The thickness of high-redshift quasar ionization fronts as a constraint on the ionizing spectral energy distribution

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ABSTRACT

High-redshift quasars (z ≳ 6) drive ionization fronts (I-fronts) into the intergalactic medium (IGM), with the thickness of the front generally increasing with the hardness of ionizing spectrum. If the thickness of the front can be measured, it can provide a novel constraint on the ionizing spectral energy distribution, uniquely available for sources prior to the end of reionization. Here we follow the propagation of an I-front into a uniform IGM, and compute its thickness for a range of possible quasar spectra and ages, and IGM neutral hydrogen densities and clumping factors. We also explore the effects of uniform and non-uniform ionizing backgrounds. We find that even for hard spectra, the fronts are initially thin, with a thickness much smaller than the mean free path of ionizing photons. The front gradually thickens as it approaches equilibrium in 10⁸–10⁹ yr, and the thickness of its outer part can eventually significantly exceed simple estimates based on the mean free path. With a sufficiently high intrinsic hydrogen column density obscuring the source [log(N_H/cm^−2) ≳ 19.2] or a sufficiently hard power-law spectrum combined with some obscuration [e.g. d log F_ν/d log ν ≳ −1.2 at log(N_H/cm^−2) ≳ 18.0], the outer thickness of the front exceeds ∼1 physical Mpc and may be measurable from the 3D morphology of its redshifted 21-cm signal. We find that the highly ionized inner part of the front, which may be probed by Lyman-line absorption spectra, remains sharp for bright quasars unless a large obscuring column [log(N_H/cm^−2) ≳ 19.2] removes most of their ionizing photons up to ≈40 eV. For obscured sources with log(N_H/cm^−2) ≳ 19.8, embedded in a significantly neutral IGM, the black Lyα trough (where the neutral fraction is ∼10⁻³) underestimates the size of the H II region by a factor of ∼4.

Key words: quasars: absorption lines – quasars: general – cosmology: observation – cosmology: theory – radio lines: general – ultraviolet: general.

1 INTRODUCTION

The spectra of z > 6 quasars (e.g. Fan et al. 2002; White et al. 2003), showing complete Gunn–Peterson (GP) absorption, have been widely analysed as a possible probe of the ionization state of the ambient intergalactic medium (IGM). The sizes of inferred H II regions surrounding these sources depend on the neutral fraction (Cen & Haiman 2000; Madau & Rees 2000) and suggest a value above a few per cent (Fan et al. 2002; Mesinger & Haiman 2004; Wyithe & Loeb 2004), although this inference is subject to some bias and significant scatter, depending on how the intrinsic H II region size is deduced from the observed spectrum (Bolton & Haehnelt 2007a,b; Maselli et al. 2007). Direct evidence for a GP damping wing in the QSO spectra (Mesinger & Haiman 2004, 2007) also suggests that the neutral fraction exceeds several per cent at least along two lines of sight. The evolution of Lyα emitting galaxies may also suggest a significant global neutral fraction (Ota et al. 2007, although the presently observed evolution may still be attributed to the evolution in the halo abundance and in the mean IGM density; Dijkstra, Wyithe & Haiman 2007).

If the IGM is significantly neutral, then the shape of the ionization front (I-front) will be well defined, i.e. the ionizing flux, over a region corresponding to the mean free path of ionizing photons, will be dominated by the quasar itself, rather than by the background. In this case, the shape of the I-front will contain information on the spectrum of the ionizing source. In particular, the thickness of the front is generally expected to increase for harder source spectra, whose typical ionizing photon has a longer mean free path (hereafter MFP). Mesinger & Haiman (2004) noted that the onset of the Lyα and β GP troughs in the spectra of z > 6 quasars occur at redshifts close to one another, corresponding to a physical separation of R_α − R_β ≲ 1 Mpc along the line of sight (LOS), possibly placing an upper
limit on the hardness of the spectrum (with mean photon energy \(E < 230\, \text{eV}\), for which the MFP in a neutral IGM at \(z \approx 6\) is \(\sim 1\, \text{Mpc}\)). Although the ratio of oscillator strengths of the Ly\(\alpha\) and \(\beta\) lines is a factor of 5.2, once density inhomogeneities and foreground Ly\(\alpha\) absorption is taken into account, the Ly\(\beta\) line effectively probes a factor of 2–3 lower neutral fraction than Ly\(\alpha\) (Fan et al. 2002; Songaila & Cowie 2002). The comparison of \(R_\beta/R_\alpha\) gives the path-length over which the neutral fraction rises by a factor of 2–3; this could naively be taken as a proxy for the thickness of the I-front.

This simple interpretation, however, is complicated by possible absorption by the GP damping wing from the IGM (Mesinger & Haiman 2004, 2007), and also by the scatter in the \(R_\beta/R_\alpha\) ratio expected to arise between different lines of sight due to density fluctuations (Bolton & Haehnelt 2007a). Nevertheless, if a sufficient number of distant quasars are detected in the future, the ratio \(R_\beta/R_\alpha\) and other features in their absorption spectra, could provide a diagnostic for a finite I-front thickness and therefore the hardness of the sources, at least statistically. Note that this test is not available at lower redshift, where the IGM is highly ionized, the MFP of ionizing photons is already \(\gtrsim 100\, \text{Mpc}\), and photoionization equilibrium is established on a time-scale of \(\left(\Gamma/\eta_H\lambda_{\text{MFP}}\right)^{-1} \sim 10^4\, \text{yr}\), much less than the expected quasar lifetime.

Other methods have been proposed to probe the finite thickness of quasar I-fronts. Zaroubi & Silk (2005) explored measuring the thickness of I-fronts through their 3D redshifted 21-cm signatures, with a low-frequency radio telescope array such as LOFAR (for a comprehensive review of current and planned high-redshift 21-cm projects, see Furlanetto, Oh & Briggs 2006). The soft spectrum of stellar radiation would produce a much sharper I-front than the very hard spectrum predicted to emerge from miniquasars; when the sources themselves are not detected, the 21-cm maps could still discriminate between stellar- and quasar-driven reionization (Oh 2001). Finally, Cantalupo, Porciani & Lilly (2008) recently suggested that collisionally excited Ly\(\alpha\) emission may be detectable from the shell of material at the I-front, over an extended solid angle behind bright quasars; the spectral shape and thickness of this emission is another possible measure of the thickness of the I-front.

At present, little is known empirically about the ionizing spectrum of quasars at \(z \gtrsim 6\). At lower redshift, quasars are found to have relatively soft power-law spectra in the extreme ultraviolet (UV), with an average spectral index of around \(s = 1.8\) (Telfer et al. 2002). However, many quasars show a strong soft X-ray excess at a few 100 eV, which cannot be explained by thermal emission from a standard accretion disc. The excess X-rays could originate from Compton scattering in a hot corona surrounding the accretion disc around the active galactic nucleus (AGN) (Porquet et al. 2004). Quasars at high redshift are also expected to be preferentially obscured due to the increased gas density, and may effectively radiate only at energies in soft X-rays bands and above (Sazonov, Ostriker & Sunyaev 2004). Shemmer et al. (2006) found that a composite X-ray spectrum of \(21 > 4\) quasars had an effective spectral index in the X-ray of \(s = 0.95\), and an intrinsic absorption column upper limit of \(N_\text{H} \leq 6 \times 10^{22} \, \text{cm}^{-2}\), consistent with the mean results from Just et al. (2007) at lower redshift.

Motivated by the suggestions above that the I-front thickness could be measurable, and by the lack of knowledge about the spectral energy distributions (SEDs) of high-z quasars, in this paper we follow the time-dependent propagation of an I-front into the IGM, and study its thickness for a range of possible spectra, quasar ages, clumping factors in the IGM, and various ionizing backgrounds. Our goal is to give a rough quantitative assessment of the conditions under which a hard spectrum may be diagnosed in future observations. Our modelling here extends the investigation of Zaroubi & Silk (2005), by exploring a range of quasar spectral parameters, by improving the treatment of helium and of secondary ionizations by energetic photoelectrons, and, most importantly, by following the time-dependent evolution of the non-equilibrium ionization structure. In an earlier study, Shapiro, Iliev & Raga (2004) used numerical simulations to study the evolution and properties of I-fronts propagating into the high-z IGM, for three different source spectra appropriate for massive Population II and III stars and quasars. Our paper extends this work by including recombination radiation from helium, and by focusing on brighter sources and covering a larger range of spectra (including obscured spectra much harder than those examined by Shapiro et al.), for which the thickness may be directly measurable.

After we completed this paper, we became aware of the work of Thomas & Zaroubi (2007) who have recently made calculations similar to some of those presented here. We will compare our results further in Section 6.

The rest of this paper is organized as follows. In Section 2, we describe our modelling of the I-fronts, including treatments of the non-equilibrium evolution, and of helium. In Section 3, we describe the salient features – evolution, shape and size – of the I-front in our fiducial model for an obscured source with a hard spectrum. In Section 4, we present our main results, discussing measurements of the thickness of the I-front. In Section 5, we reiterate the inherent limitations of our modelling approach, before finally, in Section 6 we summarize our results and conclusions.

2 MODELLING AND METHODS

In this section, we describe our model for computing the propagation of the I-front into a uniform medium. The modelling is rather standard for the most part, but we include a description of our own numerical implementation here for completeness, and in order to describe a few details about helium ionization that have typically not been included in previous works studying cosmological quasar H\(\text{II}\) regions.

2.1 Ionization and recombination

Osterbrock & Ferland (2006) give an excellent description of 1D spherical ionization structure calculations. For the most part we follow their methods, but we additionally include time evolution (non-equilibrium ionization states), secondary ionization by photoelectrons, and a full treatment of doubly ionized helium.

We use the equations of 1D radiative transfer (RT) to find the optical depth \(\tau(\nu)\) as a function of distance from the quasar \(r\) and frequency \(\nu\). The optical depth contribution from each species is calculated at its ionization threshold:

\[
\tau_{\nu,0}(r) = \int_0^r \alpha_i n_i(r') \, dr',
\]

where \(n_i(r)\) is the number density of species \(i\) and \(\alpha_{i,0}\) is the photoionization cross-section at the threshold frequency \(v_{i,0}\).\(^1\) The optical depth contribution at any frequency is then \(\tau_{\nu,i}(r) = \tau_{\nu,0,\nu}(r)/\sigma_{0,i}\).

\(^1\)Threshold ionization cross-sections were taken from Osterbrock & Ferland (2006) for H\(\text{I}\) and He\(\text{I}\) and from Hummer & Storey (1998) for He\(\text{II}\). At other frequencies, we used the fitting formulae from Yan, Sadeghpour & Dalgarno (1998) for He\(\text{II}\) and from Osterbrock & Ferland (2006) for H-like ions.
where $\sigma_i(\nu)$ is the cross-section of species $i$ at frequency $\nu$. The total optical depth is the sum of contributions from all three species

$$\tau(\nu) = \tau_{\text{H}}(\nu) + \tau_{\text{He}}(\nu) + \tau_{\text{He}^+}(\nu).$$

We ignore the effects of light travel time in calculating the ionization structure. As Cen & Haiman (2000) have pointed out, this ends up predicting the structure that is observed along the LOS. Because of the finite speed of light, the evolution of the gas at a distance $r$ from the quasar is retarded by the interval $\nu r c$. But an observer farther along the LOS will also receive photons from that point earlier by an amount $\nu r c$. So in order to correctly predict the profile as it would be observed along the LOS (e.g. in an absorption spectrum), we should add the two effects, which simply cancel each other out (White et al. 2003). If we wanted to predict the transverse structure as it would be observed, we could simply add in the appropriate delays after the evolution is calculated (Wyithe, Loeb & Barnes 2005; Yu 2005; Shapira et al. 2006).

For simplicity, we also ignore Hubble expansion. Even at $z = 6$, a quasar lifetime of $10^8$ yr is much shorter than the Hubble time. We do note, however, that the changing density of the IGM could make a discernible difference to the shape of the ionization profile, especially for the largest or thickest H II regions, which extend to several per cent of the Hubble radius.

The photoionization rate of species $i$ (per atom) is

$$\Gamma_i = \int_{\nu_{\text{HI}}}^{\infty} \frac{L_\nu}{4\pi \nu} \sigma_i(\nu) \frac{e^{-\tau(\nu)}}{\tau(\nu)},$$

where $L_\nu$ is the specific luminosity, and $r$ is the distance from the source. In our numerical ionization code, we tabulate $\Gamma_i$ as a function of $\tau_{\text{H}_{\text{I},0}},\tau_{\text{He}_{\text{I},0}}$, and $\tau_{\text{He}^+_{\text{I},0}}$ before calculating the evolution of the ionization structure. Added to that rate for hydrogen is a position-independent background photoionization rate, parametrized by the resulting equilibrium ionized fraction $X_{\text{H}_{\text{II},\text{BG}}}$:

$$\Gamma_{\text{BG}} = C\alpha_0 n_\text{H} X_{\text{H}_{\text{II},\text{BG}}}^2 / X_{\text{H}_{\text{II},\text{BG}}},$$

where $\alpha_0$ is the so-called ‘case B’ recombination rate (the recombination coefficient to all excited levels of hydrogen, evaluated at $T_{\text{gas}} = 10^4$ K unless otherwise specified) and $C$ is the clumping factor $C \equiv n^2_{\text{HI}} / n_\text{H}^2$. This background arises from pre-existing galaxies, and is expected to consist of a patchwork of H II bubbles surrounded by a relatively neutral IGM. Note that even if the ionization outside the quasar’s H II region is patchy (with a Swiss-cheese topology), as it is expected to be, in the interior of the H II region, where the low neutral fraction results in a long MFP, it will be much more uniform (and will also have a higher amplitude). There will, however, be a radial profile to the background flux, due to the clustering of galaxies around the quasar (Alvarez & Abel 2007; Lidz, McQuinn & Zaldarriaga 2007; Wyithe & Loeb 2007). We will first ignore these effects, assuming that the I-front is located sufficiently far away that this bias is small, and that we are averaging the I-front over many small galaxy bubbles. However, in Section 4.2.4, we will return to this issue, where we will also explore various models for a non-uniform ionizing background.

In addition to the quasar’s radiation and the UV background, several other processes occur in the gas that affect the ionization balance and couple the ionization states of hydrogen and helium.

Photoelectrons produced during ionization carry residual energy that can cause further ionizations (Shull & van Steenberg 1985). In our calculations we include the secondary ionization of hydrogen by photoelectrons from both hydrogen and helium, and treat it as an on-the-spot process (the latter assumption is justified similarly to the argument for case B recombination, since the collisional ionization cross-section is typically larger than the photoionization cross-section; Shull & van Steenberg 1985). We use the fitting formula provided by Dijkstra, Haiman & Loeb (2004) in the high-energy limit to calculate the fraction of energy $\phi(x)$ each photoelectron will expend in further ionizations of hydrogen. Using the high-energy limit introduces only a small error since low-energy photons cause few secondary ionizations in any case and the function quickly approaches its asymptotic value as the photon energy increases. Note that in the original calculations of $\phi(x)$, Shull & van Steenberg (1985) defined $x \equiv m_{\text{He}} / n_\text{H}$ and assumed $n\text{He}/n_\text{H} = 0.1$ (versus 0.079 in our model), and $X_{\text{He}^+} = X_{\text{He}^+}$ (where $X_{\text{He}^+} = n_{\text{He}^+}/n_\text{He}$). While neither of these conditions holds exactly in our models, they are reasonable approximations. To account approximately for the extra electrons introduced by doubly ionized helium (which was not included originally) we use $x = X_{\text{He}^+} + (n_{\text{He}^+}/n_\text{H}) X_{\text{He}^+}$ (where $X_{\text{He}^+} \equiv n_{\text{He}^+}/n_\text{He}$). It is a small effect in any case, since He III is formed only where hydrogen is already highly ionized, and $\phi$ vanishes as $x$ approaches unity.

We neglect secondary ionizations of helium which happen at less than 20 per cent of the rate of hydrogen. The mean number of secondary ionizations of hydrogen per photoelectron produced in the ionization of species $i$ is

$$n_2 = \phi(x_i) (E_i) / h\nu_{\text{H}^0,\text{H}^1},$$

where $\langle E_i \rangle$ is the mean energy of photons locally ionizing species $i$:

$$\langle E_i \rangle = \frac{1}{\Gamma_i} \int_{\nu_{\text{HI}}}^{\infty} \frac{d\nu}{4\pi \nu} \sigma_i(\nu) \frac{L_\nu}{4\pi \nu} e^{-\tau(\nu)}/\tau(\nu).$$

Similarly to $\Gamma_i$, we tabulate $\langle E_i \rangle$ as a function of $\tau_{\text{H}^0,0},\tau_{\text{He}^0,0}$ and $\tau_{\text{He}^+_{\text{I},0}}$, before integrating the ionization structure.

Photons produced during recombination of hydrogen and helium are also included in our code in the on-the-spot approximation. High-frequency recombination radiation is capable of ionizing neutral hydrogen and helium, as well as singly ionized helium, so the fraction of recombination photons ultimately ionizing each species must be calculated. In general the fraction of photons of frequency $\nu$ that ionize species $i$ is

$$y_i(\nu) = \frac{\sigma_i(\nu) n_i}{\sigma_{\text{HI}}(\nu) n_{\text{H}^0} + \sigma_{\text{He}^0}(\nu) n_{\text{He}^0} + \sigma_{\text{He}^+_{\text{I}}}(\nu) n_{\text{He}^+}}.$$

The overall fraction for a given recombination process is an average of $y_i(\nu)$ over the spectrum of the emitted radiation. In our calculations, we make the simplifying assumptions that all H I, He I and He II Lyman continua, and He II Balmer continuum photons are produced with the minimum energy. The first and last of these occur below the threshold for all species but H I. The He II Ly $\alpha$ line is treated similarly, assuming all photons have the mean energy of that line.

Certain higher He II lines produces in the recombination cascade are energetic enough to ionize hydrogen, with an average of 0.96 H-ionizing photons ultimately produced for each recombination to any excited level of He II (in the low-density limit which applies here, Osterbrock & Ferland 2006). Another source of ionizing photons is the transition from the first excited level to the ground state of He II: instead of producing a He II Ly $\alpha$ photon, it can instead occur via a two-photon process. We calculate the fraction of recombinations to all excited states of He II that end in a two-photon emission (as a function of temperature) by interpolating the tabulated values from Hummer & Seaton (1964). An average of 1.425 photons capable of
ionizing hydrogen and 0.737 capable of ionizing neutral helium are produced for each two-photon event (Flower & Perinotto 1980), the latter of which are assumed to have the threshold ionization energy for helium.

We use recombination rate coefficients from Hui & Gnedin (1997), except for the coefficient for recombinations directly to the $n = 2$ level of He II, which is taken from Ferguson & Ferland (1997). All calculations presented in this paper assume an isothermal gas of constant mean density and clumping factor.

### 2.2 The ionization structure

The ionization structure surrounding the quasar is calculated by integrating the net ionization rates over time. Before the first iteration, an array of ($X_{\text{He} \ II}, X_{\text{He} \ III}, X_{\text{He} \ IV}$) values, corresponding to a sequence of $r$ values, is initialized to ($X_{\text{He} \ II, 0}, 0, 0$). The ionization and recombination rates are calculated as described above and used to find $dX_{\text{He} \ III}/dr$, $dX_{\text{He} \ IV}/dr$ and $dX_{\text{He} \ II}/dr$. The integration time-step is calculated using

$$\Delta t = \frac{F_d}{\max(F_{\text{He} \ II}, F_{\text{He} \ III}, F_{\text{He} \ IV})},$$

where $F_d = 0.004$ is just a numerical parameter optimized by trial and error. Decreasing $F_d$ by a factor of 2 (improving the time resolution) has no important effect on the results. The time-step is only updated every 10 iterations, and to help damp numerical oscillations we actually use $\Delta t_{\text{new}} = 0.75 \Delta t_{\text{old}} + 0.25 \Delta t$ as the time-step.

In order to increase the speed and stability of the integration, the ionized fractions for the inner part of the array (at low $r$) are frozen and no longer recalculated once a stable equilibrium is achieved. Every tenth iteration we calculate the maximum radius at which the ionization states are in equilibrium, defined as $r_{\text{eq}} = \max (r)$ for which

$$X_{\text{He} \ II} \left( \frac{dX_{\text{He} \ II}}{dr} \right)^{-1} > 5 \times 10^7 \Delta t,$$

$$X_{\text{He} \ III} \left( \frac{dX_{\text{He} \ III}}{dr} \right)^{-1} > 5 \times 10^5 \Delta t,$$

$$r_{\text{H} \ I \ O} < 1000.$$

The last condition on the optical depth is introduced to exclude regions far ahead of the front, where time-scales grow long because the radiation field is so weak. For runs with a high uniform ionizing background we decreased the optical depth limit to $r_{\text{H} \ I \ O} < 100$ because of the reduced opacity. Once $r_{\text{eq}}$ is found, the next iteration is begun, and the ionized fractions at $r > r_{\text{eq}}$ are updated (and constrained to the interval $[0, 1]$). Using our fiducial parameters (described below and in Section 3), it took 76 000 iterations to evolve the structure through $5 \times 10^8$ yr.

### 2.3 Numerical parameters

As mentioned above, ionization rates and mean photon energies are tabulated as a function of the threshold optical depths of each species. The quantities are evaluated on a grid of logarithmically spaced values of $r_{\text{H} \ I \ O}$, $r_{\text{He} \ I \ O}$ and $r_{\text{He} \ II \ O}$. The dimensions of the ionization rate grids are $332 \times 301 \times 301$ values, while the mean photon energy grids are $416 \times 61 \times 61$ values. Each optical depth range extends from $10^{-8}$ up to the maximum optical depth for which $\Gamma_i / \max (\Gamma_i) > 10^{-6}$, which depends on the source spectrum.

The simulations presented here use a grid of 1300 equally spaced radius values, extending from $5 \times 10^4$ pc (all distances in this paper are in proper, not comoving, units unless stated otherwise) to $1.5 R_{\text{Str{"o}m}}$, where $R_{\text{Str{"o}m}}$ is the radius of the classic equilibrium Str{"o}mgren sphere,

$$R_{\text{Str{"o}m}} = \left( \frac{Q}{(4/3) \alpha_2 \alpha_6 C} \right)^{1/3}.$$

Note that this expression ignores helium and secondary ionizations. With $Q = 2 \times 10^7$ s$^{-1}$ and $C = 1$, $R_{\text{Str{"o}m}} = 22.2$ Mpc at $z = 6$.

We tested for convergence by doubling the resolution, which had no effect on the results. For our canonical parameters the step size works out to $\Delta r = 2.56 \times 10^{-3}$ Mpc with an outer radius of 33.4 Mpc.

We have tested our code several ways to ensure reasonable numerical performance. As mentioned above, we tested for convergence by doubling either the time or spatial resolution, neither of which had any important effect on the results. Using a soft spectrum (so that the front is sharp) we find very good agreement with analytical estimates for ionized region size and front velocity. We also find agreement with the Cosmological Radiative Transfer Code Comparison Project (‘test’ 1 in Iliev et al. 2006) calculations, and the examples presented in Osterbrock & Ferland (2006).

### 2.4 Physical parameters

The temperature of the gas is important, because it controls the recombination rates. All calculations presented in this paper assume an isothermal gas. We justify this assumption by noting that most of the photoionization heating occurs somewhat ahead of the front where the ionized fractions are small and recombination rates are therefore low, whereas the temperature inside the front is fairly uniform (as can be seen in Iliev et al. 2006; Bolton & Haehnelt 2007b). We experimented with introducing artificially varying temperature profiles in the outer regions of the front. We made the temperature a function of optical depth so that the temperature variations would be tied to the location of the front. We tried several profiles, from smooth functions mimicking the temperature profiles in the appendix of Bolton & Haehnelt (2007b), to a step function increasing the temperature by a factor of 5 beyond $\Gamma_{\text{H} \ I \ O} > 0.001$. We found that none of these had a significant effect on the profile, as long as the variation occurred outside of the region that had reached equilibrium. The ionization rate totally dominates the recombination rate in the moving part of the front, reaching parity only as the ionized fraction approaches equilibrium. We conclude that since the heating of the gas occurs before it reaches equilibrium, and since the exact recombination rate is irrelevant outside of the equilibrium region, changes in the recombination rate due to temperature variations will not be an important factor in determining the shapes of the fronts.2

We assume the number density of hydrogen atoms surrounding our sources is the mean density of the IGM at $z = 6$, $n_{\text{HI}} = 2.2 \times 10^{-7}$ cm$^{-3}$ ($1 + z^2 = 7.6 \times 10^{-3}$ cm$^{-3}$). The helium mass fraction is $0.24$, yielding $n_{\text{He}} = 6.0 \times 10^{-6}$ cm$^{-3}$. The electron temperature is $T_{\text{gas}} = 10^4$ K. For our fiducial case we use a clumping factor of $C = 1$.

2 Changes in temperature due to radiative transfer can also have dynamical effects on the gas around the I-front, but in the limit where the recombination rate is unimportant, our conclusions on the ionized fraction should also be insensitive to such dynamical effects.
3 EVOLUTION, SHAPE AND SIZE OF THE IONIZATION FRONT

In this section, we present our results for the time-evolving I-front. The spectra we have used are absorbed power laws, as shown in Fig. 1, with specific luminosity

\[ \frac{L}{c} \propto \nu^{-x} \exp \left( -N_H \left[ \frac{\sigma_H(\nu)}{n_H} + \frac{n_{\text{He}}}{n_H} \sigma_{\text{He}}(\nu) \right] \right), \]  

where \( \nu \) is the characteristic frequency of the ionizing photons. The thickness can be estimated, for example, by adopting \( n_{\text{H}} = 0.5 n_H \), and the mean frequency of ionizing photons emitted by the quasar for \( \nu \). The resulting value of \( l_{\text{MFP}} \), however, is an accurate proxy for the thickness of the I-front only for particular definitions of the thickness, and only under particular conditions. For instance, the ionizing spectrum is hardened as the photons travel outward through the gas, since low-energy photons are more readily absorbed. As a result, the outer edge of the front will be spread over a longer path than the inner edge.

Another complication is that the I-fronts around short-lived quasars are expected to be propagating outward (rather than corresponding to the static edge of an equilibrium Str"omgren sphere), which has a strong effect on the shape of the front. It is widely noted (e.g. Shapiro & Giroux 1987) that the ionization state of the gas surrounding a typical high-redshift quasar will not have time to reach equilibrium with the radiation field during a quasar lifetime of \( 10^6-10^8 \) yr,\(^3\) since the time-scale to reach equilibrium is roughly the recombination time \( t_{\text{rec}} = (C a_{\text{He}} n_{\text{H}})^{-1} = 1.62 \times 10^6 \) C\(^{-1}\) yr. This time-scale can also be thought of as the time required for the source to emit one photon for each hydrogen atom within the Str"omgren sphere. Throughout the process of establishing equilibrium, the shape of the I-front is changing; therefore we must take into account non-equilibrium effects in order to correctly predict the I-front thickness.

Fig. 2 shows the evolution of the ionization structure around our fiducial absorbed power-law source. The hydrogen front starts out quite thin, but becomes thicker and thicker as it propagates outward. When the source is turned on, the gas closest to it is very quickly ionized up to its equilibrium level, while gas a little further away is ionized much more slowly, due both to the intervening absorption and geometric dilution of the radiation. This means that the inner edge of the front is evolving faster than the outer edge, which effectively tilts the \( \chi_H \) curve, making it steeper. This creates a very thin transition region at first, which thickens as the front propagates outward and slows down. Depending on how the thickness of the front is measured, it can start out thinner than the MFP, and end up much thicker.

These effects can be seen even with a monochromatic spectrum, but, as illustrated in Fig. 3, a spectrum with a broad continuum of ionizing radiation can enhance the effect. Early on (e.g. at \( 10^3 \) yr), photons with lower energy (and therefore high ionization cross-section) will dominate the ionization at the front, while higher energy photons escape to larger distances and pre-ionize the medium (as seen in the long tail of curves representing the ionized fraction). This makes the front relatively thin because of the short MFP of these photons. As the front moves outward (e.g. at \( 10^5 \) yr), the lowest energy photons will continue to be preferentially absorbed closer to the source (and will dominate the ionization balance in the inner regions), leaving the higher energy photons to dominate in the outer parts of the front. This hardened spectrum creates a thicker front because of the longer MFP.

Based on the above features, it will be useful for the discussion below to divide a snapshot of the ionization structure at a time \( t < t_{\text{rec}} \) into three distinct regions. Closest to the quasar, in the equilibrium zone, the ionization rate has already reached equilibrium with the recombination rate. Just outside the equilibrium region is a rapid-ionization zone, where relatively neutral gas is suddenly

\(^3\)A combination of overdensity and high clumping factors in the typical quasar environment could, however, reduce the recombination time to a value perhaps as short as \( 5 \times 10^6 \) yr at \( z = 6.4 \) (Yu & Lu 2005).
the same interval: both approaches to estimating the log(l) that it is barely consistent with the range of log(l) of the spectral hardening. The intersection of the three curves at log((H I)) = −0.1 is merely a coincidence. Indeed, recall that the X H I = −0.1 to 0.9, we find (as shown in the figure) that it is barely consistent with the range of l_{MFP} over the same interval: both approaches to estimating the l_{MFP} based on an average photon energy of the source become inaccurate because of the spectral hardening. The intersection of the three curves at log((X H I)) = −0.1 is merely a coincidence. Indeed, recall that the ionization structure is not in equilibrium, so the width is constantly changing. The estimate of the MFP based on the mean photon energy of 239 eV and a neutral medium yields ~3 Mpc, whereas the path being exposed to intense ionizing radiation. Further out there is a pre-ionization zone, where the relatively rare high-energy photons penetrate and begin to ionize the gas, but recombination rates are low because of the low ionized fraction.

Fig. 4 shows a snapshot of the local mean ionizing photon energy (equation 6), and the corresponding MFP (calculated using the local neutral fraction), versus neutral hydrogen fraction, for the profile at 10^9 yr shown in Fig. 2. The spectrum is relatively unaffected by hardening up to X H I ≈ 0.1, but the mean energy increases rapidly after the neutral fraction reaches 0.3. Similarly, the MFP at first decreases in inverse proportion to the increasing neutral fraction, but reaches a minimum at X H I ≈ 0.3 and begins to grow as the spectrum hardens. This explains why the outer tail of ionization is so thick compared to the inner face of the front. If we measure the thickness of the front from X H I = 0.1 to 0.9, we find (as shown in the figure) that it is barely consistent with the range of l_{MFP} over the same interval: both approaches to estimating the l_{MFP} based on an average photon energy of the source become inaccurate because of the spectral hardening. The intersection of the three curves at log((X H I)) = −0.1 is merely a coincidence. Indeed, recall that the ionization structure is not in equilibrium, so the width is constantly changing. The estimate of the MFP based on the mean photon energy of 239 eV and a neutral medium yields ~3 Mpc, whereas the path corresponding to the range 0.1 < X H I < 0.9 in the equilibrium case is much longer, ~15 Mpc.

Fig. 5 shows two different measurements of the thickness of the front versus the logarithm of the time. The definitions of these thicknesses will be justified in Section 4, but for now we note that the outer part of the front grows thicker all the way up to about t_{rec}, while the inner part of the front comes into equilibrium much sooner.

The presence of helium also has important effects on the hydrogen ionization structure, as can be seen in Fig. 6. The influence is due to the coupling of the ionization states by recombination radiation. By
reprocessing high-energy photons (which, in the absence of helium, would escape to large distances) into lower energy recombination radiation (which is absorbed on the spot, mostly by hydrogen), helium lowers the hydrogen neutral fraction in the equilibrium zone. The difference is a factor of $\sim 3$ in the region where $X_{\text{HI}} \lesssim 10^{-2}$ at $10^8$ yr; this region is relevant in the analysis of the proximity zone of the quasar in Ly$\alpha$/β absorption. In particular, neglecting helium can result in predicting a much thicker front, depending on how thickness is measured (and a factor of several too large $R_\beta/R_\alpha$ ratio; see below).

Secondary ionizations have a similarly important effect, but on the outer tail of the ionization structure, as shown in Fig. 7. Neglecting secondary ionizations can reduce the thicknesses we would predict in the outer part of the front by several Mpc.

### 3.2 The effects of spectral hardness

As evident from the above discussion, the shape and hardness of the spectrum can have dramatic effects on the ionization structure. Generally a harder spectrum will produce thicker fronts, although as we shall see below, this is not always the case for certain definitions of front thickness. The mean photon energy is not enough to characterize the shape of the ionization structure it will produce. For instance, even a relatively weak high-energy component can produce an enhanced pre-ionization region, while a low-energy component can increase the ionized fraction of the equilibrium region but have little effect on the thickness of the rapid-ionization zone. Enhancing the effect of a high-frequency component is the fact that energetic photons can cause multiple secondary ionizations, especially in a relatively neutral medium.

A harder spectrum will also generally produce a ‘shallower’ ionized region, in the sense that the ionized fraction will be lower in the inner part of the ionized region since the ionization cross-section is lower for high-energy photons. At the quasar ages we are considering this effect can be considered to affect mainly the equilibrium region.

Two parameters control the shape of the spectrum in our models. Increasing the spectral index $x$ makes the spectrum softer, while increasing the intrinsic hydrogen column density $N_H$ cuts off more low-energy emission, hardening the spectrum.

For reference, Fig. 8 shows the fronts produced by a spectrum with no intrinsic absorption ($N_H = 0$). As expected, the fronts are much sharper than those in Fig. 2.

### 3.3 The size of the ionized region

Before discussing the thickness of the I-fronts in detail in the next section, it is useful to discuss the overall size of the H II region. As mentioned in Section 1, the size of the H II regions could be probed either in 21-cm studies, or by Lyman-line absorption spectra of individual sources. The former technique is sensitive to $X_{\text{HI}} \sim 1$, whereas the latter technique (with typical deep Keck spectra) probes the much lower neutral fraction $X_{\text{HI}} \sim 10^{-3}$. In Fig. 9, we therefore show the size of the ionized region measured out to $r_{0.5}$, where $X_{\text{HI}} = 0.5$ (top panel), and to $r_{-3}$, where $X_{\text{HI}} = 10^{-3}$ (bottom panel). The shaded plots show the H II region sizes at $3.16 \times 10^7$ yr (corresponding roughly to the Salpeter time, and to the expected ages of bright quasars; see e.g. Martini 2004), as a function of the intrinsic absorption $N_H$ and spectral index $x$.

Remember that the softest spectrum is in the lower right-hand corner of the graph, while the hardest spectrum is in the upper...
Spectra are normalized to produce the same number of photons with increasing left-hand corner. The trend in both panels is for the radius to decrease as more of the photons escape from the ionized region because of their longer MFP. Decreasing the spectral index $s$ (which also produces a harder spectrum), on the other hand, results in a larger H II region, since the harder spectrum is less attenuated by the intrinsic absorption, meaning $Q_{\text{abs}}$ is larger.

Considering both H II region size measurements together leads to an interesting conclusion. Several recent papers (Mesinger & Haiman 2004; Bolton & Haehnelt 2007a; Lidz et al. 2007; Maselli et al. 2007) have explored the accuracy of $R_\alpha$ and $R_\beta$, defined as the radii where the flux in the redshifted Ly$\alpha$ and Ly$\beta$ region of the spectrum falls below some fixed threshold, as a proxy for the location of the I-front. They found that $R_\alpha$ and $R_\beta$ are biased measurements, underestimating the ‘true’ distance to the I-front (which we might choose to locate at $r_{0.5}$) by typically 20–30 per cent. Here we discover another effect to worry about: as the spectra get harder (and especially as the obscuring column increases), the radius of the highly ionized region $r_{-3}$ decreases much more quickly than the half-ionization radius $r_{0.5}$. This is because the harder photons are ineffective at maintaining a high ionized fraction because of the low ionization cross-section, instead tending to escape into more neutral gas farther out. This produces a thicker front and a more neutral H II region. For hard spectra, this significantly increases the bias, with the underestimate reaching values as high as a factor of $\approx 8$ for the spectra with the largest obscuring column.

### 4 MEASURING THE THICKNESS OF THE I-FRONT

#### 4.1 Front thickness in 21-cm and in Lyman absorption spectra

As mentioned above, we are interested in two different regions of the I-front: the highly ionized inner face of the front at $10^{-3} \lesssim X_{\text{HII}} \lesssim 10^{-2.5}$ which is approximately the region probed by Lyman-series absorption spectra, and the less ionized outer tail of the front at $0.1 \lesssim X_{\text{HII}} \lesssim 0.9$, which is the region potentially accessible to redshifted 21-cm observations.

Mesinger & Haiman (2004) proposed the idea that the difference between $R_\beta$ and $R_\alpha$, as defined in the previous section, could be useful to probe the spectral hardness, with the two values increasingly separated for harder spectra. In a subsequent study, Bolton & Haehnelt (2007a) simulated a large set of quasar Ly$\alpha$ and $\beta$ absorption spectra and studied the possibility of using the transmission window created by the ionized region around the quasar to constrain the mean ionization fraction of the IGM. They found that density fluctuations induce a large scatter in their measured quantity, which is the ratio of radii inferred from each spectrum $R_\beta/R_\alpha$. However, according to their simulations, $R_\beta/R_\alpha = 1.2$ would be distinguishable from $R_\beta/R_\alpha = 1$ at the 2 $\sigma$ level with about 20 high-quality quasar spectra. As a proxy for this ratio, we use $r_{-2.5}/r_{-3}$, the ratio of radii at which $X_{\text{HII}} = 10^{-2.5}$ and $10^{-3}$, which correspond roughly to the points where flux would be lost in the Ly$\beta$ and Ly$\alpha$ absorption spectra, respectively, for a typical deep Keck spectrum of a $z = 6$ quasar.

In contrast to the Lyman-line absorption spectra, the 21-cm observations will be sensitive, at $z = 6–10$, to features corresponding to neutral fractions of the order of unity, with regions that have $X_{\text{HII}} \lesssim 0.1$ corresponding to ‘holes’ in tomographic 21-cm maps. Although the effective spatial resolution of such maps is highly dependent on the specific interferometric instrument and its configuration, a rough target value for next-generation facilities may be $\sim 1$ physical Mpc (see e.g. the review by Furlanetto et al. 2006). We adopt here $d_{0.1}$, the difference between the radius at which $X_{\text{HII}} = 0.1$ and $X_{\text{HII}} = 0.1$, as a proxy for the thickness of the I-front that may be measurable with 21-cm instruments.

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**Figure 8.** Ionized and neutral hydrogen fractions for a source with no intrinsic absorption ($N_\text{H} = 0$, dashed) or with $\log(N_\text{H}/\text{cm}^{-2}) = 19.2$ (solid). Spectra are normalized to produce the same number of photons $Q_{\text{abs}} = 8.3 \times 10^{53} \text{ s}^{-1}$. Other spectral parameters are the same as in Fig. 2.

**Figure 9.** The size of the ionized region in Mpc out to $X_{\text{HII}} = 0.5$ (left), and $X_{\text{HII}} = 0.001$ (right) versus the intrinsic absorption $N_\text{H}$ (in cm$^{-2}$) and the spectral index $s$ at $3.16 \times 10^{7} \text{ yr}$ and with $Q = 2 \times 10^{57} \text{ s}^{-1}$. Each block represents one simulation, with the size indicated in numerals and by the shading. The key to the shading appears at the top of each graph.
Figure 10. I-front thickness measures at $3.16 \times 10^7$ yr as measured by $d_0.1$ (in Mpc, top) and $r_{-2.5}/r_{-3}$ (bottom).

Fig. 10 depicts our measures of the I-front thickness around a quasar with an age of $\sim 3.16 \times 10^7$ yr, on the same grid of parameters used in Fig. 9. The first panel shows $d_0.1$, which exceeds our estimated detection threshold of $\sim 1$ Mpc for a large region of the parameter space. The thickness increases with increasing spectral hardness up till $\log(N_H/cm^{-2}) = 19.8$, after which it decreases as $N_H$ increases, due to the overall shrinking of the ionized region discussed in Section 3.3, and shown in Fig. 9. This will be the pattern for most of the grids we will discuss: the $d_{0.1}$ widths will always increase with decreasing spectral index, and will grow with increasing absorption up to a point, but will eventually shrink for large enough $N_H$.

The $r_{-2.5}/r_{-3}$ ratio in the second panel is almost totally insensitive to the spectral index. Making the spectral index smaller does make the front slightly thicker, but it also moves the front outward by a small amount, which keeps the ratio constant. The ratio increases dramatically between $\log(N_H/cm^{-2}) = 18.6$ and $\log(N_H/cm^{-2}) = 19.2$, becoming large enough to be potentially detectable (according to the criterion defined above based on Bolton & Haehnelt 2007a), thanks to the fact that the hard spectra $r_{-3}$ reaches equilibrium faster, while $r_{-2.5}$ continues to move outward a little longer, which stretches out the ratio. The intrinsic absorption must be at least $\log(N_H/cm^{-2}) = 19.2$ for the ratio to exceed 1.1. The ratio exceeds 1.2 for any spectral index at $\log(N_H/cm^{-2}) \geq 19.8$.

Note that the contours for the two size measures in the $N_H$–$s$ plane have different orientations. This is not surprising, since variations of $s$ and $N_H$ can affect the profile differently at different locations in the front. This suggests that a combination of 21-cm and Lyman-series absorption measurements could break the degeneracy inherent in the separate observations and allow both parameters to be constrained simultaneously.

4.2 Parameter variations

We next examine how our results change when we vary other model parameters.

4.2.1 Source lifetime

In Fig. 11, we show the same thickness measures as in Fig. 10, but for quasar three times older, at $t = 10^8$ yr. The figure reveals that the outer tail of the front ($d_{0.1}$) has generally gotten thicker, but otherwise follows the same trends we saw at $3.16 \times 10^7$ yr. The inner face ratio $r_{-2.5}/r_{-3}$ has remained small and almost unchanged for the softest spectra with $N_H \leq 10^{18.6}$ cm$^{-2}$. These spectra create steep fronts and deep equilibrium regions with $X_{HI} < 0.001$, so even at $10^8$ yr $r_{-2.5}/r_{-3}$ is still measuring the steep slope of the rapid ionization zone. There is a sharp increase in the front thickness at all spectral indices between $N_H = 10^{18.6}$ and $10^{19.2}$ cm$^{-2}$. This is because for...
the harder spectra the equilibrium region reaches \( X_{\text{HI}} > 10^{-3} \) (but is usually still below \( X_{\text{HI}} = 10^{-2.5} \)) before 10\(^8\) yr, meaning that \( r_{-3} \) is the distance to a fixed point in the equilibrium zone, while \( r_{-2.5} \) is the distance to a point in the still-receding I-front. This produces the high ratios seen in the figure.

4.2.2 Source luminosity

Reducing the (pre-intrinsic-absorption) ionizing photon luminosity \( Q = 2 \times 10^{37} \text{s}^{-1} \) to \( 2 \times 10^{28} \text{s}^{-1} \) produces the widths shown in Fig. 12. Reducing the luminosity by a factor of 10 reduces the time-scale by a factor of 10 and the Strömgren radius by a factor of \( 10^{1/3} = 2.15 \). The shape of the pre-ionization and rapid-ionization zones (since they are largely unaffected by recombinations) are therefore almost identical to the \( Q = 2 \times 10^{37} \text{s}^{-1} \) models at 3.16 \( \times 10^9 \) yr (not shown), when the same total number of photons has been emitted. And indeed the \( d_{0.1} \) values are very close, and consequently are lower than the \( Q = 2 \times 10^{37} \text{s}^{-1} \) models at 3.16 \( \times 10^7 \) yr by a factor of about 1.5–2. The same reasoning does not apply to the \( r_{-2.5}/r_{-3} \) ratio, which end up with similar values. The lower luminosity means that \( r_{-3} \) is frozen into the equilibrium zone earlier, but \( r_{-2} \) also moves out more slowly, so the ratio ends up similar to the higher luminosity case.

![Figure 12](https://academic.oup.com/mnras/article-abstract/385/3/1561/1012910)

Figure 12. Widths with \( Q = 2 \times 10^{36} \text{s}^{-1} \) at \( 3 \times 10^7 \) yr as measured by \( d_{0.1} \) (in Mpc, top) and \( r_{-2.5}/r_{-3} \) (bottom).

4.2.3 Clumping factor

The clumping factor effectively increases the recombination coefficient, which has the effect of raising the neutral fraction in the equilibrium zone, but has little effect on the rapid-ionization or pre-ionization regions, (as emphasized in Cen & Haiman 2000), and as can be seen in Fig. 13. Increasing the clumping factor also decreases the recombination time and Strömgren radius. With \( C = 5, t_{\text{rec}} = 3.2 \times 10^9 \) yr, while with \( C = 20, t_{\text{rec}} = 8.1 \times 10^7 \) yr (both at \( z = 6 \)), meaning that the ionization structure could approach equilibrium within a quasar lifetime.

Fig. 14 reproduces the grids of spectral parameters with a clumping factor of \( C = 5 \). The thickness measures follow the same trends seen with \( C = 1 \). Increasing the clumping factor produces almost the same grid of \( d_{0.1} \) values because it has little effect on the high-energy photons that pre-ionized the outer region.

The \( r_{-2.5}/r_{-3} \) ratios on the \( C = 5 \) grid are quite a bit higher than with \( C = 1 \). The ratio exceeds 1.2 for all spectra with \( N_{\text{HI}} \geq 10^{8.6} \text{cm}^{-2} \). A clumping factor of \( C = 20 \) (also not shown) produces a very similar grid for the more obscured spectra, and produces even higher ratios for \( \log(N_{\text{HI}}/\text{cm}^{-2}) \leq 19.2 \).

4.2.4 The ionizing background

The IGM is expected to have already undergone some non-negligible ionization by galaxies, and possibly by fainter quasars, by the time the massive black holes producing the observable \( z \geq 6 \) quasars appear. The ionizing background may have both a smooth X-ray component (e.g. Oh 2001; Venkatesan, Giroux & Shull 2001) from pre-existing fainter quasars, and a ‘swiss-cheese’-like component of smaller ionized bubbles surrounding (clusters of) galaxies, the latter of which may be highly clustered around the massive haloes hosting our quasars of interest (e.g. Alvarez & Abel 2007; Lidz et al. 2007; Wyithe & Loeb 2007).

Here we first calculate a grid of thickness measures with a purely uniform background \( \Gamma_{\text{BG}} = 4.4 \times 10^{-17} \text{s}^{-1} \) (see the discussion of radiation transfer below), producing an equilibrium \( X_{\text{HI,BG}} = 0.75 \). We will then study three variations of this model, to address the following effects: (i) modification of the background flux due to radiative transfer effects caused by the ionization by the quasar, (ii) a non-uniform (swiss-cheese) background ionization topology and (iii) enhanced ionization near the quasar due to clustering of pre-existing galaxies.

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In the presence of a background, there are fewer neutral hydrogen atoms to ionize, and the I-fronts travel farther in a given amount of time. The lower neutral hydrogen density also means the MFP is longer, so the fronts are somewhat thicker. The equilibrium neutral fraction is relatively unaffected as long as it is well below $1 - X_{\text{HI}}$, $\text{BG}$. Setting $X_{\text{HI}}$, $\text{BG} = 0.75$ obviously makes our previously defined measure for the thickness, $d_{0.1}$, unusable, so we here instead examine the distance from $X_{\text{HII}} = 0.9$ to 0.8 (and we can still use $r_{-2.5}/r_{-3}$). Both of these thickness measures are shown in Fig. 15, again at $3.16 \times 10^7$ yr, as a function of spectral slope and obscuring column density.

The new measure of the outer part of the front behaves much like $d_{0.1}$ did for the grids with no background (except that it is obviously smaller overall). The figure also shows that $r_{-2.5}/r_{-3}$ is somewhat larger than for the no-background case. The reduced neutral hydrogen density allows the front to move more quickly, but has little affect on the equilibrium ionized fraction where $X_{\text{HI}} \ll 1 - X_{\text{HI}}$, $\text{BG}$. This means that the inner (most highly ionized) edge of the front slows as it approaches the equilibrium value, while farther out the front is still receding at a faster rate, effectively thickening the front.

There is an inconsistency in the way the background ionization rate was added to the quasar flux above, however (which is shared by many other similar studies in the literature). We specified an ionization rate per neutral hydrogen atom $\Gamma_{1}$, $\text{BG}$ which is constant, equivalent to a uniform background flux that does not depend on the ionization state of the gas. In fact, the flux from a homogeneous population of emitters will depend on the MFP, and hence on the ionization state of the gas. The more highly ionized the gas is, the farther ionizing photons will travel through it, meaning that more distant sources can contribute to the local flux. In fact, the MFP within a highly ionized HII region might exceed the size of the region, meaning that the background will be the sum of the flux from all the sources inside the region, and the background will grow as the region expands.

In a homogeneous medium with a total photon emission coefficient of $j$ (photons per unit time per unit volume), the total incident flux (integrated over all angles) is simply

$$ J = \frac{j}{n_{\text{H}}(1 - X_{\text{HII}})\sigma} = j \text{MFP}, $$

(14)

where $\sigma$ is the absorption cross-section for the photons. Since $\Gamma_{1} = j\sigma$, the background ionization rate should clearly depend on the ionization state of the gas. Similarly, the flux in the centre of a sphere of radius $r$ (where $\text{MFP} \gg r$ and $j = 0$ outside the sphere) is $J = jr$.

4 Usually an emission coefficient is defined as the amount of power emitted per unit solid angle per unit volume. Here we use a somewhat different definition which is convenient for the task at hand.
In our model the medium is obviously not homogeneous, since \( X_{\text{HII}} \) varies with position and time (and later we will be interested in a variable \( j \) as well). Solving for the background flux \( J \) exactly in an inhomogeneous medium requires computationally expensive 3D radiation transfer (and still 2D in the azimuthally symmetric case), so we have implemented an approximate radiative transfer algorithm to estimate the effect using a 1D calculation. We assume all of the background photons are at 13.6 eV and calculate the flux using the equation

\[
J(r) = J_0(r) + J_{\text{in}}(r) + J_{\text{out}}(r),
\]

\[
J_0(r) \equiv j(r)l_{\text{MFP}}(r)\left\{1 - \exp[-\Delta r/l_{\text{MFP}}(r)]\right\},
\]

\[
J_{\text{in}}(r) \equiv \frac{1}{2} \int_0^{r+\Delta r} j(r') \left(\frac{r'}{r}\right)^2 e^{(\Delta r/r - 1)/\Delta r} dr',
\]

\[
J_{\text{out}}(r) \equiv \frac{1}{2} \int_{r+\Delta r}^{\infty} j(r') e^{(\Delta r/r - 1)/\Delta r} dr',
\]

where the first term is the flux from within one radial step \( \Delta r \), the second term is the estimated flux from within \( r - \Delta r \), the third term is the estimate flux from outside of \( r + \Delta r \) and \( \tau_0(r) \) is the optical depth at 13.6 eV as defined by equation (1). The ad hoc factor \((r'/r)^2\) is used to decrease the contribution to the flux from spherical shells at small \( r \) (roughly approximating the decrease in the total emitting volume in three dimensions at small radii). At \( r > l_{\text{MFP}} \) uniform \( j \) and \( X_{\text{HII}} \), equation (15) reproduces the analytical result (equation 14).

Fig. 16 compares the ionization structures with and without the approximate RT algorithm. The photon emission coefficient is \( j = \sigma_B n_H X_{\text{HII}} \approx 8.3 \times 10^{-22} \text{ s}^{-1} \text{ cm}^{-3} \). For quasar ages of \( \lesssim 5 \) yr, the radiation transfer makes no difference to the ionization structure. The central ionized region is simply too small to allow a large additional background to build up. At 10 yr, RT decreases the neutral fraction, but only for \( -4 \lesssim \log(X_{\text{HII}}) \lesssim -1.5 \). This is because the ionized region has grown large enough for the diffuse background to become significant, but the quasar flux still dominate close the quasar, and the MFP is still very small for 13.6 eV photons once the neutral fraction gets large, so the extra flux is confined to the inner part of the front. We conclude that radiation transfer of flux from a uniform ionizing background could be important for Lyman-series observations of old quasars or with high backgrounds, but will be less important for 21-cm observations.

Next, let us examine the effect of a patchwork of pre-existing ionized bubbles along our LOS. This is the type of background profile that results from the ‘chessy-sheese’ topology of small ionized bubbles (generated by neighbouring galaxies and possibly AGN) embedded in a neutral IGM. Naively, we might choose to fill 75 per cent of the IGM with ionized bubbles in order to compare this scenario with the smooth background of Fig. 16, but here we have to be careful about what quantities we want to compare. The recombination rate in a fully ionized region is \( \alpha_R n_H^2 = 1.48 \times 10^{-21} \text{ s}^{-1} \text{ cm}^{-3} \), so if a fraction \( f_{\text{ion}} \) of the universe is contained in ionized bubbles, then the average photon emission coefficient needed to maintain equilibrium is \( j = \alpha_B n_H^2 f_{\text{ion}} \). Equating this to the coefficient for the smooth \( X_{\text{HII,BG}} = 0.75 \) case we obtain \( f_{\text{ion}} = 0.75^2 = 0.56 \). In fact we will need an even higher background in the bubbles in order for them to be highly ionized, as we will discuss below.

Next we need to determine the size of the ionized bubbles. Furlanetto, Zaldarriaga & Hernquist (2004) calculated that when 56 per cent of the IGM was contained in galactic \( \text{H} \alpha \) regions, the \( \text{H} \alpha \) region radius distribution peaked at \( \sim 4 \) Mpc comoving, or about 0.6 physical Mpc at \( z = 6 \). We have set up a background ionization profile consisting of evenly spaced ionized regions with a diameter of 1 Mpc, occupying 56 per cent of the IGM volume (and therefore separated by neutral regions of 0.79 Mpc along the LOS). The neutral fraction within the bubbles is initially set to \( 10^{-3} \). The background needed to maintain this level of ionization is

\[
j = \frac{\alpha_B n_H X_{\text{HII,BG}}^2}{\alpha_R (1 - X_{\text{HII,BG}})} = 2.01 \times 10^{-21} \text{ s}^{-1} \text{ cm}^{-3},
\]

where \( r = 0.5 \) Mpc is the radius of the bubble. This is 35 per cent higher than the background in the smooth case. We again use equation (15) to approximate radiation transfer for the background photons.

The resulting ionization structure is shown in Fig. 17. Without the background, the fronts in the interbubble regions would be essentially the same shape as they are in totally neutral IGM, except sliced and shifted apart where the bubbles occur, since the ionizing radiation traverses the bubbles unabsorbed (except by helium and the small amounts of residual hydrogen) so the front can pick up where it left off on the other side. The presence of helium and the geometric dilution cause some changes in the shape, but the background radiation transfer has a greater effect. Once the front has swept past a bubble, its background photons can escape, and they stream out to contribute to the ionization of the interbubble regions.

This type of background structure may have interesting observational manifestations. Within the interbubble regions, the front is somewhat thinner than with either no background or a smooth background. The front is thinner than in the no-background case because the background photons contributing to the movement of the front have a short MFP. The front is thinner than in the smooth-background case because it is ‘trapped’ by the fully neutral interbubble regions where the MFP is short, so it is slowed down, meaning that a more highly ionized part of the front (e.g. \( r < 3 \)) can ‘keep up’ better with a more neutral part (e.g. \( r > 2.5 \)), resulting in a thinner front over all. There will be brief windows when \( r = 3 \) is still trapped in the residual neutral gas on one side of a bubble, while \( r > 2.5 \) is on the far side, but it would require detailed simulations of absorption spectra to determine the observability of such a situation. The shape of the front at neutral fractions more relevant to 21-cm observations.
Figure 17. Comparison of the neutral fraction with no ionizing background (solid), with a smooth ionizing background (and approximate radiation transfer) chosen to produce $X_{\text{H II}},\text{BG} = 0.75$ (dashed) and with a ‘swiss-cheese’ background (dotted) of 1 Mpc ionized bubbles separated by 0.79-Mpc neutral regions, which would produce a similar average ionization. Spectral parameters are the fiducial ones used in Fig. 2. The panels show the ionization structures at $10^7$, $3 \times 10^7$ and $10^8$ yr, respectively.

again tends to suggest smaller thickness measurements, but it seems likely that the thicknesses could still be measurable.

The signature of the hard quasar spectrum is also still quite visible on large scales, for instance in the separation between $X_{\text{H I}} \sim 10^{-4}$ and 0.1. This suggests that a combination of 21-cm and Lyman-series observations, particularly when smoothed on large scales or averaged over many quasars, could place constraints on the ionizing SED of the quasar or quasars. If the patchy ionization structure is resolved in future, high-resolution 21-cm interferometer, such as SKA, could resolve such clusters of galaxy bubbles outside the quasar’s H II region, the next generation of experiments will likely not have sufficient resolution. In this case, the I-front will appear extended due to the presence of galaxies.

In order to explore the effect of such a pre-ionization profile on our conclusions, we implemented an ionizing background designed to qualitatively mimic the background ionization structure predicted by Wyithe & Loeb (2007) when the IGM far from the quasar is at $X_{\text{H II}},\text{BG} \sim 0.7–0.8$. This scenario pre-existing galaxies produce an H II region centred on the quasar; outside this H II region, there is a tail of excess partial ionization, slowly approaching the background level of the neutral fraction in the IGM.

To produce the first panel in Fig. 18, we set up an ionizing background to produce a 1 Mpc radius inner ionized region (initially set at $X_{\text{H II}} = 2 \times 10^{-3}$ with $j = 4.41 \times 10^{-21} \text{s}^{-1} \text{cm}^{-3}$). Outside of that, the profile is set to

$$X_{\text{H II},\text{BG}} = 0.75 + \left[ \frac{(r/\text{Mpc}) + 1.91}{1.81} \right]^{-3},$$

where $r$ is the radial distance.

Finally, we consider the effect of clustering of background sources around the quasar. Wyithe & Loeb (2007) have explored the mean ionization structure around a quasar resulting from the biased clustering of galaxies around its host halo (not addressing the discreteness of the bubbles in the radial profile). They point out that even outside the I-front, the IGM is ionized 10–20 per cent more than the global mean ionized fraction. While a high-resolution 21-cm interferometer, such as SKA, could resolve such clusters of galaxy bubbles outside the quasar’s H II region, the next generation of experiments will likely not have sufficient resolution. In this case, the I-front will appear extended due to the presence of galaxies.

In order to explore the effect of such a pre-ionization profile on our conclusions, we implemented an ionizing background designed to qualitatively mimic the background ionization structure predicted by Wyithe & Loeb (2007) when the IGM far from the quasar is at $X_{\text{H II}},\text{BG} \sim 0.7–0.8$. This scenario pre-existing galaxies produce an H II region centred on the quasar; outside this H II region, there is a tail of excess partial ionization, slowly approaching the background level of the neutral fraction in the IGM.

To produce the first panel in Fig. 18, we set up an ionizing background to produce a 1 Mpc radius inner ionized region (initially set at $X_{\text{H II}} = 2 \times 10^{-3}$ with $j = 4.41 \times 10^{-21} \text{s}^{-1} \text{cm}^{-3}$). Outside of that, the profile is set to

$$X_{\text{H II},\text{BG}} = 0.75 + \left[ \frac{(r/\text{Mpc}) + 1.91}{1.81} \right]^{-3},$$

where $r$ is the radial distance.

Figure 18. Comparison of the neutral fraction with a uniform ionizing background (solid) and a biased background from pre-existing galaxies clustered around the quasar (dashed). Approximate background RT is used in both cases. Spectral parameters are the fiducial ones used in Fig. 2. The three sets of curves correspond to source ages of $\log(t/\text{yr}) = 4, 7$ and 8, respectively.

In the first panel, the central pre-ionized bubble has a radius of 1 Mpc, while in the second panel the radius is 2 Mpc.
with $j = \alpha_B n_H^2 X_{\text{H}\beta, \text{BG}}^2$ for $r > 1$ Mpc. In the second panel the radius of the pre-ionized region is increased to 2 Mpc and the outer profile is shifted accordingly.

Fig. 18 illustrates what happens to the I-front as it passes through such a biased background. The dashed curves show the I-front expanding into the pre-ionized region, contrasted with the case when the pre-ionization is uniform (solid curves). The figure reveals that once the front has passed beyond the high-background inner region, it quickly begins to approach the shape of the ionization profile in a uniform background, though the extra flux from the sources clustered close to the quasar keeps it ahead of the front in the uniform case. The presence of helium is particularly important in this case because it determines the speed at which the front can propagate through the pre-ionized region (since helium is assumed to be unaffected by the background and therefore still neutral). We have actually chosen rather small sizes for our central pre-ionized region. Wyithe & Loeb (2007) predict central regions of $r \sim 2$–8 Mpc when $X_{\text{H}\beta, \text{BG}} \sim 0.7$–0.8. A larger region implies a larger background flux once the front has passed the inner region. This would prolong the time during which the front shape is affected by the background bias. Even a region as small as 2 Mpc results in fronts whose inner parts are significantly less broad at $10^7$ yr, as seen in the second panel.

5 CAVEATS

Before we summarize our conclusions, let us briefly review the limitations of the methods we have employed in reaching them.

The one-the-spot approximation – in which we assume that ionizing photons produced by recombination are absorbed at their point of origin – is strictly valid only where the MFP of the recombination photons is much shorter than other length scales of interest, such as the thickness of the front.\footnote{The situation is slightly different for soft (e.g. stellar) spectra, in which the mean ionizing photon from the source is also close to the threshold. In that case both the source spectrum and the recombination radiation are concentrated near the threshold. See Osterbrock & Ferland (2006).} This condition is violated where the neutral fraction is very low, in the inner part of the ionized region. It is also less accurate for helium-derived photons, since they are generally more energetic. The result is a slight overestimate of the ionization rates, and therefore a slight underestimate of the neutral fraction, close to the quasar. The effect is less important for harder ionization rates, and therefore a slight underestimate of the neutral fraction is very low, in the inner part of the ionized region. \footnote{The highly ionized inner part of the front, which may be probed by Lyman-line absorption spectra, remains thin for bright quasars unless a large obscuring column [log($N_H$/cm$^{-2}$) $\gtrsim$ 19.2] removes most of their ionizing photons up to $\sim$40 eV. Otherwise the lowest energy photons with the shortest MFPs always dominate ionization at the inner face of the front resulting in a small thickness.}

It is also less accurate for helium-derived photons, since they are generally more energetic. The result is a slight overestimate of the ionization rates, and therefore a slight underestimate of the neutral fraction, close to the quasar. The effect is less important for harder spectra (because they leave higher neutral fractions overall), and is unimportant in the outer part of the front. For instance, the mean free path at $13.6 \text{eV}$, $\lambda_{\text{MFP}}(\nu_0) < 0.01$ Mpc for $X_{\text{H}} > 0.07$.

We have ignored the propagation time for photons (due to the finite speed of light). Our results accurately predict the observed structure along a LOS aimed directly at the quasar, in an absorption spectrum, for example. To simulate 2D projections of the ionization structure (like 21-cm maps), we would need to apply a simple transformation (see citations in Section 2.1). In fact, since the thickness of the I-front varies with time, in principle, a comparison of the thickness in transverse and radial directions, in addition to the angular dependence of the overall bubble size due to finite-speed-of-light effects (Wyithe et al. 2005; Yu 2005; Shapiro et al. 2006), will contain information about the age of the quasar.

We have assumed the density of the IGM surrounding the quasar is homogeneous on a macroscopic scale, with smaller variations accounted for by a uniform clumping factor. Quasars are actually expected to form in biased environmental conditions, with high gas density and a high density of neighbouring haloes. The largest effect would be along lines of sight that intersect high-density Lyman-limit systems, which could stall the propagation of the I-front and shield the gas further along the LOS from ionizing photons. The less extreme effects of density inhomogeneities would be somewhat ameliorated by certain observational necessities. In order to get a large enough signal-to-noise ratio to meaningfully constrain the structure of quasar H II regions, it may be necessary to stack 21-cm images of multiple bubbles. Similarly, measurements of the spectra of many quasars would be combined in order to constrain the ionization structure with Lyman-series absorption observations. In either case, density inhomogeneities would add to the random ‘noise’, but could, to some extent, be averaged out. Width measurements may be more robust under such conditions than the simple size measurements discussed by Maselli et al. (2007); however, more study is needed to determine that conclusively.

As mentioned in Section 2.4, we have assumed the IGM is isothermal, justifying this by pointing out that most of the heating will occur before recombinations become important. Therefore, as long as we choose the gas temperature to match conditions expected inside the H II region, this assumption should have little effect on our results.

Finally, we should remind the reader that since we did not actually simulate absorption spectra, we have not taken into account the effect of the GP trough damping wing (from the neutral hydrogen surrounding the ionized region), which could be very important for the observational determination of $R_p/R_c$. In fact, Mesinger & Haiman (2004) essentially use this effect to constrain the neutral hydrogen fraction in the IGM.

6 DISCUSSION AND CONCLUSIONS

We have found that high-redshift quasars residing in a partially neutral IGM could produce I-fronts with an observable thickness, given a sufficiently hard ionizing spectrum. We discovered that simulating the time-dependent evolution of the front is crucial for making accurate predictions of the ionization structure, and that the presence of helium in the IGM and secondary ionizations by high-energy photoelectrons can both have significant effects on the ionization structure.

With an intrinsic hydrogen column density log($N_H$/cm$^{-2}$) $\gtrsim$ 19.2 or a sufficiently hard power-law spectrum combined with some obscuration [e.g. spectral index $s \lesssim 1.2$ at log($N_H$/cm$^{-2}$) $\gtrsim 18.0$], the outer thickness of the front exceeds $\sim 1$ physical Mpc and may be measurable from the 3D morphology of its redshifted 21-cm signal.

The highly ionized inner part of the front, which may be probed by Lyman-line absorption spectra, remains thin for bright quasars unless a large obscuring column [log($N_H$/cm$^{-2}$) $\gtrsim$ 19.2] removes most of their ionizing photons up to $\sim$40 eV. Otherwise the lowest energy photons with the shortest MFPs always dominate ionization at the inner face of the front resulting in a small thickness.

Highly absorbed ionizing spectra leave a relatively large neutral fraction within the H II region, which means that the Lyman-series optical depths can be large even within the front. For sources with log($N_H$/cm$^{-2}$) $\gtrsim$ 19.8, the Ly$\alpha$ trough (where the neutral fraction is $\gtrsim 10^{-3}$) underestimates the size of the H II region by a factor of $\gtrsim 4$. The bias can get as large as a factor of $\approx$8 within out parameter space. This is in addition to other effects that bias this measurement by a much smaller amount, as already discussed by several authors (Bolton & Haehnelt 2007a; Lidz et al. 2007; Maselli et al. 2007).

These obscured spectra also result in a large difference between the sizes measured by the Ly$\alpha$ trough, and those measured by the
Lyβ trough (where the neutral fraction is $\gtrsim 10^{-2.5}$). We estimate that $R_\beta/R_\alpha$ could be higher than 1.2 for log($N_H$/cm$^{-2}$) $\gtrsim 19.8$ with a quasar age of $3 \times 10^7$ yr.

We explored the effects of uniform and non-uniform ionizing backgrounds, finding that even with a large uniform background the thickness of the I-front has the potential to constrain the spectral parameters of the quasar. An I-front propagating into a ‘swiss-cheese’ background of small pre-ionized bubbles obviously makes for a more complicated ionization structure, but again, the shape of the front on both large and small scales is controlled largely by the quasar’s ionizing SED. The greatest challenge is presented by a quasar turning on within a large pre-existing ionized region due to galaxies clustered around the quasar. In this case, the thickness of the front does not reflect the quasar’s spectrum until the quasar has pushed the front a significant distance farther into the IGM. A measurement of a thin front around a quasar cannot, therefore, be interpreted as definitive evidence of a soft or unabsorbed quasar spectrum. On the other hand, measuring a thick front does suggest a highly absorbed quasar spectrum, because the galactic sources producing the pre-quasar ionization should be soft.

Shapiro et al. (2004) and Thomas & Zaroubi (2007) have also used 1D radiative transfer calculations (with slightly different numerical methods) to explore high-redshift ionization structures, with the addition of self-consistent temperature calculations. Thomas & Zaroubi (2007) also included collisional ionization, and an evolving mean IGM density, while Shapiro et al. (2004) (who were focused on the evaporation of minihaloes by the I-front) included gas dynamics and trace metals. Like the present work, Thomas & Zaroubi (2007) included secondary ionizations, and both papers included helium, and calculations of the time evolution of the front. Neither of the two papers included the ionization of hydrogen by helium recombination radiation, and they explored only blackbody (stellar) and power-law or truncated power-law (quasar or ‘miniquasar’) sources, rather than the ultra-luminous obscured quasars that we are interested in here (though the miniquasar spectra are fairly similar to some of our spectra). Shapiro et al. (2004) found, as we did here, that I-fronts around sources with harder spectra are thicker. However, they studied sources at higher redshift ($\alpha = 9$), which were much less luminous, and the hardest spectrum they examined (a $10^5$ K blackbody, representing Population III stars) was still softer than most of the spectra in the range included in the present paper. As a result, they found fronts much thinner (up to $\sim 0.01$ Mpc; see their figs 7 and 8) than most of those discussed in the present paper. Among the many interesting findings of Thomas & Zaroubi (2007) are several relevant to the present study. Even with their harder power-law spectrum ($\alpha = 1$ extending from 200--10$^5$ eV), they did not find extended ionization tails outside of the front, due to the combination of shorter lifetimes and higher redshift (when the IGM density was higher). They do, however, find an extended kinetic temperature structure coupled to the spin temperature so as to be observable with 21-cm instruments, and find that such observations could be useful in discriminating between various source spectra.

Finally, we found that the contours of degeneracy in our parameter space for measurements using 21-cm observations are oriented differently from those for measurements using Lyman-series absorption spectra. This suggests that studies combining both types of observations have the potential to break the degeneracy and constrain both the intrinsic absorption column and spectral index of a quasar’s ionizing radiation at $z>6$.

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