PROBING THE REIONIZATION HISTORY USING THE SPECTRA OF HIGH-REDSHIFT SOURCES

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ABSTRACT

We quantify and discuss the footprints of neutral hydrogen in the intergalactic medium (IGM) on the spectra of high-redshift (z ∼ 6) sources, using mock spectra generated from hydrodynamical simulations of the IGM. We show that it should be possible to extract relevant parameters, including the mean neutral fraction in the IGM and the radius of the local cosmological Strömgren region, from the flux distribution in the observed spectra of distant sources. We focus on quasars, but a similar analysis is applicable to galaxies and gamma-ray burst (GRB) afterglows. We explicitly include uncertainties in the spectral shape of the assumed source template near the Lyα line. Our results suggest that a mean neutral hydrogen fraction, x_H, of unity can be statistically distinguished from x_H ≈ 10^{-2} by combining the spectra of tens of bright (M ≈ -27) quasars. Alternatively, the same distinction can be achieved using the spectra of several hundred sources that are ∼100 times fainter. Furthermore, if the radius of the Strömgren sphere can be independently constrained to within ∼10%, this distinction can be achieved using a single source. The information derived from such spectra will help in settling the current debate as to what extent the universe was reionized at redshifts near z ∼ 6.

Subject headings: cosmology: theory — galaxies: formation — galaxies: high-redshift

1. INTRODUCTION

The epoch of cosmological reionization is a significant milestone in the history of structure formation. Despite recent observational breakthroughs, the details of the reionization history remain poorly determined. The Sloan Digital Sky Survey (SDSS) has detected large regions with no observable flux in the spectra of several z ∼ 6 quasars (Becker et al. 2001; Fan et al. 2003; White et al. 2003). The presence of these Gunn-Peterson (GP) troughs sets a lower limit on the volume-weighted et al. 2003; White et al. 2003). The presence of these Gunn-Peterson (GP) troughs set a lower limit on the volume-weighted neutral hydrogen fraction of x_H ≳ 10^{-3} (Fan et al. 2002). This strong limit implies a rapid evolution in the ionizing background from z = 5.5 to z ∼ 6 (Cen & McDonald 2002; Fan et al. 2002; Lidz et al. 2002; Pentericci et al. 2002) and suggests that we are witnessing the end of the reionization epoch, with the intergalactic medium (IGM) becoming close to fully neutral at z ∼ 7 (but see Songaila & Cowie 2002 for a different conclusion). On the other hand, recent results from the Wilkinson Microwave Anisotropy Probe (WMAP) have uncovered evidence for a large optical depth to electron scattering, τ_e ∼ 0.17 ± 0.04 (Bennett et al. 2003) in the cosmic microwave background anisotropies. Assuming a step-function model for the reionization history, this result would indicate that reionization began at z ∼ 17 ± 4 (Kogut et al. 2003; Spergel et al. 2003). Although physically motivated “double” reionization scenarios, proposed prior to the WMAP result (Cen 2003a; Wyithe & Loeb 2003a) are consistent with the combined observations, the details of the reionization process remain far from being clear.

Numerous recent theoretical works have addressed resolutions of the apparent discrepancy (see, e.g., Haiman 2004 for a review). Successful models incorporate various feedback effects, such as that due to metal enrichment (Cen 2003b; Wyithe & Loeb 2003b) or associated with the UV radiation produced by the early ionizing sources (Haiman & Holder 2003). Alternatively, the high-redshift “tail” of ionization has been attributed to an early population of X-ray–producing black holes (Ricotti & Ostriker 2004; Madau et al. 2004) or even to something more exotic, such as decaying particles (Hansen & Haiman 2004). These competing reionization scenarios each predict a different evolution of the neutral fraction beyond z ∼ 6. It would therefore be quite beneficial to observationally determine the values of x_H at the intermediate redshifts of 6 ≤ z ≤ 30.

As a first step toward this goal, differentiating between a neutral and a mostly ionized universe at redshifts just beyond z ∼ 6, would already aid in discriminating between several models (Haiman & Holder 2003). To do this however, one requires a more detailed statistic than the presence or absence of a Gunn-Peterson trough. In this paper, we utilize the transmitted flux distribution of a hypothetical z ∼ 6 source near its Lyα wavelength. While most of the flux on the blue side of Lyα is simply extinguished for a wide range of neutral fractions (10^{-3} ≤ x_H ≤ 1), detectable flux can be transmitted close to the line center, at wavelengths corresponding to a local H_II region around the source (e.g., Cen & Haiman 2000; Madau & Rees 2000). The spectrum on the blue side, as well as the flux processed by the damping wing of IGM absorption and transmitted on the red side of the Lyα line (Miralda-Escudé 1998), depends on the neutral hydrogen fraction of the IGM in which the source is embedded. As a result, the flux distributions can be used as a probe of the neutral fraction in the IGM.

There are two immediate apparent difficulties with the above approach. First, it requires an estimate of the intrinsic spectrum of the source. Second, it requires an ab initio model of the density (and velocity) fields surrounding the source, which will influence the transmitted flux distribution. Since both of these quantities are impossible to predict accurately from first principles for any specific source and line of sight (LOS), a single spectrum is unlikely to provide tight constraints on the neutral
fraction. However, the neutral hydrogen fraction can still be inferred statistically by studying the spectra of a sample of sources. The purpose of this paper is to quantify the accuracy to which \( x_\text{H} \) can be determined in a future sample of high-redshift sources, taking the above complications into account. We use a hydrodynamical simulation to generate mock spectra of sources for different assumed values of the neutral hydrogen fraction of the IGM and quantify the statistical confidence to which these transmitted spectra can be distinguished from each other.

The rest of this paper is organized as follows. In § 2 we discuss the basic signatures of neutral hydrogen in the IGM that should be imprinted on the spectrum of a background source. In § 3 we describe the method we use to produce mock spectra. In § 4 we present the statistical comparison between the various mock spectra and assess the accuracy with which the input neutral fraction can be recovered in each case. In § 5 we discuss the relative merits of using different source types (quasars, galaxies, or gamma-ray burst afterglows) and some related issues. In § 6 we explore the benefits of independently constraining the radius of the Strömgren sphere. Finally, we summarize the implications of this work and offer our conclusions in § 7.

We use redshift, \( z \), and the observed wavelength, \( \lambda_{\text{obs}} \), interchangeably throughout this paper as a measure of the distance away from the source along the LOS. These can be related by \( (1 + z) = \lambda_{\text{obs}}/\lambda_\alpha \), where \( \lambda_\alpha = 1215.67 \) Å is the rest-frame wavelength of the Ly\( \alpha \) line center. The proper distance from a source at redshift \( z_s \) to a point at redshift \( z \), is determined by \( r = \int_0^z dz' c(\text{d}t/\text{d}z') \), where \( c(\text{d}t/\text{d}z') \) is the line element in a given cosmology and the comoving distance is \( (1 + z) \) times the proper distance. For reference, in our case a proper distance of 6 Mpc corresponds to about \( \Delta \lambda_{\text{obs}} \approx 100 \) Å.

Throughout this paper we assume a standard ΛCDM cosmology, with \( (\Omega_\Lambda, \Omega_M, \Omega_\text{b}, n, \sigma_8, H_0) = (0.71, 0.29, 0.047, 1, 0.85, 70 \text{ km s}^{-1} \text{ Mpc}^{-1}) \), consistent with the recent results from WMAP (Spergel et al. 2003). Unless stated otherwise, all lengths are quoted in comoving units.

2. SPECTRAL SIGNATURES OF NEUTRAL HYDROGEN

In this section we summarize the spectral signatures of neutral hydrogen in the IGM. The spectrum emitted by a source at redshift \( z_s \), \( F_\alpha(\lambda) \), will be modified around the Ly\( \alpha \) wavelength by absorption by neutral hydrogen atoms along the LOS, so that we observe \( F(\lambda) = F_\alpha(\lambda/[1 + z]) \exp(-\tau(\lambda, z_s)) \). The total optical depth due to Ly\( \alpha \) absorption, \( \tau \), between an observer at \( z = 0 \) and a source at \( z = z_s \), at an observed wavelength of \( \lambda_{\text{obs}} = \lambda_\alpha(1 + z_s) \), is given by

\[
\tau(\lambda_{\text{obs}}) = \int_0^z dz \frac{c}{\text{d}z'} n_H(z) x_\text{H}(z) \sigma(\lambda_{\text{obs}}/1 + z),
\]

where \( c(\text{d}t/\text{d}z') \) is the line element in a given cosmology, \( n_H(z) \) is the hydrogen number density at a redshift \( z \), \( x_\text{H}(z) \) is the neutral hydrogen fraction at redshift \( z \), and \( \sigma(\lambda_{\text{obs}}/1 + z) \) is the Ly\( \alpha \) absorption cross section. Since high-redshift sources sit in their own highly ionized Strömgren spheres, the total optical depth at a given \( \lambda_{\text{obs}} \) can be written as the sum of contributions from inside and outside the Strömgren sphere, \( \tau = \tau_\text{r} + \tau_\text{D} \). The resonant optical depth, \( \tau_\text{r} \), is given by

\[
\tau_\text{r}(\lambda_{\text{obs}}) = \int_{z_s}^{\infty} dz' c(\text{d}t/\text{d}z') n_H(z') x_\text{H}(z') \sigma(\lambda_{\text{obs}}/1 + z'),
\]

and the damping-wing optical depth for the IGM outside the Strömgren sphere can be obtained from

\[
\tau_\text{D}(\lambda_{\text{obs}}) = \int_{z_\text{end}}^{\infty} dz' c(\text{d}t/\text{d}z') n_H(z') x_\text{H}(z') \sigma(\lambda_{\text{obs}}/1 + z'),
\]

where \( z_{\text{HII}} \) corresponds to the redshift of the edge of the Strömgren sphere and \( z_{\text{end}} \) denotes the redshift by which H i absorption is insignificant along the LOS to the source. For a smooth IGM, we would simply have \( n_H(z) = n_{\text{HII}}(1 + z)^2 \), and since the fall-off of the cross section is rapid compared to the change in the average neutral fraction, we can also approximate \( x_\text{H} \approx \text{constant} \) for the smooth IGM in equation (3). Conversely, the fall-off of the cross section is slow compared to the small-scale fluctuations in the IGM, averaging out their contributions to \( \tau_\text{D} \). For these reasons, in this paper we approximate \( x_\text{H} \approx \text{constant} \) and assume a smooth IGM (hereafter \( x_\text{H} \) will denote the neutral fraction outside of the H ii region while \( x_\text{H} \) will denote the neutral fraction within the H ii region). The value of \( z_{\text{end}} \) was chosen to be \( z_{\text{end}} = z_{\text{HII}} - 0.5 \). As long as we are not looking through another source’s Strömgren sphere close to \( z_{\text{HII}} \), we find that the exact value of \( z_{\text{end}} \) is irrelevant because most of the contribution to \( \tau_\text{D} \) comes from within \( \Delta z < 0.5 \) of \( z_{\text{HII}} \). In particular, a choice of \( z_{\text{end}} = z_{\text{HII}} - 0.25 \) results in an average change in \( \tau_\text{D} \) of only \( \sim 4\% \) compared to our fiducial model with \( z_{\text{end}} = z_{\text{HII}} - 0.5 \). The difference between equations (2) and (3) are the following: (1) the limits of integration; (2) the determination of \( x_\text{H} \), which assumes ionization equilibrium with the cosmological background flux \( J_{\text{BG}} \) outside the Strömgren sphere with the approximation of \( x_\text{H} \approx \text{constant} \), and equilibrium with the sum of the background and the local source fluxes, \( J_{\text{BG}} + J_s \) inside the H ii region with a fluctuating \( x_\text{H} \); and (3) at the relevant wavelengths where \( \tau_\text{r} \) is significant, the integral in equation (2) is dominated by the resonant cross sections, whereas at all wavelengths where flux is transmitted, the damping wing dominates equation (3). As a result of this last property, \( \tau_\text{r} \) fluctuates strongly with wavelength, reflecting the local density field, whereas the damping wing contribution is smooth, since it averages the contributions to the damping wing from a relatively wide redshift interval.

The two optical depths are represented in Figure 1 for the case of a bright quasar embedded in a neutral IGM at \( z_s = 6 \). The opacities were obtained from a simulation (described below) for a typical LOS toward a source residing at a cosmological density peak. Also shown is \( R_5 \), the radius of the Strömgren sphere, corresponding to the region of transmitted flux blueward of the Ly\( \alpha \) line center. It is worthwhile to note that there are different wavelength regions where either the resonant or the damping-wing absorption dominates. These regions can shift according to the epoch being studied, since \( \tau_\text{D} \) scales linearly with \( x_\text{H} \), and also according to the quasar’s luminosity \( L \), since \( \tau_\text{r} \propto L^{-1} \) (see eq. [4]). For example, since the damping wing is less dominant close to the line center for lower \( x_\text{H} \), details of the gas density and velocity distribution can be studied in this regime. Shortward of the edge of the Strömgren sphere, no flux is observed for \( 10^{-3} < x_\text{H} < 1 \), since the attenuation is large (ranging from \( e^{-10^9} \) to \( e^{-10^7} \) for the values of the neutral fraction studied in this paper).
Simple modeling predicts several distinctive signatures that \( x_H \) should leave on a spectrum (see also Fig. 2 and accompanying discussion below). Most importantly, on average, a neutral universe would be expected to have a smoother spectrum on the blue side of the line, owing to the larger contribution to the total optical depth from the IGM, which is a smooth function (see Fig. 1).

In addition, the symmetry of the observed spectrum around the Ly\( \alpha \) line center should be affected by \( x_H \). Since \( \tau_R \to 0 \) on the red side of the Ly\( \alpha \) line, the observed spectrum should trace out the emitted spectrum for low values of \( x_H \). For low values of \( x_H \), the red side of the line has negligible absorption, while the blue side is still affected by resonance absorption. This makes the observed spectrum highly asymmetric. In comparison, in a neutral universe, the presence of a strong damping wing (\( \tau_D \)) causes additional strong suppression on the red side of the line, as well, making the line more symmetric (though overall weaker). Note that if we were to model out \( \tau_R \), leaving only the damping wing contributing to optical depth, a neutral universe would have a more asymmetric spectrum, because the damping wing would impose a sharper slope in the transmitted spectrum near the Ly\( \alpha \) line.

Furthermore, in a composite spectrum, one expects there to be a sharp drop in observed flux at the edge of the Strömgren sphere if the universe is mostly ionized. This occurs since the gradual cusp of the damping wing (immediatelyward of the sharp rise in \( \tau_D \); see Fig. 1) is subdominant if the universe is mostly ionized, making the transition from resonance-dominated to damping-wing-dominated optical depth more sudden (see feature at 8390 Å, in the lower panel of Fig. 3).

On the other hand, if the universe is neutral, the damping-wing cusp dominates at the edge of the Strömgren sphere and creates a gradual drop-off in the observed flux (see Fig. 3, upper panel). This effect is only observable if the Strömgren
sphere is not large enough that $\tau_R$, whose mean value scales as the square of the distance from the source, blocks off the observed spectrum by itself.

The above effects manifest themselves in all high-redshift sources (quasars, galaxies, GRB afterglows), and furthermore, they also scale predictably with the source strength and environment. As we will see below, the effects are difficult to detect or quantify for a single high-redshift spectrum, because of the uncertainty in the shape of the source’s intrinsic emission and because of the stochastic nature of the density field along a given LOS. However, with many sources such statistics can be usefully analyzed.

3. SIMULATION OF SPECTRA

We use a $\Lambda$CDM hydrodynamical simulation box at redshift $z_s = 6$ as the home of our source quasar. The simulations are described in detail in (R. Cen et al. 2004, in preparation), and we only briefly summarize the relevant parameters here. The box is 11 $h^{-1}$ Mpc on each side, with each pixel being about 25.5 $h^{-1}$ kpc. This scale resolves the Jeans length in the smooth IGM by more than a factor of 10. The simulation also includes feedback in the form of realistic galactic winds. Stellar particles are treated dynamically as collisionless particles, except that feedback from star formation is allowed in three forms: UV ionizing field, supernova kinetic energy, and metal rich gas, all being proportional to the local star formation rate. Supernova energy and metals from aging massive stars are ejected into the local gas cells where stellar particles are located. Supernova energy feedback into the IGM is included with an adjustable efficiency (in terms of rest-mass energy of total formed stars) of $\epsilon_{SN}$, which is normalized to observations (R. Cen et al. 2004, in preparation).

We first identified the densest region in the box, as the natural location of a high-redshift source, such as a quasar. This corresponds to a pixel with an overdensity of $n/(\langle n \rangle \sim 10^4$ relative to the background and to the center of a collapsed dark matter halo with mass $M_{halo} \approx 2 \times 10^{10} M_{\odot}$. Density and velocity information was then extracted from 92 different lines of sight (LOSs), approximately evenly spaced in solid angle, originating from this pixel. The step size along each LOS was taken to be 5.1 $h^{-1}$ kpc, which resolves the Ly$\alpha$ Doppler width by more than a factor of 40. The exact value of the step size was chosen somewhat arbitrarily and does not influence the results as long as it adequately resolves the Doppler width. At each step, the density and velocity values were averaged for the neighboring pixels and weighted by the distance to the center of the pixels. We extended each LOS by the common practice of randomly choosing a LOS through the box and stacking the pieces together (Cen et al. 1994).

The neutral hydrogen fraction inside the Strömgren sphere, $x_{HI}(z)$, was calculated at each step in the LOS, and for several values of an isotropic background flux, $J_{BG}(\nu)$ (in units of ergs s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ sr$^{-1}$), corresponding to a particular $x_{HI}$. Assuming ionization equilibrium and $x_{HI}(z) \ll 1$ inside the Strömgren sphere,

$$x_{HI}(z) = \frac{n_{HI}}{\sum_{\nu} \frac{m_e c}{h} \int_{\nu_{th}}^{\nu} \sigma_{HI} / \sigma / h \nu d\nu} \cdot (4)$$

where $\nu_{th}$ and $\sigma$ are the ionization frequency and cross section of hydrogen, respectively, and $\alpha_B$ is the hydrogen recombination coefficient at $T = 15,000$ K, $r$ is the luminosity distance between the source and redshift $z$, and $L_{\nu}$ is the quasar’s intrinsic luminosity in ergs s$^{-1}$ Hz$^{-1}$. The luminosity was taken to be $L_{\nu} = 2.34 \times 10^{31} (\nu / \nu_{HI})^{-1.8} [(1 + z)/(1 + z_I)]^{-0.8}$, which results from redshifting a power-law spectrum with a slope of $-1.8$, normalized such that the emission rate of ionizing photons per second is $2 \times 10^{57}$, matching the Elvis et al. (1994) template spectrum and the brightness typical of the SDSS quasars. The background flux, $J_{BG}(\nu)$, is also assumed to follow a $-1.8$ power-law spectrum. Results are insensitive to the shape of the background flux, since the dominant effect of $J_{BG}(\nu)$ comes from the damping wing, and that only depends on the value of $x_{HI}$. Since the quasar’s luminosity is dominant for the values of interest inside the Strömgren sphere, we find that equation (4) can be very well approximated by

$x_{HI}(z) = 4\pi^2 n_{HI} \int_{\nu_{th}}^{\nu} \left( \frac{L_{\nu}}{\sigma / h \nu} \right) d\nu$

For several combinations of $z_{HI}$ (corresponding to a Strömgren sphere radius, $R_S$) and $x_{HI}$, the integrals in equations (2) and (3) were evaluated for each LOS. To expedite analysis, $\tau_D$ was also calculated using the approximation (Miralda-Escudé 1998):

$$\tau_D = 6.43 \times 10^{-9} x_{HI} \left[ \frac{\pi e^2 f_{\nu, HI}(z)}{m_e c H(z)} \right] \times \left[ \int \frac{1 + z_{HI}}{1 + z} - \int \frac{1 + z_{end}}{1 + z} \right],$$

where

$$I(x) = \frac{x^{9/2}}{1 - x} + \frac{9}{7} x^{7/2} + \frac{9}{5} x^{5/2} + 3 x^{3/2} + 9 x^{1/2} - \ln \left[ \frac{1 + x^{1/2}}{1 - x^{1/2}} \right]. \quad (5)$$

Equations (3) and (5) give very similar results for wavelengths away from resonance (i.e., inside the Strömgren sphere), but equation (5) is much quicker to compute.

The Voigt profile was used to approximate the Ly$\alpha$ absorption cross section (Rubicky & Lightman 1979). We assumed a temperature of 15,000 K for gas inside the Strömgren sphere. Outside the Strömgren sphere, for the case of a mostly ionized universe, an IGM temperature of $T = 10^4$ K was used, while the temperature in a neutral universe was taken to be $T = 2.73 \times 151 ((1 + z)/(151))^2$ K, valid for $z < 150$ (Peebles 1993). Our results are insensitive to the exact temperature used. The Doppler width of the Ly$\alpha$ absorption cross section scales as $\nu_D \propto T^{1/2}$, but the total integrated area under the cross section is independent of temperature.

Finally, to simulate observations, we had to smooth the raw spectra we compute. Physical smoothing due to gas pressure, present in the simulations on scales of $\sim 10$ km s$^{-1}$ (Gnedin 2000) corresponds to smoothing on a wavelength range of $\Delta \lambda_{obs} = \Delta \lambda_{0}(1 + z_f)$, or $\sim 0.3$ Å at $z_f = 6$. However, current spectral resolutions achieved for high-redshift quasars (APO, Keck) are about a factor of 3 worse than this value. In order to simulate a realistic spectral resolution of $\sim 1$ Å, all resulting spectra were smoothed over 1 Å bins (20 steps in a LOS) by averaging $e^{-r}$ over each bin.

2 Spectra of GRB afterglows originating in high redshift galaxies might not have noticeable $\tau_R$, since the host galaxies could be too young or too faint to produce a significant Strömgren sphere (Burkana & Loeb 2004; Lamb & Haiman 2004).
4. INTERPRETATION OF SPECTRA

For illustrative purposes, in Figure 2 we show four different examples for the spectrum of a source with \( R_s = 43 \) Mpc. We show spectra assuming two different values of \( x_H = 1 \) or 0.008, corresponding to \( f_R(\omega_0) = 0 \) and \( 8 \times 10^{-25} \) ergs s\(^{-1}\) cm\(^{-2}\) Hz\(^{-1}\) sr\(^{-1}\), respectively. This range for the background flux is approximately what is allowed by the current analysis of known \( z \approx 6 \) quasars (e.g., Fan et al. 2003; Cen & McDonald 2002). The value of \( R_s \) was chosen because it is representative of the brightest SDSS quasars, and it corresponds to the radius of a sphere encompassing \( \approx 2 \times 10^{27} \) ionizing photons s\(^{-1}\) times \( 10^{15} \) hydrogen atoms (Cen & Haiman 2000). The value of the source’s Strömgren sphere radius is left as a free parameter to be determined by the inversion method (described below).

Also, shown in Figure 2 is the effect of the damping wing in smoothing out the spectrum. The flux decrement due to resonance absorption, \( e^{-\tau_{R}} \), is shown with discrete points, and the total flux decrement, \( e^{-\tau_{R}-\tau_{D}} \), is represented with a solid line for two different LOSs (top and bottom). Flux decrements from a neutral universe (left panels) are visibly smoother than those of a mostly ionized universe (right panels), as predicted. The sharp absorption features in the figures are produced by \( \tau_R \), while the general trend of increasing optical depth away from the line center is a combination of both \( \tau_R \) and \( \tau_D \).

In Figure 3 we show the composite mean spectra from 92 LOSs, for the two different values of \( x_H = 1 \) (top panel) and 0.008 (bottom panel). For illustrative purposes, a Gaussian+continuum emission template is overlaid (solid line), and the resulting mean observed spectrum is shown underneath (dashed line). The emission template was chosen somewhat arbitrarily, in order to resemble the typical spectrum of observed quasars (e.g., Vanden Berk et al. 2001), and is comprised of a flat continuum emission added to a Gaussian of width 2500 km s\(^{-1}\) and a peak-to continuum ratio of \( \approx 5 \). From Figures 2 and 3, we can see that the composite mean spectra for these regimes exhibit the traits discussed in § 2: spectra from a neutral universe are smoother on the blue side of the line and more symmetric around the line center (at 8509.69 \( \AA \)); however, if the \( \tau_R \) contribution is statistically modeled out, the \( x_H = 0.008 \) spectra would be more symmetric; also there is a sharp drop in the composite observed flux at the edge of the Strömgren sphere in the \( x_H = 0.008 \) universe that is not present in the neutral universe composite spectrum. The latter feature is only statistically detectable from a large sample of LOSs and was not used in our analysis below. In the analysis below, we ignore the \( \approx 5 \) \( \AA \) range redward of the edge of the Strömgren sphere, since in this region, the exact structure of the transition region from the Strömgren sphere to the IGM contributed significantly to \( \tau_D \), and the transition region can have a large spectrum-to-spectrum variability.

4.1. Inverting the Observed Spectrum to Find \( x_H \)

We are now presented with an interesting problem: supposing the only information we have is the observed spectrum, can we extract the quantities of interest, namely, \( x_H \) and \( R_s^2 \)? For the purposes of an idealized analysis, we will first assume that we know the shape of the intrinsic emission template to infinite precision (however, we do not assume knowledge of the amplitude of the template). In the next section, we shall relax this restriction. The other major assumption we implicitly make is that we can accurately predict the distribution of \( \tau_R \), using the small-scale power statistics from the simulation box. This assumption can be checked by studying more extensive simulations in the future (see discussion in § 5 below).

Before diving into the details, we first outline the main steps of the procedure. We start with a simulated observed spectrum. Then we guess values for \( R_s^2 \), and the IGM neutral hydrogen fraction, \( x_H \). Next we approximate the amplitude of the source’s intrinsic emission, \( A' \), implied by the choices of \( R_s^2 \) and \( x_H \), using the red side of the Ly\( \alpha \) line where resonance absorption can be neglected. From the observed spectrum, we divide out the assumed intrinsic emission (\( A' \) times known spectral shape), and the assumed damping-wing flux decrement, \( e^{-\tau_{D}(\omega, R_s, x_H)} \), calling the result \( S'(\omega_{\text{obs}}) \). If our choices of \( R_s^2 \) and \( x_H \) were correct, \( S'(\omega_{\text{obs}}) \) should represent the resonance absorption flux decrement alone. Hence, we compare a histogram of the implied resonance optical depths, \( -\ln [S'(\omega_{\text{obs}})] \), to the known histogram of resonance optical depth (obtained from the simulation). We then repeat this procedure with different choices of \( R_s^2 \) and \( x_H \), finding the ones whose implied resonance optical depths most closely match the known histogram. We shall now elaborate on this procedure below.

We start with the mock observed flux, of the form

\[
F(\omega_{\text{obs}}) = A e^{-\tau_R(\omega_{\text{obs}}) - \tau_D(\omega_{\text{obs}}, R_s, x_H)} T(\omega_{\text{obs}}),
\]

where \( A \) is the amplitude of the adopted normalized emission template \( T(\omega_{\text{obs}}) \), and \( \tau_R(\omega_{\text{obs}}) \equiv \tau_R(\omega_{\text{obs}}, R_s, x_H) \) also takes into account the small contribution of \( J_{BG} \) to \( \lambda_{H\alpha} \). Since we assume that we know the shape of the source’s intrinsic emission, for simplicity we shall set \( T(\omega_{\text{obs}}) = 1 \). Actual features in the spectrum will only effect the signal-to-noise ratio (S/N) of detection under this optimistic assumption (see discussion below). Next, we guess values for \( R_s^2 \) and \( x_H \). For these values, \( \tau_D(\omega_{\text{red}}, R_s^2, x_H) \) is calculated for a wavelength, \( \lambda_{\text{red}} \), on the red side of the line. We then estimate the amplitude of the intrinsic emission template, which these values would imply at \( \lambda_{\text{red}} \):

\[
A' = \left( A e^{\tau_D(\omega_{\text{red}}, R_s^2, x_H)} - \tau_D(\omega_{\text{red}}, R_s^2, x_H) \right),
\]

where for increased accuracy, \( A' \) can be averaged over several values of \( \lambda_{\text{red}} \), corresponding to a smooth amplitude in the red side of the observed spectrum. Since our simulated spectra are well-behaved, averaging was not needed, and \( A' \) was evaluated at an arbitrarily chosen \( \lambda_{\text{red}} = 8514 \, \AA \). It should be noted that, when using real spectra, one has to be careful to choose \( \lambda_{\text{red}} \) values that are not near other emission lines.

Next, we divide the input flux by \( A' \) and extract an estimate of the resonant optical depth, \( \tau_D(\omega_{\text{obs}}) \), using the damping-wing contribution, \( e^{-\tau_D(\omega_{\text{obs}}, R_s^2, x_H)} \), for observed wavelengths on the blue side of the line:

\[
\tau_D(\omega_{\text{obs}}) = -\ln \left( F(\omega_{\text{obs}}) A'^{-1} e^{\tau_D(\omega_{\text{obs}}, R_s^2, x_H)} \right),
\]

which reduces to

\[
\tau_D(\omega_{\text{obs}}) = -\ln \left( A e^{\tau_D(\omega_{\text{obs}}) - \tau_D(\omega_{\text{obs}}, R_s^2, x_H)} \right) - \ln \left( \frac{A'}{A} \right),
\]

where \( \tau_D^2(\omega_{\text{obs}}, R_s^2, x_H) \) and \( \tau_D(\omega_{\text{obs}}, R_s, x_H) \). The first term on the right-hand side of equation (8) represents our misestimate of the damping-wing contribution on the blue side, and the second term represents our misestimate of the continuum inferred from the red side.
Then, a final correction is applied to remove the contribution of the assumed background flux corresponding to our guess of \(x_{\text{HI}}, J_{\text{BG}}(\nu)\), to the neutral hydrogen fraction inside the Strömgren sphere, \(x_{\text{HI}}(z)\), defined by equation (4):

\[
\tau'_R(\lambda_{\text{obs}}) = \tau_R(\lambda_{\text{obs}}) \frac{\int_{\nu_1}^{\nu_2} [L_{\nu}/4\pi\tau^2 + 4\pi J_{\text{BG}}(\sigma/h\nu)] d\nu}{\int_{\nu_1}^{\nu_2} (L_{\nu}/4\pi\tau^2)(\sigma/h\nu) d\nu},
\]

where \(\tau'_R(\lambda_{\text{obs}})\) is our estimate for the resonance optical depth at \(\lambda_{\text{obs}}\), for our guess of \((x_{\text{HI}}, R_S)\), and normalized to the resonance optical depth in a neutral universe (i.e., \(J_{\text{BG}} = 0\) in eq. (4)) for purposes of comparison.

A histogram of \(\tau'_R\) is constructed and compared to the known template histogram of \(\tau_R\), extracted from the combined data from 92 smoothed mock spectra, created by embedding the source in a neutral universe (see Fig. 4). In order to exclude spectral pixels that would be too faint for an actual flux measurement, the inferred values of \(\tau'_R > 16\) were discarded from the analysis. This choice is motivated by the current limits available from the \(z \sim 6\) SDSS quasars. The current best lower limit on the optical depth just blueward of the Ly\(\alpha\) line is actually worse (\(\tau \sim 6\); White et al., 2003), but since the higher Lyman series lines have lower opacities, a better lower limit, \(\tau \sim 22\), is available from the Ly\(\beta\) region of the spectrum (White et al. 2003). In principle, the Ly\(\beta\) (and Ly\(\gamma\)) spectral regions could be added to our analysis. A \(\chi^2\) test statistic is used to compare the two templates:

\[
\chi^2 = N_{\text{points}} \sum_{i=1}^{N_{\text{bins}}} \frac{(f_i - F_i)^2}{f_i},
\]

where \(N_{\text{points}}\) is the number of \(\tau'_R\) values extracted from the spectrum, \(f_i\) and \(F_i\) are the fraction of values expected and received in bin \(i\), respectively. The deviations are approximately Gaussian, \(\sigma^2 = N_{\text{points}} f_i\).

This procedure is then repeated for many choices of \(R_S\) and \(x_{\text{HI}}\) (shown below), and the \(\chi^2\) test statistic in equation (10) is minimized.

The results of this procedure can be seen in Figures 5 and 6 and are quite encouraging. These figures show likelihood contours for combinations of \((x_{\text{HI}}, R_S)\) for two cases of the true parameters, \((x_{\text{HI}}, R_S) = (1, 43\ Mpc)\) and \((x_{\text{HI}}, R_S) = (0.008, 43\ Mpc)\). The statistical constraints shown in these figures are obtained from one typical LOS to a single source. Both cases had a minimum reduced \(\chi^2\) \(\sim 1\) for 22 degrees of freedom (dof), corresponding to two fitted parameters [dof = \((N_{\text{bins}} - 1) - 2\)]. The \(x_{\text{HI}} \times R_S\) probability grid in Figures 5 and 6 consists of \(25 \times 35\) grid points, respectively.

In the case of a neutral universe (Fig. 5, left), the correct values of \((x_{\text{HI}}, R_S)\), to within an error of (30\%, 5\%), respectively, are identified by our procedure at 90\% confidence. We do not display these contours, as they would be represented by a point in the figure. Confidence contours of 99\% are shown, and these constrain the IGM neutral fraction to \(x_{\text{HI}} \gtrsim 0.1\). The irregular, island contours in the left panel of Figure 5 are the result of the unique features of a single LOS and get smoothed out when averaged over several LOSs, as seen in the right panel. The right panel of Figure 5 shows the probability contours, averaged over five different random LOSs. The correct \((x_{\text{HI}}, R_S)\) values were chosen with 99\% confidence, to within an error of (30\%, 5\%), respectively. The 99.73\% and 99.99\% contours (solid and dashed lines, respectively) are shown, ruling out a \(x_{\text{HI}} \leq 0.1\) universe at better than 3\(\sigma\) and an \(x_{\text{HI}} \leq 0.7\) universe at 3\(\sigma\). As expected, confidence contours get tighter as more LOSs are analyzed.

For the case of an ionized universe with \(x_{\text{HI}} \sim 0.008\) in Figure 6, the 1\(\sigma\) uncertainty contours (not shown) enclose the correct parameters, but the contours obtained from the single LOS are not as tight as in the neutral universe case, as was predicted in the introduction. Nevertheless, a neutral universe was ruled out at the 99\% confidence level, as shown in Figure 6.

It is worthwhile to note that the isocontours in Figures 5 and 6 go from bottom right to top left, indicating a degeneracy between small \(x_{\text{HI}}\), small \(R_S\), and large \(x_{\text{HI}}\), large \(R_S\) solutions. This is to be expected since the contribution of \(\tau_R\) to the observed spectrum can be diminished both by moving the edge of the Strömgren sphere further away from the source (increasing \(R_S\)) and by having a more highly ionized IGM (decreasing \(x_{\text{HI}}\)). Because of the limited spectral range used, the determination of the amplitude of the host’s intrinsic emission, \(A'\), is most affected by this degeneracy; however, since the shapes of the damping wings are different in these scenarios, the degeneracy is not exact and can be lifted by increasing the number of sources used in the analysis.

A useful by-product of this procedure is that it produces an estimate of the amplitude of the intrinsic emission \((A' = A)\) for the correct choice of \((x_{\text{HI}}, R_S)\).

An interesting issue of biasing can be raised here. Since the quasar sits in an overdense region, histograms of \(\tau'_R\) could have a rather large scatter close to the line center due to the increased spread in the density distributions and the peculiar motion of the gas within the infall region around the halo (e.g., Barkana & Loeb 2003). This biasing effect was studied, and on average, we find that the density field reaches within 15\% of the mean density \(\sim 5\) \(\text{A}\) blueward from the observed line center, for our
redshift $z = 6$ quasar. However, the distribution of densities at a fixed distance has a high-end tail, comprised of a few LOSs. Although we can model this bias for our quasar, one would need the density profiles surrounding many host sources to fully explore these statistics for a larger sample of quasars. This is feasible in principle, in large future simulations. However, for the purposes of generality, in the present paper the blue side of the spectra was cutoff $5 \, \text{Å}$ blueward of the line center and omitted from our analysis. Environment biasing will be discussed in detail in § 5.3.

Another uncertainty can arise if the redshift of the Ly$\alpha$ line center is not well determined. An offset in the line center of $\pm1000 \, \text{km s}^{-1}$ (typical of quasar jets), results in an effective $R_S$ offset of only $\pm1.3$ comoving Mpc. A larger systematic offset of $\Delta z \sim 0.01$–0.05 in the line center, corresponding to $\Delta R_S \sim 4$–20 Mpc, can be present if an associated metal line with a well-determined redshift has not been detected. This can represent a nonnegligible misestimate in the radius of the ionized region (especially for faint sources) and underscores the importance of accurate redshift-determinations from metal-line detections. Nevertheless, we note that even these relatively large $R_S$ uncertainties do not have a major impact in distinguishing among the $x_{HI}$ values of interest, which are separated by 2 orders of magnitude. This can be seen explicitly by noting that a vertical change of order $\Delta R_S \sim 4$–20 Mpc along the probability isocontours, seen in Figures 5 and 6, corresponds to less than an order of magnitude change in the value of the neutral fraction. This is the case even for fainter sources, as discussed below.

4.2. Simulating Error in the Emission Template

The assumption of knowing the shape of the quasar’s intrinsic emission is not as outlandish as it might seem. Vanden Berk et al. (2001) created a composite quasar spectrum from $\sim150$ SDSS spectra of quasars around $z \sim 3$. Even though there were variations in amplitude, the normalized, mean template was defined around the Ly$\alpha$ line to better than 5%. Although spectrum-to-spectrum variations are considerable in the core of Ly$\alpha$ and blueward, most of these variations are accounted for by the Baldwin effect (the decrease of emission line width with increasing luminosity) and the absorption by the Ly$\alpha$ forest, both of which can be statistically removed. Hence, for this paper, we assumed spectrum-to-spectrum variations of $\pm20\%$; a typical value of the rms scatter in the continuum level immediately redward of Ly$\alpha$ (Vanden Berk et al. 2001). Fan et al. (2003) demonstrate that the high-redshift quasars follow Ly$\alpha$ emission-line and continuum spectral shapes that are remarkably similar to that of their low-redshift counterparts. More precisely, the high-redshift sample size is small, but the spectra of the present handful of $z \sim 6$ quasars are consistent
with being drawn from the Vanden Berk et al. distribution of spectral shapes (X. Fan 2003, private communication).

Here we address the effect of the uncertainties of the assumed spectral template in two ways: we assume (1) an unknown overall "tilt" in the spectrum or (2) an unknown pixel-to-pixel, uncorrelated, normally distributed scatter around a well-determined mean spectrum. These uncertainties add extra parameters in our analysis and make the constraints on the neutral fraction less tight. However, as we will argue below, tight statistical constraints on the neutral fraction can still be obtained with a sufficiently large sample of high-redshift sources.

4.2.1. Tilt in the Emission Template

The uncertainty in the emission template was first modeled with a pivoting procedure, chosen to be hinged at the wavelength used for the amplitude estimation in equation (7), \( \lambda_{\text{piv}} = \lambda_{\text{red}} = 8514 \) Å. This mimics an incorrectly chosen power law for the quasar's continuum emission (and also a tilt in the \( \lambda_{\text{Ly}} \) emission-line profile). Such a tilt would also characterize an uncertainty in the power-law index of GRB afterglow spectra (see § 5.2).

Thus, the observed flux is assumed to be of the form \( F(\lambda_{\text{obs}}) = A(\lambda_{\text{obs}}/\lambda_{\text{piv}}) e^{-\alpha(\lambda_{\text{obs}} - \lambda_{\text{piv}})} \). Furthermore, equation (8) is modified to

\[
\tau_R(\lambda_{\text{obs}}) = - \ln \left( e^{\alpha(\lambda_{\text{obs}}/\lambda_{\text{piv}})} - e^{-\tau(\lambda_{\text{obs}})} \right) - \ln \left( A^2 \right),
\]

where \( \alpha^* \) is now a guess for the spectral slope \( \alpha \).

The shape of this power-law tilt is similar but is not mathematically degenerate with the shape of the damping wing. It therefore causes constraints to degrade. Here we characterize this degradation using

\[
\langle N_{\text{hit}} \rangle \approx \frac{1}{\sigma_{\text{hit}}},
\]

where \( \langle N_{\text{hit}} \rangle \) is an estimate of the number of data points (i.e., spectral resolution bins) required to distinguish between the two spectrum shapes; \( \sigma_{\text{hit}} \equiv \Delta \tau_{\text{Damp}}/\sigma_{\tau_R} \), with \( \Delta \tau_{\text{Damp}} \equiv \langle |(A/\lambda^2) e^{-\tau_R(\lambda_{\text{obs}})} - (A/\lambda^2) e^{-\tau(\lambda_{\text{obs}})}| \rangle \) being a measurement of the typical spread of the estimated \( \tau_R \) obtained from differences in the shape of the power law and the shape of the damping-wing flux decrement, and \( \sigma_{\tau_R} \approx 0.1 \) is the width of the template \( \tau_R \) histogram.

We find that the tilt in the emission template obtained with a misestimate of \( \alpha \) is not degenerate with the shape of the damping wing for our quasar. The largest value of \( \langle N_{\text{hit}} \rangle \), obtained from our parameter space occurred for the degeneracy between the fiducial values of \( x_{\text{hit}} = 0.008 \) and \( R_0 = 43 \) Mpc and the parameter choice of \( x_{\text{hit}} = 1 \), \( R_0 = 99 \) Mpc with a tilt misestimate of \( \alpha - \alpha^* \approx -3 \). For these values, \( \langle N_{\text{hit}} \rangle \approx 10^3 \), corresponding to, e.g., 10 similar quasar spectra with 100 usable independent spectral resolution elements.

4.2.2. Pixel-by-Pixel Errors

The uncertainty in the emission template was next modeled assuming uncorrelated, Gaussian distributed errors. Such pixel-by-pixel uncertainties could also represent the noise associated with the flux detection in each bin. Hence, the value of the emission template, \( T(\lambda_{\text{obs}}) \), in the input flux in equation (6), now becomes a Gaussian distributed random variable with a mean value for each wavelength given by \( \langle T(\lambda_{\text{obs}}) \rangle \). The inversion equation to replace equation (8) then becomes

\[
\tau_R(\lambda_{\text{obs}}) = - \ln \left( e^{\alpha(\lambda_{\text{obs}}/\lambda_{\text{piv}})} - e^{-\tau(\lambda_{\text{obs}})} \right) - \ln \left( T(\lambda_{\text{obs}}) / \langle T(\lambda_{\text{obs}}) \rangle \right).
\]

In the case of small deviations from the template value, \( T(\lambda_{\text{obs}})/\langle T(\lambda_{\text{obs}}) \rangle \approx 1 \), \( \tau_R(\lambda_{\text{obs}}) \) is approximately Gaussian distributed around \( - \ln \left( e^{\alpha(\lambda_{\text{obs}}/\lambda_{\text{piv}})} - e^{-\tau(\lambda_{\text{obs}})} \right) - \ln \left( A^2 \right) \).

To test the robustness of our results to these pixel-by-pixel errors, a random LOS was drawn from our pool of LOSs, a Gaussian distributed emission template, \( T(\lambda_{\text{obs}}) \), was generated to create the mock spectrum, and the inversion procedure outlined in § 4.1 was performed, using equation (13) to generate the \( \tau_R^{\prime} \) histograms. This procedure was repeated, updating the \( \chi^2 \) values in the parameter space with each newly processed LOS (each new LOS representing a different source in a hypothetical sample) until we were able to distinguish a neutral universe from a \( x_{\text{hit}} < 0.008 \) universe with 99% confidence.

The results for the number of sources needed for the 99% confidence constraints are summarized in Table 1. The emission uncertainties refer to the standard deviation of the pixel-by-pixel Gaussian distributed errors in the emission template. With a 20% uncertainty in the intrinsic emission template, an average of \( \langle N_{\text{LOS}} \rangle \approx 34 \) LOSs were required to rule out a neutral universe when the true value of the neutral hydrogen fraction was \( x_{\text{hit}} = 0.008 \). In the \( x_{\text{hit}} = 1 \) regime, only ~three spectra on average were required to rule out a \( x_{\text{hit}} < 0.008 \) universe with 99% confidence. This should be expected, since as discussed previously, the neutral IGM leaves a heavier footprint on the quasar spectra for a reasonably sized Strömgren sphere.

| Emission Uncertainty | \( \langle N_{\text{LOS}} \rangle \) with \( x_{\text{hit}} = 1 \) | \( \langle N_{\text{LOS}} \rangle \) with \( x_{\text{hit}} = 0.008 \) |
|---------------------|---------------------------------|---------------------------------|
| 20%                 | 3.42 ± 1.95                     | 33.6 ± 20.8                     |
| 10%                 | 3.39 ± 2.15                     | 24.6 ± 20.0                     |
| 5%                  | 2.45 ± 1.13                     | 16.8 ± 14.2                     |

Aside from the implicitly assumed calibration and elimination of the Baldwin effect, the adopted 20% uncertainty does not make use of any information (such as correlations with other observables) from the observed spectrum being processed to further improve constraints. Preliminary results from a principal component analysis (PCA) of the spectrum-to-spectrum variations suggest that one might be able to characterize the variance in the emission template with only three eigenvalues (D. E. Vanden Berk 2003, private communication). It is likely that with such characterization of the variance and the usage of information redward of \( \lambda_{\text{Ly}} \), the template uncertainty can be reduced, thus reducing \( \langle N_{\text{LOS}} \rangle \). With a 10% pixel-by-pixel uncertainty, an average of 25 LOSs were needed to rule out a neutral universe for \( x_{\text{hit}} = 0.008 \), and 3 to rule out...
an $x_{\text{HI}} < 0.008$ universe for $x_{\text{HI}} = 1$. A $5\%$ uncertainty brings the average number of required spectra down to 14 and 2, for $x_{\text{HI}} = 0.008$ and $x_{\text{HI}} = 1$, respectively. These results, as well as the rms deviations, are summarized in Table 1.

5. MERITS OF DIFFERENT SOURCE TYPES

Although the preceding analysis was done with simulated quasar spectra similar to the bright SDSS high-redshift quasars, it can be repeated on other high-redshift sources, namely, quasars with lower luminosities, high-redshift galaxies, and GRB afterglows. The properties of the sources scale predictably with their luminosities, with the two most pertinent to this analysis being the size of the source’s Strömgren sphere and the shape of the source’s intrinsic emission spectrum.

5.1. Strömgren Sphere Size

The size of the source’s Strömgren sphere, $R_S$, approximately scales as the source’s (luminosity)$^{1/3}$. A fainter quasar, of similar age, might therefore have fewer measurable spectral points inside the Strömgren sphere with which to create the $\tau_R$ histogram, which weakens constraints. On the other hand, since the Strömgren sphere is smaller, the damping wing has a stronger effect on the spectrum, which strengthens constraints.

To estimate the overall effect on the determination of the neutral fraction, we repeated the pixel-by-pixel analysis outlined in § 4.2.2 on a 100 times fainter quasar $\{L_v = 2.34 \times 10^{29} \psi/v_{\text{HI}}^{1} (1 + z)/(1 + z_p)^{-0.8}\}$ with a correspondingly smaller Strömgren sphere ($R_S \approx 9.3$ Mpc). From simulated spectra of such mock quasars in a neutral universe, we find that a $x_{\text{HI}} < 0.008$ universe is ruled out at 99% confidence with $\approx 3$ LOSs. This result is therefore comparable to that available from the brighter quasars (shown in Table 1). This can be understood by realizing that even though fewer spectral points are available for the analysis of a fainter source (since the Strömgren sphere is smaller), these points are those close to the edge of the Strömgren sphere, where the damping wing has a sharper slope, and are given more statistical weight because of the lack of points far away from the edge of the Strömgren sphere, where the damping wing is flatter. On the other hand, we find that approximately $10^2 - 10^3$ faint quasar LOSs are needed on average, for the emission template uncertainties of 5%–20%, in order to break the degeneracy between the damping wing of a small $x_{\text{HI}}$, small $R_S$ and a large $x_{\text{HI}}$, large $R_S$ parameter choice. Since the probability isocontours go from bottom right to top left in the parameter space of Figure 5, limiting parameter space to $R_S < 100$ Mpc (as we had implicitly done above) allowed for a stronger degeneracy in an ionized universe in the case of a small $R_S$ than in the case of the larger $R_S$ quasar used throughout the preceding analysis in this paper. If instead we limit parameter space to $R_S < 30$ Mpc, the fainter sources are able to distinguish between a neutral universe and a $x_{\text{HI}} < 0.008$ universe, using again a comparable number (i.e., tens) of sources to the brighter quasars shown in Table 1. Whether limiting the size of the Strömgren sphere to 30 Mpc is a reasonable prior assumption depends on the actual inferred neutral fraction. The size of the Strömgren sphere scales as $x_{\text{HI}}^{-2/3}$, and for sources that are $\approx 100$ times fainter than the $z \approx 6$ SDSS quasars, they would require $\approx 10^2$ yr to reach a 30 Mpc size even if embedded in an IGM with neutral fractions as low as $x_{\text{HI}} = 0.008$.

An implicit drawback of fainter sources is that they have smaller S/N than bright sources, thereby reducing the effective detection threshold. Becker et al. (2001) and White et al. (2003) state the 1 $\sigma$ lower limits to the $\text{Ly}\alpha$ optical depth inferred from the $\text{Ly}\alpha$ trough to be $\tau_{\text{lim}} \approx 5$ or 6 for the Keck ESI spectra of $z \approx 6$ quasars. As stated previously, the analysis in this paper ignored inferred values of $\tau_R > 16$. Because of the sharp drop in the high-end tail of the $\tau_R$ histograms (see Fig. 4), the inversion procedure presented in § 4.1 is not sensitive to the exact value of the detection limit. In our template histogram, only 5% of the values were within the range $6 < \tau_R < 16$, approximately corresponding to data points used in the analysis, which are undetectable with $\tau_{\text{lim}} \approx 6$. However, a 100 times fainter quasar would have its optical depth detection threshold reduced by $\ln(100) = 4.6$ to obtain equivalent S/N for the same integration time. For our mock spectra, this would eliminate an additional 20% of the $\tau_R$ values, in the range of $1.4 < \tau_R < 6$. Hence, fainter sources have a smaller range of usable $\tau_R$ values than brighter sources. Nevertheless, higher S/N observations would decrease this effect.

Sources that are too faint to have many detectable spectral points on the blue side of the line, such as faint galaxies and GRB afterglows, would not be useful in this $\tau_R$ histogram analysis but would still have a strong damping-wing imprint on their spectrum redward of $\text{Ly}\alpha$. As mentioned previously, redward of $\text{Ly}\alpha$, $\tau_R$ is negligible, and the small-scale power analysis presented in § 4.1 is irrelevant. If the sources are intrinsically faint enough, the slope of the damping wing redward of $\text{Ly}\alpha$ is sufficient to distinguish between a small $R_S$, small $x_{\text{HI}}$ case and a large $R_S$, large $x_{\text{HI}}$ scenario with only a few sources. As emphasized recently by Lamb & Haiman (2001) and Barkana & Loeb (2004), GRB afterglows with a clean power-law intrinsic spectrum would be especially well suited to such an analysis, provided they can be identified in future data sets (e.g., of Swift).

As an example, the usefulness of the red side of the $\text{Ly}\alpha$ line in determining $x_{\text{HI}}$ was also investigated for our simulated faint quasar with $R_S \approx 9.3$ and $x_{\text{HI}} \approx 0.008$, assuming pixel-to-pixel Gaussian scatter in the emission template. In principle, sufficiently far on the red side of the $\text{Ly}\alpha$ line, where resonant absorption does not contribute, this analysis could be performed without a numerical simulation. However, owing to the cosmic infall, some of the pixels immediately on the red side of the $\text{Ly}\alpha$ line center correspond to foreground gas between us and the quasar (the resonant absorption extends, in our case, up to $7–8$ $\Lambda$ to the red; see Fig. 8). For this reason, we did use the simulation in the analysis. Alternatively, to avoid uncertainties due to modeling the cosmological infall, one could omit the spectral regions that are blueward of the infall regime. Here we utilized the flux in the observed wavelength range of $8514–8544$ $\Lambda$ and performed a simple comparison. A more robust analysis of the red side would involve $\chi^2$ minimization in the three-dimensional parameter space of $(x_{\text{HI}}, R_S, A)$, where $A$ is the amplitude of the intrinsic emission. However, for purposes of comparison to the $\tau_R$ histogram analysis presented in § 4.1, it was sufficient to obtain an estimate of $A$ using an assumed region in the observed spectrum with an accurately known template shape, and calculating $A'$ as outlined in § 4.1 and equation (7). For a choice of $x_{\text{HI}}$ and $R_S$, we therefore obtain an estimate of the flux decrement due to resonance absorption,

$$d_B(\lambda_{\text{obs}}) = F(\lambda_{\text{(obs)})} \times \frac{e^{-\tau_R(\lambda_{\text{obs})}}}{A'(T(\lambda_{\text{obs)}))} e^{-\tau_D}, \quad \text{for} \quad \lambda_{\text{obs}} \leq \lambda_{\text{obs}}.$$  

$^3$ There is a small bias associated with the fact that the detection limit, $\tau_{\text{lim}}$, is a limit on the total optical depth, $\tau \equiv \tau_R + \tau_D$, and not just $\tau_R$. 

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For the correct parameter choices, \( d_R(\lambda_{\text{obs}}) \approx e^{-\tau(\lambda_{\text{obs}})} \approx 1 \), since \( \tau_R \to 0 \) on the red side of the line and redward of the infall regime. The mean flux decrement, \( \langle d_R(\lambda_{\text{obs}}) \rangle \), averaged over several randomly chosen LOSs, was compared to the average decrement obtained from the simulated spectra at each wavelength, \( \langle e^{-\tau(\lambda_{\text{obs}})} \rangle \), with the \( \chi^2 \) statistic

\[
\chi^2_R = \sum_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} \frac{[\langle e^{-\tau(\lambda_{\text{obs}})} \rangle - \langle d_R(\lambda_{\text{obs}}) \rangle]^2}{\sigma^2_m},
\]

where the summation limits were chosen to be \( \lambda_{\text{min}} = 8514 \) and \( \lambda_{\text{max}} = 8544 \) \AA, and \( \sigma_m \) is the standard deviation of the intrinsic emission template divided by the square root of the number of LOSs used in determining the mean decrement, \( \langle d_R(\lambda_{\text{obs}}) \rangle \). LOSs were chosen at random, and the mean decrement and test statistic in equation (15) were updated until a neutral universe could be ruled out at 99% confidence.

Results from this procedure are quite comparable to the \( \tau_R \) histogram analysis on the blue side of the Ly\( \alpha \) line for our faint quasar with \( R_5 \approx 9.3 \) and \( \chi^2 \approx 0.008 \). On average, we find that \( 10^2 \)–\( 10^3 \) LOSs were needed to rule out a neutral universe at 99% confidence for template uncertainties of 5%–10%, just as in the \( \tau_R \) histogram analysis. Although the red side is cleaner (negligible resonant absorption), it is further away from the edge of the Stro¨mgren sphere, so the damping-wing shape is flatter and is therefore harder to detect. However, our results suggest that if a larger wavelength range is available for the analysis, or if the source has a smaller Stro¨mgren sphere (\( \sim \) a few megaparsecs), analyzing the red side of the Ly\( \alpha \) line could prove more efficient than the blue side in determining \( \chi^2 \).

Furthermore, very faint sources have other tracers of \( \chi^2 \). For example, Haiman (2002) showed that the shift in the peak of the observed Ly\( \alpha \) emission line (relative to other emission lines), or its measured asymmetry, as a function of the source luminosity, can be used as a probe of the IGM neutral hydrogen fraction.

### 5.2. Intrinsic Emission

Our knowledge of the source’s intrinsic emission varies considerably with source type. Again, it is only the imperfect knowledge of the shape of the emission spectrum that complicates the analysis presented here (i.e., knowledge of the overall amplitude of the spectrum is not needed). On average, quasars seem to have a moderately well-constrained emission template around Ly\( \alpha \), with an uncertainty of \( \sim 20\% \), once the spectrum is normalized and systematics such as the Baldwin effect are accounted for. It is possible that this uncertainty could be further decreased with a principal component analysis (PCA), which has yielded well-characterized spectrum-to-spectrum dispersions on the red side of the Ly\( \alpha \) line (D. E. Vanden Berk 2003, private communication). In comparison, the spectral shape of emission from galaxies is more poorly defined around Ly\( \alpha \) (Steidel et al. 2001). One would therefore need larger samples of Ly\( \alpha \) emitting galaxies at both lower redshifts and higher redshifts for a better empirical calibration of their spectral shape and its dispersion. Such samples may soon be available from extensive Ly\( \alpha \) searches using Hubble Space Telescope (Rhoads et al. 2002) and Subaru (Taniguchi 2003). GRB afterglows have a smooth power-law spectrum shape. There appears to be a scatter in the power-law index of roughly \( \sim 10\% \) in photometric data on low-redshift bursts. The sample of higher redshift bursts, whose spectral shape can be studied in more detail around the Ly\( \alpha \) line, is still too small to quantitify spectrum-to-spectrum dispersions, but they appear to closely follow power laws (Mirabal et al. 2003). Note that a pure power-law uncertainty is not degenerate with the shape of the damping wing (see § 4.2.1). The major issue with GRB afterglows will be whether the high-redshift afterglows can be identified among the lower redshift events (see, e.g., Lamb & Reichart 2000 and Barkana & Loeb 2004 for recent discussions).

### 5.3. Environment Bias

The source’s host environment has a large effect on the observed spectrum near the line center, as emphasized recently by Barkana & Loeb (2004). To accurately model this effect and to test semianalytical models (Barkana 2004), hydrodynamical simulations are needed to generate the local density and velocity fields. In Figures 7 and 8 we show the effect of this biasing for our mock quasar. Figure 7 shows the histograms of the spherically averaged (within our set of 92 lines) radial component of the peculiar velocity fields constructed from 2 \& \( \Delta \) bins in \( \lambda_{\text{obs}} \), at increasing distances away from the quasar. Most of the radial velocities closest to the host pixel exhibit strong infall, with the probability distribution function (PDF) peaking at peculiar radial velocities of \( v \approx -100 \) km s\(^{-1} \). However, there is a significant high-velocity tail in the
The velocity PDFs at each can be approximately reproduced by convolving the dashed curve with the dashed vertical line denotes the Ly\alpha field from the simulation, but not the velocity field. The solid curve includes and not including velocity information. The dashed curve includes the density between the averaged Ly\alpha spectrum, and creates a more gradual decline in the optical depth redward of the center. After about 10\textsuperscript{8} km s\textsuperscript{-1} away from the line center, just as in the former halo.

These proximity effects have a strong impact on the resonance optical depth, \(\tau_R\), as shown in Figure 8. The dotted curve shows \(\tau_R\) calculated assuming the mean IGM density, \(n_H(z) = n_{H,0}(1 + z)^3\), and not including velocity information. The dashed curve includes the density field from the simulation, but not the velocity field. The solid curve includes both the density and velocity information from the simulation box. The long-dashed vertical line denotes the Ly\alpha line center at 8509.69 Å. The solid curve can be approximately reproduced by convolving the dashed curve with the velocity PDFs at each \(\lambda_{\text{obs}}\). Including velocity information smooths out the spectrum, and creates a more gradual decline in the optical depth redward of Ly\alpha. Further away on the blue side from the host overdensity, the difference between the averaged \(\tau_R\) curves becomes statistically negligible.

These figures merely emphasize that density biasing due to the host environment is important, and it requires a larger simulation with a statistical sample of density peaks to quantify. We plan to carry out such an analysis in detail in a future paper. In particular, the analysis presented in this paper should be performed for a larger number of density peaks in other simulation boxes for the density bias to be statistically analyzed. In actual data analysis, it should help that the host environment should scale with the halo size, and therefore with the source’s luminosity.

On the other hand, the biased region does not encompass the majority of the spectrum, as mentioned in § 4.1. For our mock quasar, the biased region extends only ~5 Å away from the line center. However, since our halo is smaller than that expected to host typical z ~ 6 quasars, the biased region could be larger for a more realistic, more massive halo. Using a semianalytical model, Barkana & Loeb (2004) recently derived the gas density and velocity distributions around the relevant halos. They find (see their Fig. 1) that for halo masses typical of those expected to host the bright SDSS quasars, the biased region should extend about ~1 Mpc (proper). This translates to a wavelength range of ~20 Å and still influences less than one-sixth of the region used in our analysis. Our initial results therefore suggest that one can extract \(\tau_R\) histograms from spectra even without modeling the density bias, by ignoring this part of the spectrum around the line center, as was done in this paper.

It is interesting to ask which part of the optical depth distribution carries the most statistical power—the low or the high—optical depth pixels, since the low optical depth pixels are preferentially effected by biasing effects. We addressed this issue by computing the statistical power of fractions of our \(\tau_R\) histograms. We found that similar constraints are obtained by using only pixels with \(\tau_R < 0.1\) and by using only pixels with \(\tau_R > 0.1\) (see Fig. 4). Approximately one-third of the underdense \((\tau_R < 0.1)\) pixels used in our analysis are expected to lie within the biased region discussed above. It would clearly be beneficial to have accurate statistics of the biasing of host halos, but this is impractical given current computational constraints. The simplest way to deal with the issue is to remove the biased region from the analysis (as was attempted in this paper). Since the majority of pixels are not affected, as discussed above, we expect our results to be fairly insensitive to biasing.

As a final test of local bias, we created a new template distribution of \(\tau_R\) values by using LOSs generated from a new and independent simulation box. The densest region in the new box, from which LOSs originated, corresponds to a dark matter halo of mass \(M_{\text{halo}} \approx 1 \times 10^{10} M_\odot\), about half the mass of the densest halo in the simulation box used throughout the rest of this paper. The two template distributions can be seen in Figure 9, with squares representing the new histogram and crosses showing the old histogram (i.e., Fig. 4, top left). The two histograms are fairly similar (their difference is much smaller than those between the models being compared to one another in Fig. 4). Our old template is somewhat wider, as would be expected from the larger density contrast that we find in that simulation box. The density field around the new halo reaches within 15% of the mean density ~5 Å blueward from the line center, just as in the former halo.

6. ADDING ADDITIONAL CONSTRAINTS: LIMITS ON \(R_S\)

As discussed above, the dominant factor in this analysis is the degeneracy between small \(x_{\text{H}_2}\), small \(R_S\), and large \(x_{\text{H}_2}\), large \(R_S\) parameter choices. Hence, it would be quite useful to be able to independently restrict allowed values of \(R_S\). This is
We have not utilized in this paper is that the mass host halo being somewhat wider because of the larger density contrast in the simulation box. The two distributions are similar, with the histogram corresponding to a larger different simulation box, in order to investigate uncertainties in the template. However, a particularly important piece of information that could be constructed as a function of \( \tau_{\text{obs}} \) instead of lumping histograms into a single histogram regardless of wavelength. In general, if a large number of spectra were available, this would contain more information and would help characterize density biases, which should be a strong function of distance away from the source.

More specifically, however, Mesinger & Haiman (2004, hereafter MH04) recently presented a method, which takes only a crude account of the wavelength dependence of the opacity, using essentially only the location of the Ly\( \alpha \) and Ly\( \beta \) GP troughs, to find a robust determination of \( R_S \). Since the different hydrogen Lyman transitions have disparate oscillator strengths, simultaneously considering the measured absorption in two or more Lyman lines can be an effective way to probe a sudden growth of the Ly\( \alpha \) optical depth near the boundary of the Strömgren sphere. In MH04, we applied this technique to model the general behavior of the observed spectrum of SDSS J1030+0524 close to the onset of the Ly\( \alpha \) and Ly\( \beta \) GP troughs. We obtained a tight and robust constraint on \( R_S \) (better than 5\%), arising from the sharpness of growth of the Ly\( \alpha \) optical depth. If this (or any other) method can be used to independently constrain \( R_S \) to within \( \sim 10\% \), it would break the degeneracy between small \( x_1 \), small \( R_S \) and large \( x_1 \), large \( R_S \) parameter choices. Specifically, if \( R_S \) is known to within \( \sim 10\% \), a neutral universe could be distinguished from an \( x_1 \) \(<\) 0.008 universe with 99\% confidence using an average of only one source, following the method presented in this paper (note that an independent constraint on the neutral fraction can be derived from the size of the H \( \text{\textsc{ii}} \) region, by utilizing the estimated ionizing flux of the source; Wyithe & Loeb 2004). The usefulness of knowing \( R_S \) can be seen from Figure 2, where all panels have the same \( R_S \) and there is a large difference between the flux decrements arising from a neutral (left panels) and an ionized (right panels) IGM. This is a highly encouraging result, and the we plan to apply both the method in MH04 and the method presented in this paper to the current sample of SDSS quasars.

### 7. Conclusions

Through an analysis of mock quasar absorption spectra based on a detailed cosmological hydrodynamic simulation, we have shown that it is possible to detect the effects of the damping wing of absorption by neutral hydrogen atoms in the IGM on top of the resonant absorption from within the local H \( \text{\textsc{ii}} \) region of the quasar. We have described an inversion method that we have developed to extract an estimate of the mean neutral fraction of hydrogen in the IGM and of the size of the Strömgren sphere around a high-redshift source. The method is designed to differentiate between sources embedded in an IGM with \( 10^{-3} \) \(<\) \( x_1 \) \(<\) 1, and we have found that it can distinguish among neutral fractions in this range with only a few bright quasars.

We have explicitly incorporated into our analysis an error in the intrinsic emission template, consisting of either an uncertainty in its spectral power-law index, or Gaussian, uncorrelated, pixel-to-pixel variations at each wavelength. With both of these errors, we find that a neutral universe can be statistically distinguished from a \( x_1 = 0.008 \) universe in our parameter space, using tens of bright quasars, a sample that can be expected by the completion of the SDSS. Alternatively, similar statistical constraints can be derived from the spectra of several hundred sources that are \( \sim 100 \) times fainter. For example, the Large-aperture Synoptic Survey Telescope should be able to deliver many new faint quasars that could serve as targets for low-resolution spectroscopy (A. Mesinger et al. 2004, in preparation).

Furthermore, if the size of the source’s Strömgren sphere can be independently constrained to within \( \sim 10\% \) (such as with the method presented in MH04), the analysis presented here can distinguish between sources embedded in an IGM with \( 10^{-3} \) \(<\) \( x_1 \) \(<\) 1, using a single source. We plan to perform such analysis on the current sample of high-redshift sources.

The recent discovery of Gunn-Peterson troughs in the spectra of several \( z \sim 6 \) quasars in the SDSS only impose the restriction of \( 10^{-3} \) \(<\) \( x_1 \) \(<\) 1 on the neutral fraction at this redshift. Further distinguishing between the values allowed in this range, especially between a neutral and a mostly ionized universe, would provide invaluable new constraints that can differentiate among various competing reionization scenarios.

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