Inhomogeneous recombinations during cosmic reionization

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ABSTRACT
By depleting the ionizing photon budget available to expand cosmic HII regions, recombining systems (or Lyman limit systems) can have a large impact during (and following) cosmic reionization. Unfortunately, directly resolving such structures in large-scale reionization simulations is computationally impractical. Instead, here we implement a sub-grid prescription for tracking inhomogeneous recombinations in the intergalactic medium. Building on previous work parameterizing photo-heating feedback on star-formation, we present large-scale, semi-numeric reionization simulations which self-consistently track the local (sub-grid) evolution of both sources and sinks of ionizing photons. Our simple, single-parameter model naturally results in both an extended reionization and a modest, slowly-evolving emissivity, consistent with observations. Recombinations are instrumental in slowing the growth of large HII regions, and damping the rapid rise of the ionizing background in the late stages of (and following) reionization. As a result, typical HII regions are smaller by factors of $\sim 2$–3 throughout reionization. The large-scale ($k \lesssim 0.2 \text{ Mpc}^{-1}$) ionization power spectrum is suppressed by factors of $\gtrsim 2$–3 in the second half of reionization. Therefore properly modeling recombinations is important in interpreting virtually all reionization observables, including upcoming interferometry with the redshifted 21cm line. Consistent with previous works, we find the clumping factor of ionized gas to be $C_{\text{HII}} \sim 4$ at the end of reionization.

Key words: cosmology: theory – early Universe – reionization – dark ages – intergalactic medium – galaxies: formation – high-redshift – evolution

1 INTRODUCTION
Reionization is a story of sources and sinks of ionizing photons. Historically, the most famous protagonists of this tale have been the sources: the tiny ($\lesssim$ percent level) fraction of baryons which are able to condense and form stars inside the first galaxies. A fraction of the ionizing photons emitted from these stars (and accreting black holes) manage to escape their host galaxies and begin ionizing the surrounding intergalactic medium (IGM). Driven by the birth and evolution of galaxies, these cosmic HII regions grow and overlap, eventually permeating all of space and completing the last major phase change of our Universe: hydrogen reionization.

On the other hand, the “sinks” of ionizing photons have received comparably less attention. An ionizing photon escaping a galaxy can have one of two fates: (i) it can ionize a neutral atom beyond the surrounding HII region, contributing to its growth; or (ii) while passing through the surrounding HII region it can encounter and reionize an atom which was previously ionized but subsequently recombined. These later sinks (often dominated by so-called Lyman limit systems, LLSs, though they can also include less dense, more diffuse structures) could substantially delay reionization by depleting the photon budget available for expanding the HII regions (e.g. Miralda-Escudé et al. 2000; Ciardi et al. 2006; McQuinn et al. 2007; Finlator et al. 2012; Kaurov & Gnedin 2013b). Furthermore, sinks can substantially alter reionization morphology, imposing a limit to the size of isolated HII regions (e.g. Furlanetto & Oh 2005; Mesinger et al. 2012; Alvarez & Abel 2012). Understanding their impact is crucial in interpreting all observations of the epoch of reionization.

LLSs are better understood at lower redshifts ($z \lesssim 4$), post-reionization. Radiative transfer calculations (McQuinn et al. 2011; Rahmati et al. 2013), together with observations of quasar Ly$\alpha$ spectra (e.g. Prochaska et al. 2010; Songaila & Cowie 2010), confirm that the general properties of LLSs can be understood in terms of the local Jeans length (Schaye 2001), although the detailed properties are difficult to simulate as they (and especially even more dense systems) can occur very near galaxies. Most IGM recombinations are sourced by gas with densities near the critical threshold required for self-shielding (e.g. Miralda-Escudé et al. 2000; Furlanetto & Oh 2005).

Unfortunately, extending this simple picture of sinks to the epoch of reionization is not straightforward. From a modeling standpoint, as always the main difficulty lies in the enormous dynamical range required. One needs to fully resolve the internal structure of the dominant population of self-shielded regions (with

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typical sizes of $\sim$ ten proper kpc; e.g. Schaye 2001 in cosmological simulations which sample reionization structure on scales of $\gtrsim$ hundreds of comoving Mpc (e.g. Furlanetto et al. 2004). Although single-box simulations of reionization have made significant progress lately (for example, see the recent review in Trac & Gnedin 2011), tackling this full range of scales remains computationally out of reach for the foreseeable future.

Moreover, the properties of the recombining gas are sensitive to the local density and radiation fields, both of which can be very inhomogeneous and can evolve rapidly during reionization. Conclusions regarding the role of sinks must therefore be robust to astrophysical uncertainties in these quantities.

Here we implement a sub-grid model of recombinations inside large-scale, semi-numerical simulations of reionization. Each cell’s recombination history depends on the local values of density, ionizing UV background (UVB), and reionization history. Building on Sobacchi & Mesinger 2013a,b, our simulations also include the effects of photo-heating on the star formation rate; therefore, we include reionization feedback on both the sources and the sinks. We investigate the relative impact of inhomogeneous recombinations on the reionization history and morphology, as well as the evolution of the UVB, emissivity, mean free path to ionizing photons and the clumping factor (see below) of the ionized gas.

This paper is organized as follows. In Section 2 we describe our large-scale reionization simulations. In Section 3 we present our sub-grid prescriptions to model UVB feedback on galaxies (3.1), and the small-scale structure of the IGM (3.2). In Section 4 we present our results, investigating the role of sinks and sources on IGM properties during reionization. In Section 5 we present our conclusions. Throughout we assume a ΛCDM cosmology with parameters ($\Omega_m$, $\Omega_\Lambda$, $\Omega_b$, $h$, $\sigma_8$, $n$) = (0.28, 0.72, 0.046, 0.70, 0.82, 0.96), as measured by the Wilkinson Microwave Anisotropy Probe (WMAP; Bennett et al. 2013), and also consistent with recent results from the Planck satellite (Planck Collaboration 2013). Unless stated otherwise, we quote all quantities in comoving units.

2 LARGE-SCALE SIMULATIONS OF REIONIZATION

To model cosmological reionization, we use a parallelized version of the publicly available semi-numerical simulation, 21CFAST. We generate the IGM density and source fields by: (i) creating a 3D Monte Carlo realization of the linear density field in a box with sides $L = 300$ Mpc and $N = 1600^3$ grid cells; (ii) evolving the density field using the Zeldovich approximation (Zeldovich 1970), and smoothing onto a lower-resolution $N = 400^3$ grid; (iii) using excursion-set theory (Press & Schechter 1974; Bond et al. 1991, Lacey & Cole 1993, Sheth & Tormen 1999) on the evolved density field to compute the fraction of matter collapsed in halos bigger than a threshold $M_{\text{min}}$ (see Section 3.1), thus contributing to reionization (see Mesinger & Furlanetto 2007, Mesinger et al. 2011 for a more detailed description of the code).

The ionization field is computed by comparing the integrated number of ionizing photons to the number of baryons plus recombinations, in spherical regions of decreasing radius $R$ (i.e. following the excursion-set approach of Furlanetto et al. 2004). Specifically, a cell located at spatial position and redshift $(x, z)$, is flagged as ionized if:

$$\xi f_{\text{coll}}(x, z, R, M_{\text{min}}) \geq 1 + \bar{n}_{\text{rec}}(x, z, R)$$

where $f_{\text{coll}}(x, z, R, M_{\text{min}})$ is the fraction of collapsed matter inside a sphere of radius $R$ residing in halos larger than $M_{\text{min}}$, and $\xi$ is an ionization efficiency, defined below. As we detail below, each cell keeps track of the local values of $M_{\text{min}}(x, z)$ and $\bar{n}_{\text{rec}}(x, z)$, computed according to the cell’s density and ionization history. The latter is the main improvement of this work. When computing the ionization criterion in eq. (1), $M_{\text{min}}$ and $\bar{n}_{\text{rec}}$ are also averaged over scale $R$.

Starting from the box size, the smoothing scale is decreased, and the criterion in eq. (1) is re-evaluated. It is important to note that most previous excursion-set approaches add a maximum starting scale, $R_{\text{max}}$, generally corresponding to a chosen value for the mean free path to ionizing photons through the ionized IGM, $\lambda_{\text{HII}}(1 + z) = R_{\text{max}}$. This value is usually treated as homogeneous and redshift independent. In this work we remove this free parameter, as our procedure explicitly computes the local mean free path. At the cell size, $R_{\text{cell}}$, the partial ionizations from sub-grid sources are evaluated, and the cell’s ionized fraction is set to $\xi f_{\text{coll}}(x, z, R_{\text{cell}}, M_{\text{min}})/(1 + \bar{n}_{\text{rec}})$ (Mesinger et al. 2011). Neglecting recombinations, this algorithm results in ionization fields which are in good agreement with cosmological radiative transfer algorithms on $\gtrsim$ Mpc scales (Zahn et al. 2011).

The ionizing efficiency from eq. (1) can be written out as:

$$\xi = 30 \left( \frac{N_\gamma}{4000} \right) \left( \frac{f_{\text{esc}}}{0.15} \right) \left( \frac{f_{\text{f}}}{0.05} \right) \left( \frac{f_0}{1} \right),$$

where $N_\gamma$ is the number of ionizing photons per stellar baryon, $f_{\text{esc}}$ is the fraction of UV ionizing photons that escape into the IGM, $f_{\text{f}}$ is the fraction of galactic gas in stars, and $f_0$ is the fraction of baryons inside the galaxy with respect to the cosmic mean $\Omega_b/\Omega_m$ (note that some works include the total number of homogeneous recombinations inside the definition of $\xi$). Although our models depend only on the product in eq. (2), we show on the RHS some reasonable values for the component terms. $N_\gamma \approx 4000$ is expected for PopII stars (e.g. Barkana & Loeb 2005). On the other hand, the parameters $f_{\text{esc}}$, $f_{\text{f}}$, and $f_0$ are extremely uncertain in high-redshift galaxies (e.g. Gnedin et al. 2008; Wise & Cen 2009; Ferrara & Loeb 2013), though our fiducial choices are in agreement with high-redshift galaxy luminosity functions (e.g. Robert-son et al. 2013).

As discussed in Sobacchi & Mesinger 2013a), formally we should be averaging over the local values of $f_{\text{coll}}$, instead of $M_{\text{min}}$, i.e. $\langle f_{\text{coll}}(M_{\text{min}}) \rangle_{R} \neq f_{\text{coll}}(\langle M_{\text{min}} \rangle_{R})$. However, only computing $f_{\text{coll}}$ locally in each cell could yield spurious, resolution-dependent results, since we are using the evolved (instead of the linear) density field: an application of the conditional mass function which has only been tested empirically within the context of the excursion-set approach to reionization (Zahn et al. 2011, Mesinger et al. 2011). In Sobacchi & Mesinger 2013a we show that under maximally pessimistic assumptions, this approach results in a mis-estimate of the effective collapse fraction of at most 10–20%, comparable to the uncertainty in the high-redshift mass function itself. 

There are likely $\sim$two orders of magnitude separating the halo masses corresponding to the atomic cooling threshold and the current sensitivity limits of high-redshift ($z \sim 6 – 10$) Lyman break galaxy (LBGs) sur-
2.1 Incorporating an Inhomogeneous UVB

In order to determine the ionization state of the IGM, it is necessary to know \( M_{\text{min}}, \lambda_{\text{mp}} \) and \( n_{\text{rec}} \) (see eq. [15] and [13] respectively), which all depend on the photoionization rate in the local HII region. The mean emissivity (number of ionizing photons emitted into the IGM per unit time per baryon) can be written as:

\[
\epsilon \approx f_{\text{H}} f_{\text{esc}} N_{\gamma} \frac{df_{\text{coll}}}{dt} \approx \xi \frac{df_{\text{coll}}}{dt},
\]

The photoionization rate is proportional to the local ionization mean free path, \( \lambda_{\text{mp}} \) (set by either recombinations or reionization morphology), multiplied by the emissivity. Assuming that the emissivity is spectrally distributed as \( \nu^{-\alpha} \) (in this paper we use \( \alpha = 5 \), corresponding to a stellar-driven UV spectrum; e.g. [1]), we can write the average photoionization rate in a given HII region as

\[
\Gamma_{\text{HII}}(x, z) \approx (1 + z)^2 \lambda_{\text{mp}} \sigma_{\text{H}} \alpha \frac{\lambda_{\text{mp}}}{\alpha + \beta} \bar{n}_b \xi \frac{df_{\text{coll}}}{dt},
\]

where \( \bar{n}_b \) is the mean baryon number density inside the HII region, and we have assumed a photoionization cross-section \( \sigma(\nu) = \sigma_{\text{H}}(\nu/\nu_0)^{-\beta} \) with \( \sigma_{\text{H}} = 6.3 \times 10^{-18} \text{cm}^2 \) and \( \beta = 2.75 \).

Due to the clustering of dark matter halos, the relevant intensity at galaxy locations will be higher than the average UVB intensity inside the local HII region. Therefore when calculating \( M_{\text{crit}} \) in eq. [5], we use \( \Gamma_{\text{halo, HII}} = \Gamma_{\text{HII}} \times \Gamma_{\text{HII}} \), with \( f_{\text{bias}} = 2 \), consistent with results from Sobacchi & Mesinger (2013b).

3 IMPLEMENTING SUB-GRID PHYSICS

Unlike previous studies, our approach self-consistently follows the local star-formation and recombination rates based on each cell’s density, ionization history, and local UVB. The recombination rate is computed using the full distribution of HI in the IGM. Before we describe the details, we present the general steps of our algorithm. Starting from a high-redshift (here taken to be \( z_{\text{init}} = 15 \)) snapshot of the large-scale density field:

(i) Using the excursion-set procedure and criteria described above, we identify local HII regions around each cell, computing the associated UVB with \( \lambda_{\text{mp}} = R \) (eq. [2]).

(ii) If a cell is newly ionized, its ionization redshift and UVB intensity are recorded in order to account for photo-heating feedback on star formation, according to eq. [5] (Sobacchi & Mesinger 2013b).

(iii) Treating each cell as a large-scale background (e.g. [3]), we model its density sub-structure with an empirical density distribution, calibrated to numerical simulations (eq. [6] Miralda-Escudé et al. 2000).

3.1 UVB Feedback on Ionizing Sources

We implement UVB feedback as in Sobacchi & Mesinger (2013a). In this approach, the minimum mass of halos contributing to reionization is expressed in terms of two star-formation criteria: \( M_{\text{min}} = \max \left( M_{\text{cool}}, M_{\text{crit}} \right) \). \( M_{\text{cool}} \) corresponds to the virial temperature \( T_{\text{vir}} \approx 10^4 \text{K} \) below which gas cannot cool through atomic hydrogen (molecular hydrogen cooling is expected to be strongly suppressed during the very early stages of reionization; e.g. Haiman et al. 1997).

In reionized regions, the gas reservoir to form stars can be depleted from the additional heating from the UVB (lowering \( f_{\text{b}} \) from eq. [2] e.g. Shapiro et al. 1994 Miralda-Escudé & Rees 1994 Hu & Gnedin 1997). Halos with masses above \( M_{\text{crit}} \) retain enough gas (defined so that \( f_{\text{b}} \gtrsim 1/2 \)) to continue efficiently forming stars inside HII regions. Using a functional form motivated by linear theory, in Sobacchi & Mesinger (2013b), we obtain the following empirical formula:

\[
M_{\text{crit}}(x, z) = M_0 \left( \frac{\Gamma_{\text{halo, HII}}}{(10^{-12} \text{ s}^{-1})^{1/2}} \right)^a \left( 1 + \frac{z}{10} \right)^b \left[ 1 - \left( 1 + \frac{z}{1 + z_{\text{IN}}} \right)^{c+d} \right]^{e+d}
\]

where \( z \) is the collapse (i.e. current) redshift, \( z_{\text{IN}} \) is the redshift when the halo is first exposed to the UVB, and \( (M_0, a, b, c, d, e) = (3.0 \times 10^9 M_\odot, 0.17, -2.1, 2.0, 2.5) \) are fitted to suites of 1D collapse simulations exploring a wide parameter space. Eq. [5] allows us to self-consistently keep track of the local value of \( M_{\text{min}} \) in each cell.

3.2 Small Scale Structure of the IGM

We assume that the density sub-structure of each large-scale simulation cell is described according to the empirical formula, developed and calibrated to numerical simulations by Miralda-Escudé et al. (2000). In this “MHR” model, the volume-weighted gas density distribution (i.e. the fraction of volume in which the gas is at overdensity \( \Delta \equiv n_b/\bar{n}_b \)) can be written as:

\[
P_{V}(\Delta, z) = A \exp \left[ -\frac{(\Delta - 2/3 - \delta_0)^2}{2 (2\delta_0/3)^2} \right] \Delta^{-\beta}
\]

where the fitted parameter \( \delta_0 = 7.61/(1 + z_{\text{crit}}) \) crudely scales as the Jeans length in the ionized IGM, which we evaluate at an effective redshift \( (1 + z_{\text{eff}}) \equiv (1 + z) \Delta^{1/3}_{\text{crit}} \) this is motivated by the self-similarity of the Einstein-de Sitter Universe, where each

6 We caution that the MHR density distribution is not calibrated to simulations at very high redshifts, nor at very high densities (which were not well-resolved by their simulation). This is approximately dealt with using an overall normalization, \( f_s \) (see eq. [12]).
large-scale patch can be treated as a background Universe. The parameter \( \beta \) is tabulated at \( z < 6 \), while we assume \( \beta = 2.5 \) at higher redshifts (corresponding to an isothermal sphere profile for high-density absorbers). \( A \) and \( C_0 \) ensure volume and mass normalization of the distribution as appropriate for each cell’s mean over-density, \( \Delta_{\text{cell}} \).

Assuming photoionization equilibrium, we calculate the neutral fraction at a given density:

\[
x_{\text{HI}} \Gamma_{\text{local}} = \chi_{\text{HeIII}} n_{\text{H}} (1 - x_{\text{HI}})^2 \alpha_B ,
\]

where \( n_{\text{H}} = \Delta n_{\text{H}} \) is the hydrogen number density, \( \alpha_B = 2.6 \times 10^{-13} \text{cm}^{-3} \text{s}^{-1} \) is the case B recombination coefficient for gas at \( T \approx 10^4 \text{K} \), and \( \chi_{\text{HeIII}} = 1.08 \) accounts for singly-ionized helium. We take into account the self-shielding of the gas through a density-dependent photoionization rate, obtained by an empirical fit to radiative transfer simulations (Rahmati et al. 2013):

\[
\frac{\Gamma_{\text{local}}}{\Gamma_{\text{HI}}} = 0.98 \times \left[ 1 + \left( \frac{\Delta}{\Delta_{\text{ss}}} \right)^{1.64} \right]^{-2.28} + 0.02 \times \left[ 1 + \left( \frac{\Delta}{\Delta_{\text{ss}}} \right)^{0.84} \right] ,
\]

where \( \Delta_{\text{ss}} \) is the overdensity above which the gas is self-shielded (Schaye 2001). Using a spectrally-averaged ionization cross-section corresponding to our UVB power index of \( \alpha = 5 \), we have:

\[
\Delta_{\text{ss}} = 27 \times \left( \frac{T}{10^4 \text{K}} \right)^{0.17} \left( \frac{1 + z}{10} \right)^{-3} \left( \frac{\Gamma_{\text{HI}}}{10^{-12} \text{cm}^{-2} \text{s}^{-1}} \right)^{2/3} .
\]

We are implicitly assuming that the density distribution of the gas responds instantaneously to photo-heating. Although this is not exactly the case (Pawlik et al. 2009), this assumption is relatively safe since the response time-scale is shorter than the typical extension of inhomogeneous reionization. Most importantly, it is likely the IGM is pre-heated by X-rays (e.g. Oh 2001; Ricotti & Ostriker 2004; Mesinger et al. 2013), dramatically reducing the time-scale for response. Nevertheless, the photon-consumption during gas relaxation remains an uncertainty.

Figure 1. CDDF of the gas calculated with different fiducial photoionization rates (in units of \( 10^{-12} \text{ s}^{-1} \)). The shaded region corresponds to observational constraints at a mean redshift of 3.7 (O'Meara et al. 2007; Prochaska & Wolfe 2009; Prochaska et al. 2009, 2010) with the compilation from McQuinn et al. 2011). Curves correspond to, solid: \( \Gamma_{\text{HI}} = 0.5 \); dashed: \( \Gamma_{\text{HI}} = 0.25 \) and \( \Gamma_{\text{HI}} = 1 \) (upper and lower curves respectively). The dotted curve corresponds to the optically thin approximation with \( \Gamma_{\text{HI}} = 0.5 \).

Figure 2. Mean effective ionizing efficiency \( \xi_{\text{eff}} = 1/(1 + n_{\text{rec}}) \) in HII regions for the fiducial run, FULL. The shaded region corresponds to the 1σ spread among HII regions.

To compare our model against observations we calculate the corresponding column density distribution function (CDDF) of the gas. This is usually expressed as the number of absorption lines per unit absorption distance \( X \) (defined in eq. 10) and column density \( N_{\text{HI}} \). The relation of the CDDF to the observed number density of absorption lines per unit redshift \( d^2 n/dN_{\text{HI}} dz \) depends on the assumed cosmology:

\[
f (N_{\text{HI}}, z) \equiv \frac{d^2 n}{dN_{\text{HI}} dz} \equiv \frac{d^2 n}{dN_{\text{HI}} dz} \frac{H(z)}{H_0} \frac{1}{(1 + z)^2} . \tag{10}
\]

We assume that the gas is in dynamical equilibrium and calculate \( N_{\text{HI}} \) as (Schaye 2001):

\[
N_{\text{HI}} = 1.6 \times 10^{21} \text{ cm}^{-2} n_{\text{H}}^{1/2} \left( \frac{T}{10^4 \text{K}} \right)^{1/2} x_{\text{HI}} . \tag{11}
\]

Assuming uniform density absorbers, the CDDF is given by Furlanetto & Oh 2005 Appendix A):

\[
f (N_{\text{HI}}, z) = f_s \Omega_0 \frac{d \Delta}{dN_{\text{HI}}} \Delta \rho^c (\Delta, z) \frac{3H_0 c (1 - Y)}{8\pi G m_\text{H}} x_{\text{HI}} N_{\text{HI}}^{-1} . \tag{12}
\]

Since the MHR distribution overestimates the amount of gas at densities \( \Delta \gtrsim \Delta_{\text{ss}} \) (e.g. Pawlik et al. 2009; Bolton & Becker 2009), we re-scale eq. (12) by \( f_s \sim 0.3 \) (given the uncertainty in the measured CDDF, \( f_s \) can not be constrained strictly; see also Furlanetto & Oh 2005 Appendix A).

In Figure 1 we compare the resulting CDDF with observational constraints at a mean redshift of 3.7 (O'Meara et al. 2007; Prochaska & Wolfe 2009; Prochaska et al. 2009, 2010). We show the CDDF calculated assuming different fiducial photoionization rates (in units of \( 10^{-12} \text{ s}^{-1} \)): \( \Gamma_{\text{HI}} = 0.5 \) (solid), \( \Gamma_{\text{HI}} = 0.25 \) and \( \Gamma_{\text{HI}} = 1 \) (dashed). The CDDF agrees well with observations, including the damped Lyα system (DLA) dip at \( N_{\text{HI}} \gtrsim 2 \times 10^{20} \text{ cm}^{-2} \). For comparison we also show the result of an optically thin approximation with \( \Gamma_{\text{HI}} = 0.5 \) (dotted). As expected, the optically thin approximation underestimate the CDDF at large column densities where the self-shielding of the gas becomes important.

3.2.1 Recombination Rate

Taking self-shielding into account, and integrating over the entire density distribution, the recombination rate per baryon in an ionized
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3.2.2 Mean Free Path of Ionizing Photons

Our formalism also allows us to compute the local mean free path through the ionized IGM, \( \lambda_{\text{mfp, HII}} \), and compare with observational estimates post-reionization. High-redshift predictions of \( \lambda_{\text{mfp, HII}} \) are also very useful in checking the empirical extrapolations used extensively in analytic models of reionization (e.g. Choudhury & Ferrara 2006).

Using the CDDF from eq. (12), we can write (Furlanetto & Oh 2005):

\[
\lambda_{\text{mfp, HII}} = \frac{H_0 (1 + z)^3 \int_0^\infty f (N_{\text{HI}}, z) \left(1 - \frac{\Delta_{\text{HII}}}{\Delta_{\text{ss}}}\right) dN_{\text{HI}}}{c}
\]

Assuming ionization equilibrium, \( \lambda_{\text{mfp, HII}} \) is set by the instantaneous recombination rate, and should be included in the time-integral of eq. (1); for numerical robustness however we also require that \( \lambda_{\text{mfp, HII}} > R \) for a region to be ionized. This added check (although we confirm that it has a negligible impact on our fiducial reionization history and morphology), helps ensure that rapidly-evolving recombination rates are not “smoothed-over” between two redshift snapshots.

Eq. (15) includes a weighted integral over the entire CDDF of the ionized IGM. A simpler, two-phase model of the ionization state was proposed by Miralda-Escudé et al. (2000), where the neutral fraction of the local density patch effectively transitions from zero at \( \Delta < \Delta_{\text{ss}} \) to unity at \( \Delta > \Delta_{\text{ss}} \). Then the fraction of the IGM occupied by absorbers is \( Q_{\text{ss}} = \int_0^{\Delta_{\text{ss}}} P(\Delta, z) d\Delta \). If absorbers are further assumed to correspond to discrete systems with a constant shape at a fixed \( \Delta_{\text{ss}} \), their radius is proportional to \( Q_{\text{ss}}^{1/3} \) and their mean separation to \( Q_{\text{ss}}^{-2/3} \). In this simple picture, the mean free path can be written as:

\[
\lambda_{\text{mfp, HII}} = \frac{\lambda_0 Q_{\text{ss}} (\Delta_{\text{ss}})^{-2/3}}{c},
\]

where \( \lambda_0 H = 60 \text{ km s}^{-1} \) is the chosen normalization, which implicitly also allows one to account for the physically non-negligible cumulative opacity of \( \Delta < \Delta_{\text{ss}} \) systems (Furlanetto & Oh 2005 Appendix A).

In Figure 3 we compare the values of \( \lambda_{\text{mfp, HII}} \) calculated using the full CDDF (eq. (15) blue solid curve) and the Miralda-Escudé et al. (2000) approximation (eq. (16) green dotted curve). Both models assume the same UVB and reionization morphology, corresponding to the FULL model, described below. At moderate redshifts (\( z \sim 7 \)), the results are surprisingly similar. Some similarity between the two approaches is expected, given that the \( \lambda_0 \) normalization in eq. (16) was chosen to match \( z \sim 3 \) observations. However, at \( z > 7 \) the Miralda-Escudé et al. (2000) approximation begins overestimating the mean free path, by up to a factor of \( \sim 2 \) at the highest redshifts we consider. With the increasing mean density at higher redshifts, more common systems (lower \( \Delta_{\text{ss}} \)) dominate.
4 RESULTS

We now investigate the relative impact of inhomogeneous recombinations on the reionization history, morphology, and other IGM properties. Our fiducial model assumes $\xi = 30$ and an atomic cooling threshold for star-forming galaxies ($M_{\text{cool}}$ corresponding to $T_{\text{vir}} > 10^4$ K). This choice of $\xi$ is simply motivated by having reionization histories match the mean value of $\tau_e$ as observed by WMAP. This integral constraint still allows for a wide range of models; therefore the fiducial choice of $\xi$ should be treated merely as a rough “guess”. Keeping these parameters fixed, the runs we compare are:

- **FULL**: self-consistent calculation of $M_{\text{crit}}$ and $n_{\text{rec}}$, as described above.
- **No Recombinations, Feedback (nRF)**: like **FULL**, but neglecting recombinations, i.e. $n_{\text{rec}} = 0$.
- **Recombinations, No Feedback (RnF)**: like **FULL**, but neglecting UVB feedback on sources, i.e. $M_{\text{min}} = M_{\text{cool}}$.
- **No Recombinations, No Feedback (nRnF)**: like **FULL**, but neglecting both recombinations and UVB feedback on sources.

Obviously, these models are not meant to be exhaustive, spanning a wide range of astrophysical parameter space. Rather they serve to further physical intuition about the impact and relative importance of inhomogeneous feedback from sources and sinks. Eventually, more physical models can be constructed, including a
but with a delay corresponding to the recombination time-scale. The combination morphology resembles the reionization morphology, and these regions host the most recombinations. In general, the large-scale reionization is more complex than our simple models (e.g. Lidz et al. 2011; Bolton & Haehnelt 2013). We also denote the strict upper limit at $z_e \approx 6$ from the dark fraction in QSO spectra (McGreer et al. 2017), and the two recent (somewhat qualitative) lower limits at $z_\text{HI} \approx 7$ suggested by (i) observations of ULAS J1120+0641 (Bolton et al. 2011) and (ii) the fall in the Ly$\alpha$ emitter fraction among LBGs (e.g. Dijkstra et al. 2011; Pentericci et al. 2011; Bolton & Haehnelt 2013).

### 4.1 Reionization History

In Figure 6 we compare the evolution of the global volume-averaged neutral fraction $x_\text{HI}$ in different reionization models. As mentioned before, both recombinations and UVB feedback delay reionization; the former by depleting the photon budget for growing the HII regions, and the later by decreasing the star-formation rate. We stress again that the fiducial choice of $\xi = 30$ is just a rough guess; reionization histories can be shifted later/earlier by decreasing/increasing $\xi$.

From Fig. 3 we also see that the reionization delay from recombinations is more significant than the one from UVB feedback on sources. By decreasing the effective ionizing efficiency (see Section 3.2.1), recombinations delay the end of reionization by $\Delta z \sim 1.3$ ($\text{nRF} \text{ vs } \text{nRF}$). The analogous delay due to feedback on sources is $\Delta z \sim 0.7$ ($\text{RF} \text{ vs } \text{nRF}$). The total effect of both recombinations and feedback on sources is to delay the completion of reionization by $\Delta z \sim 2.5$ ($\text{FULL} \text{ vs } \text{nRF}$). This delay is greater than the combined individual delays from either effect, as both preferentially impact the same, late-stage large HII regions, accelerating their transition to a recombination-limited regime. Since the impact is stronger on the end stages of (and following) reionization, $\tau_e$ is only mildly affected, with the FULL ($\text{nRF}$) model having $\tau_e = 0.07$ (0.08).

### 4.2 Reionization Morphology

We now proceed to quantify the impact of recombinations on the morphology of reionization. Understanding the morphology of reionization is important in interpreting almost all reionization observables (e.g. Lidz et al. 2007; McQuinn et al. 2008; Mesinger & Furlanetto 2008; Mesinger 2010; Schoeder et al. 2013; Dijkstra et al. 2011; Dayal et al. 2011; Mesinger et al. 2012). Furthermore, current 21cm interferometers, such as Low Frequency Array (LOFAR; van Haarlem et al. 2013), Murchison Wide Field Array (MWA; Tingay et al. 2013) and the Precision Array for Probing the Epoch of Reionization (PAPER; Parsons et al. 2010) should provide a statistical measurement of large-scale ($k \sim 0.1 \text{ Mpc}^{-1}$) reionization morphology in the next couple of years.

In the top panels of Fig. 7 we show the size distributions of the HII regions, calculated according to the procedure in Mesinger & Furlanetto (2007), randomly choosing an ionized cell and tabulating the distance to the HII region edge along a randomly chosen direction. In the middle panels we show the ionization power spectrum $\Delta s^2_x \equiv k^3/(2\pi^2) \langle |\delta_x|^2 k \rangle$, with $\delta_x = x_\text{HI}/x_\text{HI} - 1$. Panels correspond to different stages of reionization: $x_\text{HI} \approx 0.75, 0.50, 0.25$ (left to right). We compare our fiducial model FULL (solid) with the runs $\text{RF}$ (dotted), $\text{nRF}$ (dashed) and $\text{nRF}$ (dot-dashed). To facilitate direct comparisons to upcoming 21cm interferometric observations, in the bottom panels we plot the corresponding 21cm power spectrum, de-
The effect is dramatic. Recombinations decrease the typical HII region size by factors of \( \sim 2-3 \) throughout reionization. During the second half of reionization, recombinations suppress the power spectra by \( \gtrsim 50-100\% \) (RnF vs nRnF) on the \( k \sim 0.1 \text{ Mpc}^{-1} \) scales relevant for current 21cm interferometers (e.g. Choudhury et al. 2013). For the FULL model which also includes UVB feedback on sources, this suppression increases to a factor of \( \gtrsim 2-4 \)\(^{14}\) this dramatic suppression of large-scale power from recombinations.

\(^{14}\) The dearth of large-bubbles increases the cross-correlation between the ionization and density fields, which has a negative contribution to the 21cm power spectrum. This generally results in a somewhat larger suppression of the 21cm power spectra than the ionization power spectra.
tions qualitatively impacts the shape of the ionization power spectrum. Neglecting recombinations, large-scale, radiative transfer simulations (e.g. McQuinn et al. 2007; Zahn et al. 2011; Friedrich et al. 2011) predict a relatively flat or mildly decreasing power spectrum in the relevant range $k \sim 0.1 \to 0.3$, during the late stages of reionization, consistent with our nRnF model (c.f. Zahn et al. 2011). The dramatic suppression of large-scale power caused by recombinations instead results in a strongly-increasing power spectrum in this range. The amplitude and slope of the power spectrum around $k \sim 0.1 \text{Mpc}^{-1}$ are fundamental observables of the first generation 21cm interferometers (e.g. Lidz et al. 2008). Recombinations strongly affect both.

Our model explicitly tracks the sub-grid mass fraction of neutral gas inside the HII regions, finding it to be a few percent on average, consistent with post-reionization measurements (e.g. Wolfe et al. 2005). Instead if the (mass-weighted) neutral fraction of the entire $\sim 1 \text{Mpc}$ simulation cell was set to unity, the reionization morphology could be noticeably changed on small-scales (Choudhury et al. 2009; Crociani et al. 2011). Indeed, the procedure outlined in Choudhury et al. 2009 assumes that an entire $\sim 1.4 \text{cMpc}$ cell is neutral, if it begins to self-shield. They find that this large reservoir of neutral gas can drive up the small-scale 21cm power. This is contrary to our results, which are driven by the sub-grid density and ionization distributions.

4.3 Additional Properties of the Ionized IGM

One of the benefits of our formalism is that it can track IGM evolution into the late stages of reionization, and even somewhat afterward. This allows us to test our model against IGM observations at redshifts $z < 6$, before the Ly$\alpha$ forest saturates. Here we show the evolution of the mean free path, the ionizing background and the ionizing emissivity. It is useful to recall (eq. 4) that inside ionized regions (and post reionization), these quantities approximately scale as: $\Gamma_{\text{HII}} \propto \lambda_{\text{mfp}} \varepsilon$. The ionizing background can be measured from the Ly$\alpha$ forest of high-$z$ quasars (with the a-priory assumption that reionization has completed). Mesinger (2010), while $\lambda_{\text{mfp}}$ can be either measured or estimated with radiative transfer simulations. These measurements become increasingly uncertain at $z \geq 4$ (e.g. Bolton & Haehnelt 2007; McQuinn et al. 2011; Kuhlen & Faucher-Giguère 2012).

4.3.1 Ionizing emissivity and recombination rate

In Figure 8 we show the evolution of the ionizing photons emissivity $\varepsilon \equiv \xi_{\text{i}f_{\text{e,all}}}/dt$ (thick) and the recombination rate per baryon (thin) for the models FULL (solid), RnF (dotted) and nRF (dashed); the emissivity in the model nRnF is the same as in the model RnF. We plot the curves until $\lambda_{\text{mfp}}$ exceeds the box size.

The vertical ticks corresponds to the redshifts when the volume-averaged neutral fraction is $\bar{x}_{\text{HI}} \equiv \frac{1}{V} \int_0^V x_{\text{HI}} dV = 0.2$ and $\bar{x}_{\text{HI}} = 0.2^{-2}$. For comparison we show the emissivity constraints inferred from the Ly$\alpha$ forest (Bolton & Haehnelt 2007; McQuinn et al. 2011). At the earliest redshifts, all of the runs have the same emissivity, by construction. As time passes, the runs which include UVB feedback on star-formation have a reduced emissivity, consistent with $z \leq 6$ observations. Furthermore, the emissivity is somewhat (10s of per cent) higher in the run FULL than in the run nRF: if we neglect recombinations, $\bar{\Gamma}_{\text{HII}}$ increases and reionization occurs earlier, resulting in stronger UVB feedback. Overall, UVB feedback decreases the emissivity by a factor of $\sim 2$ by the end of reionization. This is relatively modest when compared to the corresponding impact on $\bar{\Gamma}_{\text{HII}}$, which can scale with the emissivity as a power law, in the late (recombination-limited) stages of reionization and afterwards (McQuinn et al. 2011 see also below).

 Runs which include recombinations reach a recombination-limited regime at $\bar{x}_{\text{HI}} \sim 0.1$ (the short, vertical ticks on the curves demarcate $\bar{x}_{\text{HI}} = 0.2, 0.01$), consistent with analytic predictions (Furlanetto & Oh 2005). Runs RnF (FULL) result in $\approx 0.9$ (1) recombinations per baryon by the end of reionization. It is important to note that an extended regime of a constant emissivity and recombination rate only occurs in the FULL model, with the combined effort of the evolutions of sources and sinks slowing down reionization sufficiently. As we shall see below, this regulates the rise in the $\lambda_{\text{mfp}}$ and $\Gamma_{\text{HII}}$ in the final stages of reionization.

We stress again that our runs are only “tuned” via the fiducial choice of ionizing efficiency $\xi = 30$ so as to match the observed $\tau_{c}$. If one plays with this free parameter, one can shift the emissivities in Figure 8 up or down. We test this explicitly with a new RnF run, but with $\xi = 15$ (not shown in the figure for the sake of clarity). The emissivity in this run is approximately consistent with observational estimates at $z \sim 5-6$, without appealing to UVB feedback on sources. However, in this case reionization happens relatively late, with a corresponding $\tau_{c} = 0.058$, inconsistent with WMAP at $\approx 2-3 \sigma$. 

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4.3.2 The mean free path and the UVB

In Figure 9, we compare the evolution of $\lambda_{\text{mfp}, \text{HII}}$ in our runs. Only the FULL run is consistent with observations at $z \sim 6$, as well as the high redshift extrapolation of the empirically-calibrated formula provided in Songaila & Cowie (2010).

$$\lambda_{\text{mfp}} = 50 \left(\frac{1 + z}{4.5}\right)^{-4.44} \text{pMpc}.$$  \hspace{1cm} (18)

which approximates the CDDDF as a power law.

The same trend can be seen in Figure 10 where we plot the evolution of $\langle \Gamma \rangle_z$, averaged over HII regions. Namely, in all runs except FULL, the mean free path and UVB grow too rapidly, too early.

In order to avoid rapid, early evolution in the UVB and mean free path, one needs both: (i) recombinations; and (ii) a fairly low emissivity, $\varepsilon \lesssim 3 \, \text{Gyr}^{-1}$. In our fiducial model, (ii) is assured by UVB feedback on star formation, which also results in an extended reionization history. As mentioned previously, in the absence of UVB feedback, a low emissivity could also result from a smaller ionizing efficiency, $\xi \lesssim 15$; however in this case reionization would occur rapidly and late, and be only marginally consistent with WMAP observations. Similarly, a low emissivity could also be obtained by increasing $M_{\text{cool}}$, physically corresponding to reionization driven by more-massive sources which generate ionizing photons more efficiently. However in this case, reionization again occurs very late, and with the added complication of an emissivity which, although low at $z \sim 6$, is evolving too rapidly to be consistent with observations of the Ly$\alpha$ forest (Miralda-Escude 2003; Fig. 12 in Mesinger et al. 2012).

4.3.3 Clumping Factor

In analytic models, recombinations are often parameterized in terms of a “clumping factor” of the ionized gas. This quantity encodes the integral over the ionization structure of the gas, facili-
tating analytic estimates of the global recombination rate using a single parameter. There are several ways of defining the clumping factor (see, e.g. Finlator et al. 2012). Here we use the following simple definition: \( C_{\text{HI}} \equiv \langle n_{\text{HI}}(x)/\bar{n}_{\text{HI}} \rangle^2 \). In Figure 11 we show the evolution of \( C_{\text{HI}} \) in the runs FULL (solid), nRF (dotted), nRF (dashed) and dot-dashed.

The evolution of \( C_{\text{HI}} \) can be understood looking at the over-density threshold for self-shielding, \( \Delta_{\text{ss}} \) (eq. 9), and the large-scale mean overdensity in HII regions, \( \Delta_{\text{HI}} \). In Figure 12 we show the evolution of \( \Delta_{\text{ss}} \) (solid) and \( \Delta_{\text{HI}} \) (dashed) in the run FULL. \( \Delta_{\text{ss}} \) is increasing with time, driven by its dependence on redshift and by the growth of \( \Gamma_{\text{HI}} \) in the late stages of reionization \( \Delta_{\text{ss}} \propto (1+z)^{-2} \Gamma_{\text{HI}}^{2/3} \). Physically, this corresponds to ionization fronts penetrating into increasingly overdense regions of the IGM (with higher recombination rates), thereby driving the rapid increase of \( C_{\text{HI}} \) during the late stages of reionization. At the end of reionization, the value of the clumping factor for the run FULL \( (C_{\text{HI}} \sim 4) \) is consistent with previous works (e.g. Pawlik et al. 2009; McQuinn et al. 2011; Shull et al. 2012; Finlator et al. 2012).

On the other-hand, during the early stages of reionization, HII regions are biased towards the large-scale overdensities which host the first generations of galaxies. Since \( C_{\text{HI}} \propto \Delta_{\text{HI}} \), the decreasing bias of the HII regions (fall in \( \Delta_{\text{HI}} \) with time) balances the rise in \( \Delta_{\text{ss}} \), resulting in a relatively flat \( C_{\text{HI}} \approx 1.5-2 \) at \( z \geq 10 \) (\( \Delta_{\text{HI}} \geq 0.5 \)) (see also, e.g. Kaurov & Gnedin 2013b; So et al. 2013).

5 CONCLUSIONS

We study the role of ionizing photon sinks during reionization by implementing a sub-grid recipe inside large-scale, semi-numerical simulations of reionization. Building on previous work, we self-consistently model the evolution of both sinks and sources of ionizing photons, using prescriptions calibrated to numerical simulations. The inhomogeneous recombination rate and emissivity in our model depend on the local density, photo-ionizing background, and reionization history.

We find that both UVB feedback on sources, and recombinations slow the growth of large HII regions, prolonging reionization and resulting in a more uniform ionization morphology. Although recombinations are more potent, both affects amplify one another as they most strongly affect the same biased regions. Such regions were the first to ionize, allowing enough time for both recombinations and photoevaporation to take effect.

In our complete model, the end of reionization is delayed by \( \Delta z \approx 2.5 \). This delay is sufficient for simple reionization models to match best estimates of the mid and end stages of reionization, as implied by recent observations of the CMB, quasar spectra, and LAEs.

Recombinations are mostly responsible for the slowing and eventual “freeze-out” of large HII regions (\( \geq 10 \) Mpc). This results in a dramatic suppression of the large-scale (\( k \leq 0.2 \) Mpc\(^{-1} \)) ionization power-spectrum by factors of \( \geq 2-3 \), even as early as \( x_{\text{HI}} < 0.5 \). Such a dramatic impact on these scales makes recombinations invaluable in interpreting upcoming data from 21cm interferometers.

Furthermore, recombinations are responsible for damping the rapid rise of the mean free path and photo-ionizing background during the late stages of reionization. The volume-averaged photoionization rate increases by a modest factor of \( \sim 2 \) (as opposed to \( \sim 5 \) ignoring recombinations) during the last, \( \bar{x}_{\text{HI}} < 0.2 \) stages of reionization.

Our complete model naturally results in an early start, and “photon-starved” end of reionization, as well as a modest, slowly-evolving emissivity (governed by UVB feedback which depletes gas from increasingly massive halos as time progresses). Although undoubtedly too simplistic, this physical picture ameliorates empirically-motivated claims for a rapid redshift evolution in galaxy properties, like the escape fraction of ionizing photons (e.g. Haardt & Madau 2012; Kuhlen & Faucher-Giguère 2012). Further progress would be aided by improved, physically-motivated models for the evolution of the ionizing emissivity.

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To be more precise, our emissivity estimates are only sensitive to the product on the RHS in eq. 2 most importantly \( f_{\text{esc}} \). As the dependence on \( f_{\text{esc}} \) is accounted for in our UVB feedback treatment via an evolving \( M_{\text{esc}}(x,z) \). Our model assumes that this product does not have a halo mass or redshift dependence. In our model, the emissivity during reionization is dominated by faint galaxies, 1-2 orders of magnitude fainter than current detection limits. Instead, at lower redshifts (\( x < 3 \)), the emissivity from star-forming galaxies is likely dominated by the observed LBGs, which do seem to have somewhat lower values of \( f_{\text{esc}} \) than our fiducial choices in eq. 2 (see for example, Fig. 7 in Kuhlen & Faucher-Giguère 2012). This is suggestive of at least a mild halo mass dependence of \( f_{\text{esc}} \) (e.g. Alvarez et al. 2012).

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