Descending from on high: Lyman-series cascades and spin-kinetic temperature coupling in the 21-cm line

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Accepted 2005 December 21. Received 2005 December 13; in original form 2005 August 17

ABSTRACT
We examine the effect of Lyman-continuum photons on the 21-cm background in the high-redshift Universe. The brightness temperature of this transition is determined by the spin temperature $T_s$, which describes the relative populations of the singlet and triplet hyperfine states. Once the first luminous sources appear, $T_s$ is set by the Wouthuysen–Field effect, in which Lyman-series photons mix the hyperfine levels. Here we consider coupling through $n \geq 2$ Lyman photons. We first show that coupling (and heating) from scattering of Ly$\alpha$ photons is negligible, because they rapidly cascade to lower-energy photons. These cascades can result in either a Ly$\alpha$ photon – which will then affect $T_s$ according to the usual Wouthuysen–Field mechanism – or photons from the $2s \rightarrow 1s$ continuum, which escape without scattering. We show that a proper treatment of the cascades delays the onset of strong Wouthuysen–Field coupling and affects the power spectrum of brightness fluctuations when the overall coupling is still relatively weak (i.e., around the time of the first stars). Cascades damp fluctuations on small scales because only $\sim 1/3$ of Ly$\alpha$ photons cascade through Ly$\alpha$, but they do not affect the large-scale power because that arises from those photons that redshift directly into the Ly$\alpha$ transition. We also comment on the utility of Ly$\alpha$ transitions in providing ‘standard rulers’ with which to study the high-redshift universe.

Key words: atomic processes – galaxies: high-redshift – cosmology: theory.

1 INTRODUCTION
One potentially promising probe of the cosmic dark ages is 21-cm tomography. It has long been known (Hogan & Rees 1979; Scott & Rees 1990) that neutral hydrogen in the intergalactic medium (IGM) may be detectable in emission or absorption against the cosmic microwave background (CMB) at the wavelength of the redshifted 21-cm line, the spin-flip transition between the singlet and triplet hyperfine levels of the hydrogen ground state. The brightness of this transition will thus trace the distribution of HI in the high-redshift Universe (Field 1958, 1959a), which gives the signal angular structure as well as structure in redshift space. These features arise from inhomogeneities in the gas density field, the hydrogen ionization fraction and the spin temperature. Madau, Meiksin & Rees (1997) showed that the first stars could cause a rapid evolution in the signal through their effect on the spin temperature. Consequently, the 21-cm signal can provide unparalleled information about the ‘twilight zone’ when the first luminous sources formed and the epoch of re-ionization and reheating commenced.

Despite the theoretical promise of this probe, it is only with improvements in computing power that building radio arrays with sufficient sensitivity, capable of correlating billions of visibility measurements, has become possible (Morales & Hewitt 2004). Three such arrays (LOFAR,1 MWA2 and PAST3) will soon be operational, opening a window on to this new low-frequency band. Before a detection can be made, however, there are still major scientific and technical challenges to be met. Ionospheric scattering and terrestrial interference are two serious issues. Also worrying is the need to remove foregrounds, which are many orders of magnitude stronger than the signal. Multifrequency subtraction techniques (Morales & Hewitt 2004; Zaldarriaga, Furlanetto & Hernquist 2004; Santos, Cooray & Knox 2005), exploiting the smoothness of the foreground spectra, have been proposed, but their effectiveness has yet to be tested. The challenges are great, but so are the opportunities. It is thus crucial to understand the nature of the 21-cm signal as we commence these searches.

Fluctuations in the 21-cm signal arise from both cosmological and astrophysical sources. Most previous work has focussed on the signal due to density perturbations (Madau et al. 1997; Loeb & Zaldarriaga 2004) or from inhomogeneous ionization (Ciardi &

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1 See http://www.lofar.org/
2 See http://web.haystack.mit.edu/arrays/MWA/
Madau 2003; Furlanetto, Sokasian & Hernquist 2004a; Furlanetto, Zaldarriaga & Hernquist 2004b). An additional source of fluctuations is the spin temperature, which describes the relative occupation of the singlet and triplet hyperfine levels. These levels may be excited by three primary mechanisms: absorption of CMB photons, atomic collisions and absorption and re-emission of Lyα photons (the Wouthuysen–Field effect; Wouthuysen 1952; Field 1959a). The first two processes rely upon simple physics, but the last one allows us to study the properties of luminous sources, which determine the background radiation field.

Barkana & Loeb (2005b, henceforth BL05) studied the signal generated by the first generation of collapsed objects. These high-redshift objects are highly biased, leading to large variations in their number density. This, combined with the $1/r^2$ dependence of the flux, causes large fluctuations in the Lyα background, which can be probed through their effect on the 21-cm transition. Exploiting the anisotropy induced by peculiar velocities (Bharadwaj & Ali 2004; Barkana & Loeb 2005a), they showed that information about the Lyα radiation field could be extracted from the power spectrum of 21-cm fluctuations and separated into those fluctuations correlated and uncorrelated with the density field. The features of these spectra allow extraction of astrophysical parameters such as the star formation rate and bias. However, it is not a trivial task to relate the emissivity to a distribution of Lyα photons. The background in the Lyα line is composed of two parts: those photons that have redshifted directly to the Lyα frequency and those produced by atomic cascades from higher Lyman-series photons. To calculate this latter component, BL05 assumed that atomic cascades were 100 per cent efficient at converting photons absorbed at a Lyman resonance into a Lyα photon, while in reality most cascades end in two photon decay from the 2S level.

In this paper, we calculate the exact cascade conversion probabilities from basic atomic physics. In addition, we discuss the possibility of level mixing by scattering of Lyα photons via a straightforward generalization of the Wouthuysen–Field effect. We then apply the cascade efficiencies to calculate the Lyα flux profile of an isolated source. The existence of discrete horizons, determined by the maximum distance a photon can travel before it redshifts into a given Lyman resonance, imprints a series of discontinuities into the profile, which can in principle be used as a standard ruler. We apply these results to the power spectra of 21-cm fluctuations during the epoch of the first stars, showing that these corrections cannot be ignored when extracting astrophysical parameters.

The layout of this paper is as follows. In Section 2, we introduce the formalism for describing 21-cm fluctuations and the dominant coupling mechanism, the Wouthuysen–Field effect. In Section 3, we discuss the possibility of direct pumping by Lyα photons. Next, in Section 4, we detail the atomic physics of radiative cascades in atomic hydrogen. The results are applied to the Lyα flux profile of an isolated source in Section 5 and to the 21-cm power spectrum from the first galaxies in Section 6. We also discuss some of the limitations of this formalism. Finally, we summarize our results in Section 7. In Appendix A, we review the equations needed to calculate analytically the Einstein A coefficients for the hydrogen atom. Throughout, we assume $(\Omega_m, \Omega_b, \Omega_\Lambda, h, \sigma_8, n_s) = (0.3, 0.046, 0.7, 0.7, 0.9, 1.0)$, consistent with the most recent measurements (Spergel et al. 2003).

During the preparation of this paper, Hirata (2006) submitted a preprint covering similar material. We have confirmed agreement where there is overlap. The main results of this work were discussed at the ‘Reionizing the Universe’ conference in Groningen, the Netherlands (2005 June 27–July 1; see http://www.astro.rug.nl/~cosmo05/program.html).

2 21-cm FORMALISM AND THE WOUTHUYSEN–FIELD MECHANISM

The 21-cm line of the hydrogen atom results from hyperfine splitting of the 1s ground state due to the interaction of the magnetic moments of the proton and the electron. The H I spin temperature $T_\alpha$ is defined via the relative number density of hydrogen atoms in the 1s singlet and triplet levels $n_1/n_0 = (g_1/g_0) \exp(-T_\alpha/T_\alpha)$, where $(g_1/g_0) = 3$ is the ratio of the spin degeneracy factors of the two levels, and $T_\alpha \equiv hc/k\lambda_{21\mathrm{cm}} = 0.0628$ K. The optical depth of this transition is small at all relevant redshifts, so the brightness temperature of the CMB is

$$T_b = \tau \left( \frac{T_s - T_{\mathrm{CMB}}}{1 + z} \right),$$

where the optical depth for resonant 21-cm absorption is

$$\tau = \frac{3e\lambda^2 A_{10}\rho_{H_1}}{32\pi k_\lambda T_\alpha (1 + z)(dv/dr)},$$

Here $\rho_{H_1}$ is the number density of neutral hydrogen, $A_{10} = 2.85 \times 10^{-15}$ s$^{-1}$ is the spontaneous emission coefficient and $(dv/dr)$ is the gradient of the physical velocity along the line of sight with $r$ the comoving distance. When $T_s < T_{\mathrm{CMB}}$ there is a net absorption of CMB photons, and we observe a decrement in the brightness temperature.

The spin temperature is determined by three coupling mechanisms. Radiative transitions due to absorption of CMB photons (as well as stimulated emission) tend to drive $T_s \rightarrow T_{\mathrm{CMB}}$. Spin flips from atomic collisions drive $T_r \rightarrow T_{\Lambda}$, the gas kinetic temperature. Finally, the Wouthuysen–Field effect (Wouthuysen 1952; Field 1958), which is the main focus of this paper, also drives $T_s \rightarrow T_k$ (see below). The combination that appears in equation (1) can be written as

$$\frac{T_s - T_{\mathrm{CMB}}}{T_k} = \frac{x_{\mathrm{tot}}}{1 + x_{\mathrm{tot}}} \left( 1 - \frac{T_{\mathrm{CMB}}}{T_k} \right),$$

where $x_{\mathrm{tot}} = x_r + x_c$ is the sum of the radiative and collisional coupling parameters. The latter is

$$x_c = \frac{4k_\lambda (T) \rho_{H_1} T_\alpha}{3A_{10} T_{\mathrm{CMB}}},$$

where $k_{\lambda = 0}$ is tabulated as a function of $T_k$ (Allison & Dalgarno 1969; Zygelman 2005). The spin temperature becomes strongly coupled to the gas temperature when $x_{\mathrm{tot}} \gtrsim 1$.

A schematic diagram of the Wouthuysen–Field effect is shown in Fig. 1; it mixes the hyperfine levels through absorption and re-emission of Lyα photons. Quantum selection rules allow transitions for which the total spin angular momentum $F$ changes by $\Delta F = 0, \pm 1$ (except $0 \rightarrow 0$), making only two of the four $n = 2$ levels accessible to both the $n = 1$ singlet and triplet states. Transitions to either of these states can change $T_s$. The coupling coefficient is

$$x_r = \frac{4P_\alpha T_s}{27A_{10} T_{\mathrm{CMB}}},$$

where $P_\alpha$ is the Lyα scattering rate (Madau et al. 1997). If resonant scattering of Lyα photons occurs rapidly enough, $T_s$ will be driven to $T_\alpha$, the colour temperature of the radiation field at the Lyα frequency (Field 1958; Madau et al. 1997). In parallel, the repeated scattering of Lyα photons by the thermal distribution of atoms brings $T_\alpha \rightarrow T_k$ (Field 1959b; Hirata 2006). Consequently, the Wouthuysen–Field
effect provides an effective coupling between the spin temperature and the gas kinetic temperature.

We can also write the Wouthuysen–Field coupling as

\[
x_a = \frac{16\pi^2 T_e^2 f_a}{27A_{10}T_{\text{CMB}}n_e} S_0 J_u,
\]

where \( f_a = 0.4162 \) is the oscillator strength for the Ly\( \alpha \) transition, \( S_0 \) is a correction factor of the order of unity (Chen & Miralda-Escudé 2004; Hirata 2006) that accounts for the redistribution of photon energies due to repeated scattering of the thermal distribution of atoms and \( J_u \) is the angle-averaged specific intensity of Ly\( \alpha \) photons by photon number. For reference, a Ly\( \alpha \) flux of \( J_a = 1.165 \times 10^{-10} \)\((1+z)/20)\ cm^{-2} \ s^{-1} \ Hz^{-1} \ sr^{-1} \) yields \( x_a = 1 \) [corresponding to \( P_a = 7.85 \times 10^{-13} (1+z)\ s^{-1} \)].

Fluctuations in the brightness temperature arise from fluctuations in the density, the Wouthuysen–Field coupling, the neutral fraction of Ly\( \alpha \) and the radial velocity component. To linear order

\[
\delta_{\text{rec}} = \beta \delta_x + \frac{x_0}{x_{\text{tot}}} \delta_{\text{int}} + \delta_{\text{tot}} - \delta_{\mu \text{rec}},
\]

where \( \delta_x \) is the fractional perturbation in \( x \), \( \delta_{\text{int}} \) is the fractional density perturbation and \( x_{\text{tot}} = x_{\text{int}}(1+x_{\text{int}}) \). \( \beta \) is a parameter describing the thermal history of the gas, which we assume to have cooled adiabatically, so that \( \beta \approx 0.2 \). Naoz & Barkana (2005) showed that \( \beta \) slightly increases and exhibits mild scale dependence, as gas temperature fluctuations do not exactly track the density fluctuations. We note that, on scales \( 0.01 \) Mpc\(^{-1} < k < 10^3 \) Mpc\(^{-1} \), \( \beta \) is approximately constant at \( z = 20 \) and choose to ignore this subtlety for ease of comparison with BL05. The first three components of equation (7) are isotropic, but the velocity fluctuation introduces an anisotropy of the form \( \delta_{\mu \text{rec}} \) in Fourier space (Bharadwaj & Ali 2004), where \( \mu \) is the cosine of the angle between the wavenumber \( k \) of the Fourier mode and the line of sight. This allows us to separate the brightness temperature power spectrum \( P_{T_\alpha} \) into powers of \( \mu^2 \) (Barkana & Loeb 2005a)

\[
P_{T_\alpha}(k) = \mu^4 P_{\text{int}}(k) + \mu^2 P_{\text{rec}}(k) + P_{\mu}(k).
\]

The anisotropy is sourced only by density fluctuations, so that \( P_{\mu} \) depends only on the matter power spectrum. \( P_{\text{rec}} \) contains cross-correlations between matter fluctuations and both \( \delta_{\text{int}} \) and \( \delta_{\text{tot}} \), making it an ideal probe of fluctuations in the radiation background. In particular, at sufficiently high redshifts such that \( x_{\text{H}_2} \ll 1 \), it probes variations in the Ly\( \alpha \) background. Linear combinations of these three terms can be used to extract detailed information about other types of fluctuations (Barkana & Loeb 2005a).

### 3 Direct Pumping by Lyman-Series Photons

Of course, the radiation background contains photons that redshift into all the Lyman transitions, not just Ly\( \alpha \). The main purpose of this paper is to examine how these affect \( T_n \). The existing literature assumes that all Ly\( n \) photons are immediately converted into Ly\( \alpha \) photons by atomic cascades (e.g., BL05). In reality, there are two different contributions to consider: one due to scattering of the Ly\( \alpha \) photon itself and the other due to its cascade products. In this section, we discuss the direct contribution of Ly\( n \) scattering to the coupling of \( T_n \) and \( T_\alpha \), which occurs in a manner exactly analogous to the Wouthuysen–Field effect. For this effect to be significant, two requirements must be fulfilled. First, the scattering rate of Ly\( n \) photons must be sufficient to couple \( T_n \) and \( T_\alpha \), the Ly\( \alpha \) colour temperature. Second, it must be sufficient to drive \( T_n \rightarrow T_\alpha \). We will argue that neither condition is satisfied in practice.

The IGM is optically thick \( \tau \gg 1 \) to all Lyman-series transitions with \( n \lesssim 100 \). Consequently, a Ly\( \alpha \) photon emitted by a star will scatter many times \( \sim \tau \sim 10^7 \) (Gunn & Peterson 1965) before it finally escapes by redshifting across the line width; each of these scatterings contributes to the Wouthuysen–Field coupling. A Ly\( \alpha \) photon can escape by redshifting across the line width, but a transition to a level other than \( n = 1 \) will also remove it. The probability for a decay from an initial state \( i \) to a final state \( f \) is given in terms of the Einstein \( A_{if} \) coefficients by

\[
P_{df} = \frac{A_{df}}{\sum A_{id}}.
\]

Appendix A summarizes the expressions needed to compute the Einstein \( A_{id} \) coefficients. For the Lyman-series transitions, \( P_{\text{rec}+1s} \approx 0.8 \) (see Table 1) so that a Ly\( \alpha \) photon will scatter of the order of \( N_{\text{scat}} \approx 1/(1-P_{\text{rec}+1s}) \sim 5 \) times before undergoing a cascade.

Because a cascade occurs long before escape via redshifting, the coupling from direct pumping is negligible. Recall that the scattering

<table>
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<th>( n )</th>
<th>( f_{\text{recycle}} )</th>
<th>( P_{\text{rec}+1s} )</th>
<th>( n )</th>
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</tr>
</tbody>
</table>
rate \( P_X \) for the photon type \( X = \text{Ly} \alpha, \text{Ly} \beta \) etc. may be expressed as (Field 1959a)

\[
n_{\text{hit}} P_X = N_{\text{scat}} n_X
\]  

in terms of the production rate of photons per unit volume \( n_X \). It is then clear that, for similar production rates (i.e., for sources with a reasonably flat spectrum), \( P_X / P_\alpha \sim N_{\text{scat}, \alpha} / N_{\text{scat}, \alpha} \sim 5 \times 10^{-6} \). This simple argument shows that the contribution from direct pumping by \( \text{Lyn} \) photons will be negligible compared to that of the \( \text{Ly} \alpha \) photons, because \( x_\alpha \propto P_\alpha \).

The second question, whether \( T_\alpha \rightarrow T_k \) is still relevant for heating of the gas by repeated scatterings. Given the reduced number of scattering events, it seems unlikely to be the case, but a full calculation using a Monte Carlo method or following Chen & Miralda-Escudé (2004) is required to rigorously answer this question. Lack of equilibrium would make \( \text{Lyn} \) scattering a more efficient source of heat, on a per scattering basis. Chen & Miralda-Escudé (2004) have shown that \( \text{Lyr} \) heating is much smaller than previous calculations indicated (Madau et al. 1997), because \( T_\alpha \approx T_k \), which reduces the heat transferred per collision. This is unlikely to be the case for the \( \text{Lyn} \).

Following Madau et al. (1997), we can estimate the maximum heating from a single \( \text{Lyn} \) scattering by assuming that all of the atomic recoil energy for a stationary atom is deposited in the gas. Momentum conservation then demands

\[
E_n = -\left\langle \frac{\Delta E}{E} \right\rangle h \nu_n P_n,
\]

where \( \langle \Delta E / E \rangle \sim 10^{-8} \) is the fraction of energy lost by a \( \text{Lyn} \) photon after scattering from a stationary hydrogen atom, and \( h \nu_n \) is the energy of the photon. Assuming the production rate of \( \text{Lyn} \) photons is comparable to that of the \( \text{Ly} \alpha \) photons and taking \( x_\alpha = 1 \), we then obtain \( E_n \approx 0.002(1 + z)/10 \) K Gyr\(^{-1} \). This is much smaller than the \( \text{Lyr} \) heating rate, even including the \( T_\alpha \approx T_k \) correction, so we do not expect \( \text{Lyn} \) scattering to be a significant heat source. Furthermore, if \( T_\alpha \approx T_k \) the rate would be much smaller than this estimate, as in Chen & Miralda-Escudé (2004).

### 4 Lyman-Series Cascades

An excited state of hydrogen may reach the ground state in three ways. First, it may decay directly to the ground state from an np state \((n > 2)\), generating a \( \text{Lyn} \) photon. Secondly, it may cascade to the metastable 2s level. Decay from the 2s level proceeds via a forbidden two photon process. Finally, it may cascade to the 2p level, from which it will produce a \( \text{Lyr} \) photon. We are primarily interested in the fraction of decays that generate \( \text{Lyr} \) photons, which will increase the \( \text{Lyr} \) flux pumping the hyperfine levels.

The fraction of cascades that generate \( \text{Lyr} \) photons can be determined straightforwardly from the selection rules and the decay rates. As an example, consider the \( \text{Ly} \beta \) system. Absorption of a \( \text{Ly} \beta \) photon excites the atom into the 3p level. As illustrated in Fig. 2, the 3p level can decay directly to the ground state, regenerating the \( \text{Ly} \beta \) photon, or to the 2s level, where it will decay by two photon emission. The selection rules forbid \( \text{Ly} \beta \) photons from being converted into \( \text{Lyr} \) photons. In contrast, the 4p level, excited by absorption of \( \gamma \gamma \), can cascade via the 3s or 3d levels to the 2p level and then generate \( \text{Lyr} \).

To calculate the probability \( f_{\text{recycle}} \) that a \( \text{Lyn} \) photon will generate a \( \text{Lyr} \) photon, we apply an iterative algorithm. The expression

\[
 f_{\text{recycle}, i} = \sum_f P_{if} f_{\text{recycle}, f}
\]

relates the conversion probability for the initial level \( i \) to the conversion probabilities of all possible lower levels \( f \). The decay probabilities are calculated using equation (9). We then iterate from low to high \( n \), calculating each \( f_{\text{recycle}} \) in turn.

In our particular case of an optically thick medium, we can ignore direct transitions to the ground state. These generate a \( \text{Lyr} \) photon, which will rapidly be re-absorbed and regenerate the np state. Therefore, such decays will not affect the net population of photons or of excited states. We incorporate this into the calculation by setting \( A_{np \rightarrow 1s} = 0 \) (Furlanetto et al. 2005).

Results for the lowest Lyman-series transitions are summarized in Table 1 and plotted in Fig. 3.\(^4\) These results are in agreement with the above calculations.

\(^4\) Code for calculating the conversion factors is available at [http://www.tapir.caltech.edu/~jp/cascade/](http://www.tapir.caltech.edu/~jp/cascade/)
with those of Hirata (2006). At large \( n \), the conversion fractions asymptote to \( f_{\text{recycle}} \approx 0.36 \) because nearly all cascades pass through lower levels. We emphasize again that the quantum selection rules forbid a Ly\( \beta \) photon from producing a Ly\( \alpha \) photon.

Finally, we briefly comment on the two photon decay from the 2s level (for a more detailed discussion, see Hirata 2006). Selection rules forbid electric dipole transitions from the 2s level to the ground state, but the second-order two photon decay process can occur with \( A_{\gamma\gamma} = 8.2 \text{ s}^{-1} \lesssim A_{2p+1s} \). At \( z \lesssim 400 \), the CMB flux density is sufficiently small that radiative excitations from the 2s level are negligible. Additionally, at the relevant densities collisional excitation to the 2p level is slow compared to the two photon process (Breit & Teller 1940). Consequently, the 2s level will preferentially decay via this two photon process. These transitions may themselves affect \( T_\alpha \), because both the 2s and 1s levels have hyperfine structure and any imbalance in the decay constants here would affect the 1s populations. However, even without detailed calculations, we can see that the resultant coupling must be small. Cascades that do not generate Ly\( \alpha \) must reach the 2s level, so the fraction of Ly\( \alpha \) photons that undergo two photon decay is \( f_{\gamma\gamma}(n) = 1 - f_{\text{recycle}}(n) \approx 0.64 \) (see Table 1). Each such decay has \( N_{\text{scat}} \approx 1 \) because the resulting photons are not re-absorbed. This is much smaller than \( N_{\text{scat}} \approx 10^6 \). Consequently, only if the coupling per scattering were many orders of magnitude larger for two photon decay than for Ly\( \alpha \) scattering could this effect be significant.

5 THE Ly\( \alpha \) COUPLING AROUND A SOURCE

We can see the effects of these recycling fractions on the Ly\( \alpha \) coupling by considering the life of a photon emitted from a given source. The photon initially propagates freely, redshifting until it reaches a Ly\( \alpha \) resonance. Because the IGM is so optically thick, the photon will then scatter several times until a cascade converts it into a Ly\( \alpha \) photon or two 2s \( \rightarrow \) 1s photons. In the latter case, the photons escape to infinity; in the former case, it scatters \( \tau \) times before redshifting out of the Ly\( \alpha \) resonance. This establishes a series of closely spaced horizons, because a photon entering the Ly\( \alpha \) resonance at \( z \) must have been emitted below a redshift,

\[
1 + z_{\text{max}}(n) = (1 + z) \left( \frac{1 - (n + 1)^{-2}}{1 - n^{-2}} \right) .
\]

(13)

The number of Ly\( \alpha \) transitions contributing Ly\( \alpha \) photons is thus a function of the distance from the source. These horizons imprint well-defined atomic physics onto the coupling strength by introducing a series of discontinuities into the Ly\( \alpha \) flux profile of a source.

Thus the Ly\( \alpha \) flux, \( J_\alpha \), arises from a sum over the Ly\( \alpha \) levels, with the maximum \( n \) determined by the distance. The sum is ultimately truncated at \( n_{\text{max}} \approx 23 \) to exclude levels for which the horizon lies below the others at large \( z \). The Ly\( \alpha \) background is thus

\[
J_\alpha(z) = \sum_{n=2}^{n_{\text{max}}} J_\alpha^{(n)}(z) = \sum_{n=2}^{n_{\text{max}}} \int_{z}^{z_{\text{max}}(n)} \frac{d\nu}{\nu} f_{\text{recycle}}(n)(1+z)^2 \frac{c}{H(z')} \epsilon(\nu'_n, z') ,
\]

(14)

where \( \nu'_n \) is the emission frequency at \( z' \) corresponding to absorption by the level \( n \) at \( z \),

\[
\nu'_n = \nu_0 \frac{1 + z'}{1 + z} ,
\]

(15)

and \( \epsilon(\nu, z) \) is the comoving photon emissivity (defined as the number of photons emitted per unit comoving volume, per proper time and frequency, at frequency \( \nu \) and redshift \( z \)). To calculate \( \epsilon(\nu, z) \), we follow the model of BL05:

\[
\epsilon(\nu, z) = \frac{\rho_0^2}{\nu} \frac{d}{d\nu} F_{\text{gal}}(z) \epsilon_\alpha(\nu),
\]

(16)

where \( \rho_0^2 \) is the cosmic mean baryon number density today, \( f_\alpha \) is the efficiency with which gas is converted into stars in galactic haloes (and with which Lyman-continuum photons escape their hosts) and \( F_{\text{gal}}(z) \) is the fraction of gas inside galaxies at \( z \). We model the spectral distribution function of the sources \( \epsilon_\alpha(\nu) \) as a separate power law \( \epsilon_\alpha(\nu) \propto \nu^{\alpha} \) between Ly\( \alpha \) and Ly\( \beta \), and between Ly\( \beta \) and the Lyman limit. In our calculations, we will assume Population III stars with spectral index \( \alpha_\epsilon = 1.29 \) between Ly\( \alpha \) and Ly\( \beta \), normalized to produce 4800 photons per baryon between Ly\( \alpha \) and the Lyman limit, of which 2670 photons are emitted between Ly\( \alpha \) and Ly\( \beta \). In contrast, for Population II stars the numbers are 0.14, 9690 and 6520, respectively (BL05). In calculating \( F_{\text{gal}} \), we use the Sheth & Torman (1999) mass function \( d\mathcal{n}/dm \), which matches simulations better than the Press & Schechter (1974) mass function, at least at low redshifts. We assume that atomic hydrogen cooling to a virial temperature \( T_{\text{vir}} \approx 10^4 \text{ K} \) sets the minimum halo mass. We will normalize \( f_\alpha \) so that \( x_\alpha = 1 \) at \( z = 20 \); this yields \( f_\alpha = 0.16 \) per cent when we include the correct \( f_{\text{recycle}} \).

To see what fraction of photons from a given source are converted into Ly\( \alpha \), we integrate \( \epsilon_\alpha(\nu) \) with the proper weighting by \( f_{\text{recycle}} \). We find that \( f_{\text{recycle}} = 0.63, 0.72 \) and 0.69 for \( \alpha_\epsilon \), (Ly\( \alpha \) \( \rightarrow \) Ly\( \beta \)) = 1.29, 0.14 and \( -1.0 \), respectively (roughly corresponding to Population III stars, low metallicity Population II stars and quasars; Zheng et al. 1997). The total flux is significantly less than, if \( f_{\text{recycle}} = 1 \), as has been generally assumed before. Thus Ly\( \alpha \) coupling will take place later if the proper atomic physics are included (typically \( \Delta z \gtrsim 1 \) for fixed source parameters; see also Hirata 2006). Of course, this is only the average value, and around a given source there will be a distance dependence. A gas element that can only be reached by photons redshifted from below the Ly\( \beta \) resonance will see an effective \( f_{\text{recycle}} \approx 1 \). In contrast, a gas element very close to the source will have \( f_{\text{recycle}} \approx 0.36 \). This will be reflected in the brightness temperature power spectrum (see Section 6).

The Ly\( \alpha \) flux profile of a galaxy with \( M_{\text{gal}} = 3 \times 10^{10} \text{ M}_\odot \) and our fiducial parameters at \( z = 20 \) is plotted in Fig. 4. In our approximation, \( J_\alpha \propto M_{\text{gal}} \). Thus obtaining \( x_\alpha \geq 1 \) at \( r = 10 \text{ Mpc} \) requires a galaxy mass of \( M_{\text{gal}} = 4.2 \times 10^{12} \text{ M}_\odot \), corresponding to a 14\% fluctuation in the density field. Obviously, individual sources do not induce strong Lyman coupling on large scales. The conversion of photons from Ly\( \alpha \) to Ly\( \beta \) steepens the flux profile beyond the simple \( 1/r^2 \) form. Notice that we have normalized \( f_\epsilon \), for each curve separately, so that \( x_\alpha = 1 \) at \( z = 20 \). Because setting \( f_{\text{recycle}} = 1 \) weights large \( n \) transitions more heavily (and hence small scales) that curve lies below the others at large \( r \). The discontinuities occur at the Ly\( \alpha \) horizons. In theory, their positions yield standard rulers determined by simple atomic physics. In practice, the weakness of the discontinuities, and the overlapping contributions of other nearby sources, makes it unlikely that these discontinuities will be observable for an isolated source (see also Section 6). Finally, we note that sharp discontinuities only occur if a photon undergoes a cascade immediately after entering a Ly\( \alpha \) resonance and if the resulting Ly\( \alpha \) photons redshift out of the Ly\( \alpha \) resonance immediately. The former is certainly true, but the latter will affect the shape significantly (Loeb & Rybicki 1999).

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We will show how the scale-dependent small-scale fluctuations in \( T \) manifest of this will occur when the Wouthuysen–Field effect (BL05). First, the number of galaxies traces, but is biased with respect to the underlying density field. As a result an overdense region will contain a factor \( 1 + b(z) \delta \) more sources, where \( b(z) \) is the (mass-averaged) bias, and will have a larger \( x_a \). Next, photon trajectories near an overdense region are modified by gravitational lensing, increasing the effective area by a factor \((1 + 2\beta/3)\). Finally, peculiar velocities associated with gas flowing into overdense regions establish an anisotropic redshift distortion, which modifies the width of the region corresponding to a given observed frequency. These three effects may be represented using a linear transfer function \( W(k) \) relating fluctuations in the coupling \( \delta_{x_a} \) to the overdensity \( \delta \):

\[
\delta_{x_a} = W(k)\delta . \tag{17}
\]

We compute \( W(k) \) for a gas element by adding the coupling due to Ly\(\alpha \) flux from each of the Ly\(\alpha \) resonances (BL05),

\[
W(k) = \frac{1}{x_a} \sum_{n=2}^{n_{\text{max}}} \int \frac{x_a^{(n)}}{z} \frac{dz}{x_a^{(n)}} D(z') \frac{dz'}{D(z)} \times \left\{ 1 + b(z') \right\} j_0(kr) - \frac{2}{3} j_2(kr)\right\}, \tag{18}
\]

where \( D(z) \) is the linear growth function and the \( j_i(kr) \) are spherical Bessel functions of the order of \( i \). The first term in brackets accounts for galaxy bias while the second describes velocity effects. The ratio \( D(z')/D(z) \) accounts for the growth of perturbations between \( z' \) and \( z \). The factor \( dz/x_a/dz' \) converts from Ly\(\alpha \) flux to the coupling. Each resonance contributes a differential coupling (see equation 6).

\[
\frac{dx_a^{(n)}}{dz'} \propto \frac{dJ_0^{(n)}}{dz'} , \tag{19}
\]

with the differential comoving flux in Ly\(\alpha \) from equation (4).

Because this correlates with the density field, it is easiest to observe via

\[
P_{x_a}(k) = 2 P_{x}(k) \left[ \frac{\beta + x_a}{x_{\text{tot}}} W(k) \right] . \tag{20}
\]
The first term probes fluctuations in $T_k$ and $κ_{1-0}$ (all encoded in $β$). We show $P_ψ$ in Fig. 5, contrasting cases that include only photons with $ν_u < ν < ν_p$, $ν_u < ν < ν_s$ and the entire Lyman continuum. For the latter two models, we show results with $f_{\text{recycle}} = 1$ and with the proper atomic physics. Note that each is separately normalized to $x_u = 1$. The dotted curve isolates $2P_β$, which clearly dominates on small scales. Note that we have applied two cut-offs to the power spectrum in this regime (BL05). The first is due to baryonic pressure, which prevents collapse on small scales. The second is the thermal width of the 21-cm line. Naoz & Barkana (2005) showed that this thermal cut-off displays a characteristic angular dependence, which, theoretically, allows fluctuations and the cut-off to be separated. To allow easy comparison with BL05, we do not include this refinement. Additionally, we expect power from the H II regions surrounding the sources to become important on scales smaller than the size of a typical H II region $r_{\text{HII}}$. We have marked this scale for an isolated galaxy in Fig. 5, but note that Furlanetto et al. (2004) predict that the H II regions could be a factor of a few larger at these early times. On sufficiently large-scales $kr ≈ 0$, the second term in equation (20) dominates, and $W(k)$ is fixed by the source bias.

Fig. 5 clearly shows that the Lyα resonances are important on intermediate scales. On large scales only the average flux matters, but as we move to smaller scales the higher-$n$ levels become important. Fig. 6 shows that the fractional reduction in $W(k)$ on small scales is $∼0.63$. Although this is near $f_{\text{recycle}}$ for Population III stars that is not the origin of this scaling. In equation (18), we can write

$$x_u = \sum_n a_n f_{\text{recycle}}(n),$$

and

$$W(k) = \frac{1}{x_u} \sum_n b_n f_{\text{recycle}}(n),$$

where the $b_n$ and $a_n$ are defined by reference to equation (18) and the integral of equation (19), respectively. The former care only about the local flux, but the latter are averaged over the entire Lyman continuum. If $f_{\text{recycle}} = \text{constant}$, they cancel out of $W(k)$ and are relevant only as an overall normalization of $x_u$. In actuality, $f_{\text{recycle}}$ is a function of $n$, reducing the power. We stress that this is because the $f_{\text{recycle}}(n)$ are essentially frequency dependent and so distort the flux profile about any isolated galaxy (see Fig. 4).

It might be hoped that the discontinuities in Fig. 4 would leave a clear feature on the power spectrum, especially one associated with the loss of all photons entering the Lyβ resonance. Such a feature, whose angular scale would be determined by simple atomic physics, could set a standard ruler that could be used to test variations in fundamental constants or to measure cosmological parameters. Sadly, as can be seen from Fig. 5, there is no truly distinct feature. Still, the power does decline around $kr$, and measuring its shape can constrain the angular diameter distance: we find that the amplitude of $P_β$ changes by a few per cent if the angular diameter distance changes by the same amount. However, such constraints would also require the astrophysical parameters to be known precisely, which will be difficult.

### 6.2 Poisson fluctuations

We turn now to brightness fluctuations uncorrelated with the underlying density perturbations, which can be extracted from the power spectrum because of the redshift-space distortions (BL05). Specifically, if the number density of galaxies is small, then Poisson fluctuations can be significant. To calculate the correlation function from Poisson fluctuations, we again follow BL05 and consider the Lyα flux from sources within a volume element $dV$ at two points A and B separated by a comoving distance $l$. The correlation function takes the form

$$ξ_p(l) = \frac{2}{π^2} \int dV \int M \frac{dn(z)}{dM} M^2 P(z') P(z) F_{\text{gal}}(z'),$$

where $z' = z'(r_β)$ is the redshift of a halo at a comoving distance $r_β$ from a gas element at redshift $z$. In this expression, we integrate over a half volume such that $r_β < r_Δ$, with the factor of 2 accounting for the contribution of sources that are nearer to B. The factors $P(z')$ serve to normalize the flux from d $V$ such that

$$\text{d}x_u = P(z') \frac{1}{r^2} \int M \frac{dn(z)}{dM} dM dV,$$

which makes explicit the expected $1/r^2$ dependence of the flux. Because of the finite speed of light, points A and B see the sources within $dV$ at different stages in their evolution. Following BL05, we account for this with the last factor, which scales the source flux by the fraction of mass that has collapsed at the observed redshift. This ignores a possible dependence of the formation rate on halo mass, but in practice high-redshift galaxies are highly biased and occur within a small mass range just above the minimum cooling mass, so this dependence will be weak. Equation (23) is easy to understand. For Poisson statistics, the variance of flux from a set of identical galaxies would be $\propto m^2 f_{\text{gal}} V$; this must then simply be weighted by the flux reaching each of the two points. Note also that, contrary to the claims of BL05, $ξ_p \propto 1/f_{\text{gal}}$, where $f_{\text{gal}}$ is the duty cycle of each galaxy, because the fluctuations are weighted by two powers of luminosity $[MP(z)]$ but only one factor of the density.
The top panel of Fig. 7 shows how the correlation function increases toward small scales. This is a result of the $1/r^2$ dependence of the flux, which weights the correlations to small scales. Including the Ly resonances amplifies this, because the horizon scales skew the flux profile to small radii (see Fig. 4). On large scales the correlation function decreases as the two points A and B share fewer sources. For $r > 2x_a$, a single source cannot affect both points so $\xi_P = 0$. Including $f_{recycle}(n)$ reduces $\xi_P$, especially on the smallest scales, because it decreases the efficiency of coupling from level $n$. The bottom panel of Fig. 7 shows that the suppression on small scales is $(0.63)^2 \approx 0.40$, because $\xi_P$ depends on two powers of the flux. Note that, on large scales, $\xi_P$ increases with the proper $f_{recycle}$. This results from the way we have normalized to $x_a = 1$, which reduces the flux of a given source on large scales as $f_{recycle}$ increases (see Fig. 4). As with $W(k)$, the scale dependence is weak except on large scales, where rapid changes occur at the appropriate horizons. Proper treatment of the recycling fractions is clearly necessary to understand the shape of $\xi_P$.

These features have similar effects on the power spectrum of fluctuations uncorrelated with the density fluctuations,

$$P_{\delta \delta}(k) = P_{\delta \delta}^0 - \frac{p^2}{4p^2} = \left(\frac{x_a}{x_{\text{in}}^2}\right)^2 P_{\delta}(k),$$

as shown in Fig. 8. On large scales, taking $f_{recycle} = 1$ slightly amplifies the power. On small scales, they significantly reduce the power by $\approx 60$ per cent. They also affect the shape of the power spectrum, especially near $k = \pi/r_{\alpha}$, where the lack of Ly $\beta$ to Ly $\alpha$ imprints a knee on the power spectrum. We also note that the sharp Ly horizons imprint weak oscillations on the power spectrum, especially if $f_{recycle} = 1$ (though these will likely be smoothed by photon diffusion).

6.3 Non-linearities in the Wouthuysen–Field coupling

To this point, we have used equation (7) to compute the brightness temperature fluctuations. This assumes that all the underlying perturbations are linear; obviously, at $x_a = 1$, this may only be marginally satisfied. When the radiation background is large, the brightness temperature becomes insensitive to the coupling strength and $P_{\delta \delta}$ will be smaller than our estimate. When will such corrections be important? One obvious test is whether the typical fluctuation $T_b$ is comparable to the maximum brightness temperature decrement between coupled and uncoupled gas, $\delta T$ (i.e., if $T_b = T_1$ in equation 1). But non-linearities may be important even if this condition is not satisfied. A universe with discrete strongly coupled regions separated by uncoupled IGM could have small rms variations, even though non-linearities are extremely important in fixing the brightness temperature of the strongly coupled regions.

Instead we must look deeper at the nature of the fluctuations. First, note from Fig. 4 that individual galaxies most likely provide only weak coupling: $x_a \ll 1$ except near to the sources, at least if small galaxies (near the atomic cooling threshold) are responsible for most of the radiation background. This is not surprising: because of Olber’s paradox, each logarithmic radius interval contributes equally to the background flux in a homogeneous universe. The higher Lyman-series photons, together with the finite speed of light, also do not dramatically increase the weighting on nearby radii. Thus, we expect a substantial fraction of the flux to come from large distances, where density fluctuations are weak. This immediately suggests that the density-dependent power spectrum described in Section 6.1 will not require substantial non-linear corrections.

More quantitatively, the fluctuations become non-linear when $\delta_{\nu} = W(k)\theta(k) \gtrsim 1$; thus we require

$$W(k) \gtrsim 1/[\sigma(R) D(z)],$$

where $\sigma(R)$ is the typical density fluctuation on scale $R \sim 1/k$. Fig. 5(b) shows, however, that $W(k)$ is of the order of unity only for $k \lesssim 0.1 \text{Mpc}^{-1}$, where the density fluctuations are themselves tiny at these redshifts. Thus, we conclude that a linear treatment is adequate for computing the $P_{\delta \delta}$ power spectrum, because it is primarily driven by large-scale fluctuations.

The Poisson fluctuations in Section 6.2 are more problematic. By definition,

$$\xi_P (r_a - r_b) = \frac{\langle x_a(r_a) x_b(r_b) \rangle}{x_a^2} - 1.$$

Thus, on scales at which $\xi_P \gtrsim 1$, the radiation background near galaxy overdensities on this scale is considerably larger than its
average value, indicating that non-linear effects are important. In the particular model we have examined, $\xi_f$ is large only on comoving scales $\lesssim 10$ kpc, so non-linear effects are negligible. However, the amplitude of the Poisson fluctuations increases rapidly as the source density decreases: in models with fewer sources at $x_a = 1$, or which strongly weight massive galaxies, non-linearities may be important. A maximum value to the variance on any scale is $\delta T^2 \propto Q (1 - Q) < 0.25 \delta T^2$, where $Q$ is the volume filling factor of regions with $x_a \geq 1$. In particular, a linear treatment for sources with $f_0 \propto n^{2/3}$ can violate this limit on scales $k \lesssim 1$ Mpc (see, e.g., figs 5 and 7 of BL05); in those cases the observed fluctuations can be much weaker than linear theory predicts (though it will also be non-Gaussian).

7 CONCLUSIONS

In this paper, we have explored the effects on the spin-kinetic temperature coupling of photons that redshift into Lyman resonances. First, we considered the effect of direct coupling via resonant scattering of Ly$\alpha$ photons. We showed that the possibility of cascades greatly reduces the number of times a Ly$\alpha$ photon scatters before escaping. Consequently, the coupling is negligible and may be correctly ignored. A side effect of the reduced scattering rate is to make the Ly$\alpha$ contribution to IGM heating extremely small, even if $T_\alpha$ is not in equilibrium with $T_k$.

Next we considered the increased Ly$\alpha$ flux that results from atomic cascades. Following the selection rules and transition rates, we calculated the probability that a Ly$\alpha$ photon is converted into Ly$\beta$ and showed that $f_{\text{recycle}} \to 0.36$ as $n$ increases. This is significantly smaller than the value $f_{\text{recycle}} = 1$ usually assumed [e.g., by BL05]. For a typical Population III source spectrum, we showed that only 63 per cent of the emitted photons will be converted into Ly$\alpha$, delaying the onset of coupling ($x_a = 1$) for a given set of source parameters.

Incorporating the correct $f_{\text{recycle}}$ modifies the flux profile of an individual source and reduces the coupling on small scales by about a factor of 3 for fixed source parameters. In addition, the cascade process imprints discontinuities on to the flux profile. Using the correct atomic physics reduces the amplitude of these discontinuities and removes one due to the Ly$\beta$ resonance. Unfortunately, their weakness is likely to frustrate attempts to use these discontinuities as a standard ruler.

We then recalculated the power spectra of BL05, incorporating the correct $f_{\text{recycle}}$. This showed a reduction in power of $\sim 37$ per cent (Fig. 5) on intermediate scales for density correlated fluctuations and of $\sim 64$ per cent (Fig. 8) on small scales for fluctuations uncorrelated with the density. It is possible to mimic this loss of power by changing the shape of the stellar spectrum. On small scales, a reduction in the star formation rate will produce a similar reduction in $T_\alpha$, changing the shape of the stellar spectrum. On small scales, a re-

APPENDIX A: CALCULATING EINSTEIN A COEFFICIENTS IN THE HYDROGEN ATOM

The simplicity of the hydrogen atom permits us to compute matrix elements for radiative transitions analytically. We are interested in the Einstein $A$ coefficients, which may be written as (Sobelman 1972)

$$A(n, l, j, n', l', j') = \frac{64 \pi^2}{3 \hbar^3} \epsilon^2 (2j' + 1) \left\{ \begin{array}{c c c} l & j & 1/2 \\ j' & l' & 1 \end{array} \right\}^2 \left\langle R_{n l}^{\epsilon,j,j'} \right\rangle ^2.$$  \hspace{1cm} (A1)

Here $\left\langle \cdots \right\rangle$ denotes the Wigner 6 -- $j$ symbol and we assume spin-1/2 particles. In this expression, the matrix element $R_{n l}^{\epsilon,j,j'}$ has the usual quantum numbers $n, l$ and $n'$, with $n - l - 1 \equiv n$. We use the

\footnotesize{\textsuperscript{6} See http://www.skatelescope.org/}.\normalsize
sets \((n, n_r, l)\) and \((n', n'_r, l')\) to describe the upper and lower levels in the spontaneous transition. In addition, we let \(l_\pm\) be the greater of \(l\) and \(l'\). Because they are separated by \(\Delta l = l' - l = \pm 1, 2l_\pm = l + l' + 1\). We next define, for \(n' \geq l_\pm \geq 0\),
\[
r = n' - l_\pm - 1 \geq 0.
\]
We also let
\[
\Delta l = l' - l = \pm 1, 2
\]
\[
u = 1 - 1/u^2 = -4n n'/ (n - n')^2;
\]
\[
w = v/(v - 1) = 4nn'/ (n + n')^2.
\]
Thus, we only need \(R_{n,l} \equiv a_0 R\), where \(a_0\) is the Bohr radius. This is given by (Rudnick 1935)
\[
R = 2^{l+l'+2}n^l l + 3 \frac{(n-n')^{n'-1}}{(n+n')^{n'+1}} \frac{(n+l)!}{(n+l')!(n-l-1)!(n'-l'-1)!} P_{\Delta l}.
\]
Here \(P_\pm\) and \(P_+\) (the subscripts corresponding to the sign of \(\Delta l\)) are terminating hypergeometric series
\[
2n'P_\pm = (-1)^{r} \left[ (n-n')^{2n'} (2l_\pm + r)/(2l_\pm + 2) \right] \times [(n+n')F(-r, -n + l_\pm + 1; 2l_\pm + 1; v) - (n-n')F(-r, -n + l_\pm; 2l_\pm + 1; v)],
\]
\[
2nP_+ = (-1)^{r} \left[ (n-n')^{2n} (2l_\pm + r)/(2l_\pm + 2) \right] \times [(n+n')F(-r, -n + l_\pm + 1; 2l_\pm + 1; v) - (n-n')F(-r, -n + l_\pm; 2l_\pm + 1; v)].
\]
These expressions can be inserted into equations (9) and (12) to compute \(P_d\) and \(f_{\text{recycle}}(n)\). They are in good agreement with existing experimental measurements.7