameters. Figure 6 compares, for each of these runs, the mean transmitted flux averaged in redshift bins $\Delta z = 0.1$ from $z = 4$ to 6 to that measured by White et al. (2003) from SDSS quasars. In all cases shown in Figure 6, the mean transmitted flux gives a reasonable fit to the SDSS data. This means that for each model, the escape fraction can be adjusted to achieve consistency with the mean transmitted flux measured from the SDSS data.

Further analysis, discussed in §§ 5.3 and 5.5, reveals some difference between the cases, such as in the distribution of $\text{H} \text{II}$ sizes and of troughs in the spectra.

When comparing the different cases, we observe, as expected, that case A has the largest $f_{\text{esc}}$. This is because we take into account all the photons in the high-density regions. The best-fit values for case B are the smallest, only around a few percent (§ 5). The significant difference in the values for $f_{\text{esc}}$ for the various clumping-factor models show how different the methods of counting photons are and how they affect the amount of ionizing flux, but the fact that we can fit all three models within reasonable error to the SDSS data shows that $f_{\text{esc}}$ is a convenient phenomenological parameter.

Fitting the effective escape fraction to get the correct shape in a flux-versus-redshift plot requires several simulation runs with varying escape fraction (see § 5.1) to close in on the correct $f_{\text{esc}}$. We mainly fit the average transmitted flux between $z = 5$ and $z = 6$, because of the larger errors on the SDSS data at higher redshifts and our focus on simulating the period of reionization.

In addition to the three different cases for the clumping factors, the best-fit values for the effective escape fraction also depend weakly on numerical resolution and box size. These effects are
usually not large, but need to be taken into account to obtain the best fits to the data.

Figure 6 shows that the case of $10^9$ yr quasar lifetime is barely distinguishable from that of infinite lifetime. In effect, $10^9$ yr is tantamount to infinite lifetime, because the age of the universe is 0.92 Gyr at $z = 6$. The best-fit escape fractions are similar: $f_{\text{esc}} = 0.065$ for $10^9$ yr, versus $f_{\text{esc}} = 0.07$ for infinite lifetime. The effective escape fraction for the shorter lifetime is slightly smaller, because for a given luminosity function, quasars with shorter lifetimes are less biased.

The normalized transmitted flux of all the runs shown in Figure 6 tends to 0.2 at $z = 4.5$ at the low-redshift end, but for the high-redshift end there is a larger variation in the flux between the different runs. The data obtained from SDSS at redshifts $z > 5$ have a larger error because there are fewer high-redshift quasar observations, so that our results lie within the error for this regime. The general trend of the SDSS data is fit well, although the spread in the timing of reionization of about $\delta z = 0.3$ along different lines of sight

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Figure 6 illustrates that the model for the clumping factors only weakly affects the evolution of the IGM during reionization. One of the slight deviations can be seen in case C, where the high-density regions are excluded from the calculation of the clumping factors. The mean transmitted flux curve shows a somewhat more rapid ionization around $z = 5.5$ to $z = 6.0$. The case C models follow the curve set by the SDSS data more closely, but at lower redshifts they tend to lower neutral fractions than case B models. Figure 6 emphasizes that independent of the choice of cell size, box size, and model, there is an escape fraction $f_{\text{esc}}$ that fits the transmitted flux of the simulation run to the SDSS data.

Figure 7 shows two sets of the same data analyzed independently by White et al. (2003) and Songaila (2004). For clarity, only the error bars on the White et al. set are displayed. Also shown is a mean transmitted flux curve from one of our simulations and the 1 $\sigma$ deviation of the flux from this mean in the various lines of sight. The fit clearly lies within the error of the observational data. The variations in mean transmitted flux from the simulation increase toward higher redshift, indicating the spread in the timing of reionization of about $\delta z = 0.3$ along different lines of sight.

For a clearer illustration of how reionization proceeds in our simulation, Figure 8 shows the evolution with redshift of the averaged photoionization rate $\Gamma$ in different simulations. For these figures, the photoionization rate $\Gamma$ of the gas was averaged over the entire simulation box instead of along a line of sight. In all the different cases shown, the rapid increase of $\Gamma$ at $z \sim 7$ is

![Figure 6](image1.png)  
**Fig. 6.—** Average flux vs. redshift for the SDSS data and some of the best fits: SDSS data from White et al. (2003; filled triangles), run 3 (black long-dashed line), run 4 (gray dotted line), run 5 (black short-dashed line), run 6 (gray dash-double-dotted line), run 7 (gray dashed line), run 8 (gray dash-dotted line), run 9 (black dotted line), run 10 (black dash-dotted line), and run 11 (black dash-double-dotted line). Notice how similar all models and resolutions appear when fitted with $f_{\text{esc}}$.

![Figure 7](image2.png)  
**Fig. 7.—** Mean transmitted flux for two different analyses of the same set of SDSS quasars: Songaila (2004; filled triangles) and White et al. (2003; open squares) compared to the mean transmitted flux calculated for run 10 (which we choose just for illustration purposes; other models have very similar variations in the mean transmitted flux with redshift), a case C $128^3$ simulation with $2 \, h^{-1}$ Mpc cell size (solid line). Shown also are the lines corresponding to 1 $\sigma$ change at each redshift for the synthetic spectra (dash-double-dotted lines).
clearly visible; in addition, the rate of increase of $\Gamma$ versus redshift is lower than predicted by small-box simulations (Gnedin 2000, 2004). This period of rapid increase corresponds to a drop in neutral gas that is spread over a range in redshift of only $\Delta z \sim 1$. 

Figure 8 illustrates how box and cell size affect the averaged photoionization rate $\Gamma$ for case B. The graph indicates a spread of about a factor of 3 as the ionization rate $\Gamma$ increases by $\sim 10^4$ and the redshift varies from $z \sim 9$ to $z \sim 4$. The main systematic difference appears to be that the photoionization rate is, on the whole (except during reionization), lower in the lower resolution simulations with $10 \ h^{-1}$ Mpc cell size. This difference can be attributed to the difference in clumping factors, and can be interpreted as an indication of the uncertainty arising from the use of the clumping-factor formalism.

The first panel of Figure 9 shows the evolution of the volume-weighted hydrogen neutral fraction during the epoch of reionization, with observational data (Fan et al. 2006) overlaid. At low redshifts the neutral fraction tends to $10^{-5}$. At $z = 9$ the simulation volume is not completely neutral, but is already 40% ionized. This results in a optical depth of about $\tau_6 \sim 6.7\%$ (the three clumping-factor models range between $\tau_6 = 6.4\%$ and $\tau_6 = 6.7\%$), so our simulation results are in agreement with the 3 yr WMAP data release (Spergel et al. 2006).

The second panel of Figure 9 shows a graph of the mean free path versus redshift for a case A simulation. We used case A clumping factors because they yield the mass-weighted neutral fraction needed to compute the mean free path. Overlaid is the mean free path inferred by Fan et al. (2006) from SDSS data. The mean free path changes drastically between $z = 7$ and $z = 5.5$, where it increases 3 orders of magnitude from 0.01 to about 10. This is the period of overlap during reionization, where the individual H ii regions grow large enough to combine. The discrepancy with the observational data at $z \lesssim 5$ arises from the fact that the clumping factors were calculated using small-box simulations with $z > 5$, which underpredicts the Lyman limit systems at lower redshifts.

Both figures show that while fitting the mean transmitted flux does not depend significantly on the clumping-factor model used, there appears to be a difference for other variables. The observational data for the neutral fraction implies earlier ionization of the IGM than the simulation. To better fit this data, we need to have a more accurate model of the density distribution of the IGM. This deviation from the observational data might prove useful in determining which clumping-factor model best describes the IGM, since the observed neutral fraction does not depend significantly on the clumping-factor models.

To analyze the process of reionization in greater detail, Figure 10 shows the scatter in the ionization of subvolumes in the simulation. The graph shows the relative dispersion of the mean neutral fraction of the IGM for various smoothing sizes. The neutral fraction was averaged over different volumes ranging from 2 to $160 \ h^{-1}$ Mpc, corresponding to volumes between 1 and 80 cells. This allows us to better understand the variation of the neutral fraction with both redshift and size of smoothing region. The highest value of relative dispersion corresponds to $z = 6.67$. The figure shows that near the epoch of reionization the variation in neutral fraction is nearly 40% on a scale of $2 \ h^{-1}$ Mpc and is progressively smaller on larger scales.

5.2. Examples of Synthetic Spectra

As described in § 3.1, we use synthetic spectra to allow comparison between the results of our simulations and observations. Small-scale variations are added to the synthetic spectra created from the simulations, as described in § 3.1. In the following paragraphs we compare the large-scale variations with the synthetic spectra composed from the convolution of large and small scales.

The top left panel of Figure 11 shows a synthetic spectrum of a quasar at $z = 6.49$, which is about the same distance as the farthest quasar observed so far, over the whole wavelength range from 9100 to 6000 Å. To be comparable to observational data,
the resolution of this synthetic spectrum is the same as for spectra obtained with the best ground-based telescopes, such as Keck. This plot shows how the large-scale neutral fraction decreases with shorter wavelengths because the universe is more ionized (Miralda-Escudé et al. 2000, Miralda-Escudé 2003), so that the average flux increases around 7500 Å or $z \sim 5.2$, as can be seen in the large-scale flux distribution and has been observed in SDSS spectra. Also, this figure shows how the transmission gaps thin out toward higher redshifts and the overall average flux decreases, similarly to the Gunn-Peterson trough found in observational spectra.

The bottom left panel of Figure 11 shows the same spectrum as in the top panel. Here we zoom into some of the large gap regions centered at 8550 Å and their surroundings to show the sparse transmitted flux in more detail. Gaps this large at a relatively low redshift should correspond to large-scale overdensities in the IGM (see also §5.5). It is also notable how dense the Ly$\alpha$ forest is at these redshifts, which shows that the IGM is not ionized enough at this epoch to be transparent. This does not imply that the IGM is neutral, because even a small fraction of neutral hydrogen increases the optical depth drastically.

The right panel of Figure 11 is a zoom to the high-redshift end of the spectrum. It shows the transmitted flux from the H II region of the quasar both on small scales (solid line) and smoothed to a resolution of 10 Å for calculating the H II region size (dash-dotted line).

5.3. Simulated H II Regions

A bright quasar can photoionize a large region around it: its H II region. The H II region is detectable in spectra as an increase in transmitted Ly$\alpha$ flux to the red side of the quasar’s Ly$\alpha$ emission line. Our spectra can be used to obtain properties of H II regions and then compare them to observed properties. To analyze the sizes of the H II regions, we calculate several characteristics of the H II regions surrounding a quasar and how they change with time. Some of these characteristics are also measurable in observed high-resolution spectra: e.g., the maximum of the mean transmitted flux near the quasar, the closest distance to the quasar at which the flux is minimal, and the area under the flux versus wavelength curve. These values give a measure of the size of the H II region and can be compared to observed data. Since flux increases, on average, with decreasing redshift due to the ionization of the IGM, the flux minimum should be a measure of the boundary of the H II region.

Small-scale fluctuations and low spatial resolution can prevent us from finding the actual minimum. Also, our simulation does not produce spherical H II regions, as can be seen in the two panels of Figure 12, causing several different values for the size of an H II region depending on the direction of the line of sight cast. The images in Figure 12 show two cross sections of the simulation box gray-scale coded by the neutral fraction from $x_{HI} = 10^{-5}$ in black to $x_{HI} = 10^{-4}$ in white ($x_{HI} = n_{HI}/n_{H}$). The top cross section lies in the $x$-$y$ plane, while the bottom one shows a $z$-$y$ projection. The slices are positioned at the position of a luminous quasar in the simulation and shows the large H II regions (black shading) surrounding it as cross sections through the simulation box.

Near the top of the left panel of Figure 12, one can clearly see a relatively spherical H II region surrounding a bright quasar. Near this large H II region there are other smaller highly ionized regions in dark gray shading, corresponding to $x_{HI} < 10^{-4}$. These regions correspond to fainter quasars and their H II regions. In the lower right part of the image is an example of a non spherical H II region around another very bright quasar. It is more difficult to obtain a reliable value for the size of the H II region because it is so irregularly shaped. Since most of our quasars produce ionized regions that are non spherical, we cast several lines of sight from each quasar to obtain a statistically relevant sample.
The second panel of Figure 12 shows a perpendicular slice of the same simulation. Here the complicated structure of the H ii region is even more pronounced, with features that resemble a plume. There are also a few white spots in the image, which correspond to highly neutral regions in the simulation. These spots would show up as regions in spectra with no transmitted flux.

Figure 13 gives a closer view of the same H ii region. The black area is the highly ionized region and has a diameter of about 8 h\(^{-1}\) Mpc; however, the ionized region extends much further (shown in darker gray). The irregular, elongated shape of the ionized region is almost completely surrounded by almost completely neutral gas on either side. This high-density gas has not yet been fully ionized and confines the H ii region to a “tunnel.” The ionizing radiation can escape from the quasar only through this tunnel, because the mean free path is much lower in the orthogonal direction. Also, Figure 13 shows several areas with low neutral fraction around the main H ii region. Most of these spots, which have a neutral fraction of about 10\(^{-3}\), are clustered together with other more ionized “blobs” shown in lighter gray.

At this redshift (z = 6.28) the universe is already very close to fully ionized, so the gray areas that have a neutral fraction of 10\(^{-3}\) to 10\(^{-4}\) (on scales of our resolution, 2 h\(^{-1}\) comoving Mpc) are the most neutral regions in the simulation at this redshift. However, this does not imply that the spectra will have a large transmitted flux, because even a neutral fraction as low as 10\(^{-4}\) is sufficient to absorb all flux from the quasar.

The IGM in the vicinity of the luminous quasars in our simulations is substantially more ionized than inferred for the vicinities of SDSS quasars by Mesinger & Haiman (2004) and Wyithe & Loeb (2003). However, at least part of this discrepancy probably results from the fact that none of our quasars are as luminous as the SDSS quasars, so our quasars are not as biased, and thus reside in less dense, hence more highly ionized, regions.

**5.4. Properties of H ii Regions**

The sizes of H ii regions, measured from the extent in wavelength of the region of increased flux, offer a point of comparison between simulations and observations.

The simulations show that a quasar’s H ii region is typically neither spherical nor sharply defined, so the notion of its size is inevitably somewhat hazy. We define the size of an H ii region for our synthetic spectra as the first minimum in the flux, with $F < 0.01$ or $F < 0.03$. The flux cutoff is calculated by smoothing the synthetic spectra, including the small-scale flux, so that the resolution is 10 Å, corresponding to 2.5 h\(^{-1}\) Mpc at $z = 6.28$. The first minimum of the flux that falls below the cutoff flux is defined as the edge of the H ii region, and thus corresponds to a region where there is no or little flux over a scale of 10 Å.

This definition reflects the fact that the degree of ionization should be high in the immediate vicinity of the quasar, should decrease moving away from the quasar, and then should increase again because of the general ionization of the universe. It is also similar to methods for determining the size of H ii regions from observational spectra.

The location of the minimum of the transmitted flux, which yields the size of the H ii region, depends on the resolution of the spectrum. To allow unbiased comparison between simulations and observations, the resolution of the synthetic spectra must match closely that of the observations.

Because the H ii regions are aspherical, different lines of sight yield different measures of its size. For each simulation, we construct synthetic spectra from three random lines of sight through each of the 50 brightest quasars. The result is an ensemble of ~150 spectra from each simulation. It is this ensemble of spectra for each simulation that we compare to observations, such as the spectrum for SDSS J1030+0524 (X. Fan 2005, private communication), throughout the paper.

For example, Figure 14 shows one of the distributions of the size of the H ii region as a function of the area under the flux versus wavelength curve. The area under the spectrum indicates the degree to which the gas in the H ii region is ionized. The distribution shown is for a simulation with case B clumping factors, 2 h\(^{-1}\) Mpc cell size, and 128\(^3\) cells at $z = 6.28$. In general, the physical distance to the minimum flux and the area under the spectrum are two properties that can be observed and then compared to our simulations if the resolution is known. For example, the values for SDSS J1030+0524 are also included in the figure (black square).

Figure 15 illustrates the measurement of the H ii region size of SDSS J1030+0524 from the high-resolution spectrum. The black dash-dotted line displays the spectrum smoothed to a spatial resolution corresponding to 10 Å. The position of the redshifted Lyα line (gray dash-dotted line) at 8852 Å and the assumed edge of the H ii region (gray dashed line) are shown as vertical lines. The line at 8748 Å shows the edge of the H ii region using the
smoothed flux and finding the first minimum that also lies below the threshold flux of 0.01. This measurement is the same as the method used on the simulation data and yields a physical size of 4.76 Mpc.

The discrepancy of the area under the spectrum, apparent from Figure 14, for the quasars from our simulation and the SDSS quasar can be attributed to the much higher luminosity of the SDSS quasar. The brightest quasar from the simulation has a luminosity of $3.09 \times 10^{12} L_{\odot}$, whereas J1030+0524 has about $1.3 \times 10^{13} L_{\odot}$. Higher luminosity quasars will emit more photons, which not only increases the size, but also reduces the ionization fraction of the gas in the H II region. Comparison of this graph to Figure 11 shows that the transmitted flux near the quasar, corresponding to the amount of ionized material, is significantly larger for the observed quasar than the transmitted flux for any of our simulated ones. This means that the gas is more highly ionized around this quasar.

Figure 16 displays the effects of simulation resolution on measuring the H II region sizes by comparing 2 and 10 $h^{-1}$ Mpc cell size runs. The two distributions are rather similar; we also find fewer H II regions for lower resolution simulations, as would be expected, because most of our H II regions are too small to be detected with a coarser resolution.

Figure 17 shows the dependence of the size of the H II regions on quasar lifetime. Of the three lifetimes shown, $10^7$, $10^8$, and $10^9$ yr, the longest, $10^9$ yr, gives results that are barely distinguishable from infinite lifetimes. This is to be expected because the age of the universe at $z = 6$ is only about 0.9 Gyr. In the case of finite lifetime, quasar lifetimes are distributed with an exponential probability distribution with the given mean, so that not all quasars have the same lifetime. Thus, even if the mean lifetime is longer than the age of the universe, a fraction of quasars still managed to turn off before $z = 6$. In the case with infinite lifetime, no quasars turn off. For the shortest lifetime, however, the increased abundance of smaller H II regions results from new quasars starting new H II regions. For longer lifetimes, the quasar can emit photons into the IGM for longer time periods after ionizing its immediate high-density surroundings, so that the H II regions for shorter lifetimes will be smaller.

The lines of sight for the spectra start at the position of the quasar and extend in a random direction through the box, and therefore we only probe one specific part of each H II region with each large-scale spectrum. Thus, using just one line of sight for measuring the size of the ionized region surrounding each quasar does not necessarily represent the actual H II region size. To improve the statistical estimate of the H II region size, we cast three lines of sight in random directions through each quasar. Thus, even if the quasar is located at the edge of a very high density region in the IGM, we should be able to detect the H II region in one of the three lines of sight cast. We used each line to measure the size of the H II region separately, and so accumulated distributions for their sizes.

Figure 18 addresses the question of shape of the H II regions. The three lines of sight for each quasar yield a maximum and a minimum size, which are shown as filled triangles. The line corresponds to spherical H II regions, in which the two parameters would be equal. The figure shows that few of the H II regions are spherical. Some of the spectra show a large discrepancy between maximum and minimum size, and for a few we do not even detect the H II region in one of the directions within the limits of our

5 Because most of the H II regions are barely resolved even with $2 h^{-1}$ Mpc resolution, using more than three lines of sight does not actually improve statistics.
Numerical resolution. Thus, the measurement of \( \text{H} \text{II} \) region sizes from one line of sight of a quasar does not provide a complete picture of the volume contained in the \( \text{H} \text{II} \) region.

One of the difficulties in determining the \( \text{H} \text{II} \) region size from this simulation is that our spatial resolution for the spectra can only be as small as the cell size of the simulation box. This causes smoothing on scales of 2–10 \( h^{-1} \) Mpc, depending on the simulation run. This means that we can easily miss or overestimate the \( \text{H} \text{II} \) region size. In Figures 16–18 we plot the physical size of \( \text{H} \text{II} \) regions, where the smallest ones correspond to only one cell. If the quasar is positioned in an extremely high density region, the ionized volume surrounding it can be too small to appear in a spectrum with such low resolution. Also, if the smoothing causes the edge of the \( \text{H} \text{II} \) region (set to be at the closest flux minimum to the quasar in accordance with the method used for the synthetic spectra) to disappear, the size of the ionized volume due to the quasar can be much smaller than determined by our method.

5.5. Troughs in the Spectra

In addition to analyzing the ionization of the IGM around luminous sources, we also investigated the distribution of low-flux regions, associated with higher neutral fraction, using the synthetic spectra. Regions in the simulation volume with high neutral fraction along the line of sight will appear as troughs in the absorption spectrum. The extent of these troughs in the spectra and their positions in space give us information about structure of the IGM between the quasar and the observer. Since only a small amount of neutral gas is required to absorb almost all of the flux, the depth of the troughs is not used for analysis.

For this analysis, we use the same sets of synthesized spectra as described in \( \frac{3}{2} \) 3.1 and scan them for regions with extremely low flux, below a threshold detectable by instruments, here set to \( 10^{-3} \). We then compile distributions of these troughs from the 150 spectra obtained from each simulation and plot their distributions. A few examples of these distributions are shown in Figures 19 and 20. These figures show only the largest troughs, which extend more than 10 \( \text{Å} \).

We scanned the spectra for troughs between \( \sim 9100 \text{ Å} \) (corresponding to \( z = 6.5 \)) and \( \sim 7200 \text{ Å} \) (corresponding to \( z = 4.9 \)). The most striking feature of this set of distributions is their similarity. For example, all the different runs display a decrease in average length of the low-flux regions toward shorter wave-lengths. This feature can be explained by the increase in the mean free path for ionizing photons due to the reionization of the universe.

Figure 19 illustrates the similarity of the distributions by taking a closer look at the trough distributions for two different clumping-factor models (case C in gray triangles and case B in black triangles). The two distributions nearly completely overlay each other. The only visible difference is a small excess of large high-redshift troughs for case C and an excess for case B at lower redshifts (\( z \sim 7700 \)). This means that there is no difference in the trough distribution between the clumping-factor models, and together with the mean transmitted flux data this allows us to pick any of the three cases for analysis.

Another notable similarity is the fact that the largest troughs for each simulation are all about the same size, 100 \( \text{Å} \). Most of these long stretches of low flux in the spectra lie above 8500 \( \text{Å} \), with a few outliers in some of the simulations. For example, Figure 19 shows two troughs of about 40 \( \text{Å} \) centered at 7800 \( \text{Å} \) for case B, which corresponds to a stretch of \( \sim 3.5 \) Mpc at redshift \( z = 5.4 \), or 14 \( h^{-1} \) Mpc in comoving units. Since a trough only appears in this distribution when the flux is \( < 10^{-3} \), these
two troughs are produced by very large regions of relatively neutral gas in the IGM. For example, Figure 11 shows a spectrum containing a large trough near $z = 6.0$ that extends for 100 Å, similar to the largest troughs shown in the distribution.

Figure 20 shows that we can, similarly to the H II region size calculations, compare our results for trough distributions from synthetic spectra with the quasar spectrum SDSS J1030+0524. Since the data of the observed spectrum contains noise, we have to set a level of uncertainty below which we assume that the transmitted flux is zero. The black triangles correspond to 3 $\sigma$ as the threshold for no transmitted flux and the open squares correspond to a threshold of 5 $\sigma$. The distribution for the troughs obtained from the simulation is shown in Figure 20 as gray triangles, and the similarities of the observation to the simulation are clearly visible. The 3 $\sigma$ detection limit yields a better agreement with the simulations, but both values show the same decrease in large troughs toward lower redshifts and similar sizes for the troughs over the whole redshift range.

In contrast to measurements of H II region sizes, the comparison of resolution sizes of the simulation (Fig. 21) does not reveal a strong dependence on resolution. The largest trough size for both cases is around 100 Å at high redshift, and both show a slow decrease in trough size toward the lower redshifts. In addition, they both exhibit a few outliers of larger size, as mentioned above. There is a slight excess of larger troughs for the 10 h$^{-1}$ Mpc simulation. This is due to the larger step size in the synthetic spectra, which removes some of the small spikes in transmitted flux that intersect large troughs.

Altogether it is clear that the differences for varying parameters of the simulations do not change the distribution of troughs in the spectra significantly. This invariance to parameter changes allows us to conclude that as long as we fit the mean transmitted flux from SDSS, we will reproduce the gross features of the Ly$\alpha$ forest as well.

5.6. Flux Decrement

In addition to looking at how the mean transmitted flux changes over time, the change in ionization of the IGM can also be observed when we consider how many pixels of the spectra fall below a certain flux at each redshift. Figure 22 shows this “flux decrement” for five different levels: $F_0 < 0.3$, $F_0 < 0.2$, $F_0 < 0.1$, $F_0 < 0.05$, and $F_0 < 10^{-3}$. Even at the low-redshift end, around $z = 4.0$, only about 40% of the pixels still have $F > 0.3$. The curve corresponding to lowest flux limit, which reflects the region in redshift where effectively all the flux is absorbed in neutral gas, displays a drop around $z = 5.5$, below which most pixels have more flux than $10^{-3}$. This means that after redshift 5.5, the universe is ionized enough to eliminate the Gunn-Peterson trough.

It is also important to note that all the distributions, except for the $F_0 < 10^{-3}$ one, reach 1.0 toward higher redshifts, meaning that there is not a significant amount of flux transmitted in this regime. Thus, we can identify the region in the spectra above $z = 5.5$ as the Gunn-Peterson trough. The change in transmitted flux appears to happen within a short period of time, supporting the idea that reionization happened quickly.

6. DISCUSSION AND CONCLUSIONS

We use cosmological simulations to model the large-scale effects of reionization, including luminous high-redshift quasars. A major issue with simulations of large volumes is that a large dynamic range needs to be covered, including cosmic structures on a diverse range of scales. To solve this problem, we have used clumping factors to approximate the small-scale structure of the cosmic gas. These clumping factors are derived from small-volume simulations that can simulate structures on kpc scales and then be used to produce results on Gpc scales with resolution up to 10 h$^{-1}$ Mpc. We developed three models for computing the clumping factors: (1) case A, in which clumping factors are weighted by volume, thus including local absorption and ionization; (2) case B, in which the clumping factors are weighted by the inverse of the density, therefore lowering the influence of high-density regions; and (3) case C, in which we disregard all volume elements with high gas density, and with that all absorption and ionization in high-density regions. All three cases yield similar results and can fit the mean transmitted flux as observed by SDSS.

We use these simulations to construct synthetic spectra of quasars comparable to observed spectra of SDSS quasars at high redshifts. These synthetic spectra are used to investigate H II region sizes of bright quasars in our simulations and to compare with H II regions of observed quasars. We found a significant scatter in the distribution for the sizes, even when looking at a large number of quasar H II regions. The H II region size depends
on quasar lifetime (Fig. 17), with larger \( \text{H} \) regions for longer quasar lifetimes, but this relation is too weak to put constraints of quasar lifetimes by observing their \( \text{H} \) regions.

The synthetic spectra can be used to make detailed comparisons between the observational data and the simulations. In this paper we limit this comparison only to the distribution of \( \text{H} \) regions around bright quasars and the distribution of troughs (regions with no flux) in the spectra. In a future work we plan to use synthetic spectra for a more detailed and elaborate comparison with the observational data.

Future improvements to our method will include, as has been mentioned in § 2.2, an account for the scatter in the modeled clumping factors. As we have discussed above, the clumping factors on scales we are interested in (several comoving Mpc) are not deterministic functions of the gas properties, and should be treated statistically.

In addition, our box volumes, although large, are still too small to contain quasars as bright as the most luminous SDSS quasars. Also, most quasars found in our simulation boxes are still too faint to be detected by even the best telescopes; constrained simulations can be used to model \( \text{H} \) regions around the quasars comparable in luminosity to those observed by the SDSS.

This weak dependence of the simulation results on the particular choice of clumping factors is the main justification of our approach. It demonstrates that as long as ionization and recombinations are counted self-consistently, the specific form of spatial averaging used to define clumping factors is not too important.

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REFERENCES

Bi, H., & Davidsen, A. F. 1997, ApJ, 479, 523
Bruscoli, M., Ferrara, A., & Scannapieco, E. 2002, MNRAS, 330, L43
Cen, R., Miralda-Escudé, J., Ostriker, J. P., & Rauch, M. 1994, ApJ, 437, L9
Chiu, W. A., & Ostriker, J. P. 2000, ApJ, 534, 507
Ciardi, B., Ferrara, A., Governato, F., & Jenkins, A. 2000, MNRAS, 314, 611
Ciardi, B., Ferrara, A., & White, S. D. 2003a, MNRAS, 344, L7
Ciardi, B., Stoeckl, F., & White, S. D. 2003b, MNRAS, 343, 1101
Croom, S. M., et al. 2005, MNRAS, 356, 415
Fan, X., Narayanan, V. K., Strauss, M. A., Becker, R. H., Becker, R. H., Pentericci, L., & Rix, H. 2002, AJ, 123, 1247
Fan, X., et al. 2006, AJ, 132, 117
Ferrarese, L. 2002, ApJ, 578, 90
Giroix, M. L., & Shapiro, P. R. 1996, ApJS, 102, 191
Gnedin, N. Y. 1995, ApJS, 97, 231
Gnedin, N. Y., & Abel, T. 2001, NewA, 6, 437
Gnedin, N. Y., & Hui, L. 1998, MNRAS, 296, 44
Gnedin, N. Y., & Ostriker, J. P. 1997, ApJ, 486, 581
Gunn, J. E. & Peterson, B. A. 1965, ApJ, 142, 1633
Haiman, Z. 2002, ApJ, 576, L1
Haiman, Z., & Loeb, A. 1999, ApJ, 519, 479
Hui, L., & Gnedin, N. Y. 1997, MNRAS, 292, 27
Hui, L., & Haiman, Z. 2003, ApJ, 596, 9
Kashikawa, N., et al. 2006, ApJ, 637, 631
Lidz, A., Hui, L., Zaldarriaga, M., & Scoccimarro, R. 2002, ApJ, 579, 491
Loeb, A., & Barkana, R. 2001, ARA&A, 39, 19
Madau, P., Haardt, F., & Rees, M. 1999, ApJ, 514, 648
Maselli, A., & Ferrara, A. 2005, MNRAS, 364, 1429
Mesinger, A., & Haiman, Z. 2004, ApJ, 611, L69
Mesinger, A., Haiman, Z., & Cen, R. 2004, ApJ, 613, 23
Miralda-Escudé, J. 2003, ApJ, 597, 66
Miralda-Escudé, J., Haehnelt, M., & Rees, M. 2000, ApJ, 530, 1
Schirber, M., & Bullock, J. S. 2003, ApJ, 584, 110
Shandarin, S. F., Melott, A. L., McDaniel, K., Pauls, J. L., & Tinker, J. 1995, Phys. Rev. Lett., 75, 7
Sokasian, A., Abel, T., & Hernquist, L. E. 2001, NewA, 6, 359
Sokasian, A., Abel, T., Hernquist, L., & Springel, V. 2003, MNRAS, 344, 607
Songaila, A. 2004, AJ, 127, 2598
Songaila, A., & Cowie, L. 2002, AJ, 123, 2183
Spergel, D. N., et al. 2006, ApJ, submitted (astro-ph/0603449)
Tegmark, M., Silk, J., Rees, M. J., Blanchard, A., Abel, T., & Palla, F. 1997, ApJ, 474, 1
White, R., Becker, R., Fan, X., & Strauss, A. 2003, AJ, 126, 1
Wyithe, J. S. B., & Loeb, A. 2003, ApJ, 586, 693