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On the spin-temperature evolution during the epoch of reionization

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ABSTRACT
Simulations estimating the brightness temperature (\(\delta T_b\)) of the redshifted 21 cm from the epoch of reionization (EoR) often assume that the spin temperature (\(T_s\)) is decoupled from the background cosmic microwave background (CMB) temperature and is much larger than it, i.e. \(T_s \gg T_{\text{CMB}}\). Although a valid assumption towards the later stages of the reionization process, it does not necessarily hold at the earlier epochs. Violation of this assumption will lead to fluctuations in \(\delta T_b\) that are driven neither by density fluctuations nor by \(H\) II regions. Therefore, it is vital to calculate the spin temperature self-consistently by treating the Ly\(\alpha\) and collisional coupling of \(T_s\) to the kinetic temperature, \(T_k\). In this paper we develop an extension to the BEARS algorithm, originally developed to model reionization history, to include these coupling effects. Here, we simulate the effect in ionization and heating for three models in which the reionization is driven by stars, mini-QSOs or a mixture of both. We also perform a number of statistical tests to quantify the imprint of the self-consistent inclusion of the spin-temperature decoupling from the CMB. We find that the evolution of the spin temperature has an impact on the measured signal especially at redshifts higher than 10 and such evolution should be taken into account when one attempts to interpret the observational data.

Key words: radiative transfer – methods: observational – cosmology: theory – diffuse radiation – radio lines: general.

1 INTRODUCTION
Physical processes that occur during reionization are numerous and complex. Nevertheless, ionization of neutral gas (hydrogen and helium) and heating of the inter-galactic medium (IGM) can be considered the two primary influences of radiating objects during reionization.

Currently, the most promising ‘direct’ probe of reionization is the redshifted 21-cm radiation emanating from neutral hydrogen during the epoch of reionization (EoR), which are to be measured using upcoming telescopes like LOFAR,1-2 MWA,3 PAPER4 and 21CMA.5 The intensity of the observed 21-cm radiation depends on the ratio between the number density of electrons in the hyperfine states in the ground state of a neutral hydrogen atom. This ratio is normally expressed in terms of the so-called 21-cm spin temperature, \(T_s\). At the onset of the formation of the first reionizing objects the spin temperature is equal to the cosmic microwave background (CMB) temperature since at these redshifts the ratio between excited and ground hyperfine state electrons is completely determined by the CMB. However, as the number of ionizing sources increases, \(T_s\) starts departing from \(T_{\text{CMB}}\); slowly at the beginning, then rapidly approaching values larger than \(T_{\text{CMB}}\). This evolution is typically ignored in most previous studies of reionization which assumes \(T_s \gg T_{\text{CMB}}\) at all times (Abel, Bryan & Norman 2000, 2002; Bromm, Coppi & Larson 2002; Yoshida et al. 2003; Mellema et al. 2006).

Recently, Baek et al. (2009) have relaxed this assumption on \(T_s\) at the dawn of reionization and explored its impact on the brightness temperature. They found a considerable deviation from assuming \(T_s \gg T_{\text{CMB}}\) at the beginning of reionization. Towards the end of reionization though, this assumption holds ground. But, in order to track the evolution of \(T_s\) accurately, like in Baek et al. (2009), it is necessary to perform a detailed 3D Ly\(\alpha\) radiative transfer (RT) calculation. The Ly\(\alpha\) photons undergo a large number (~103) of scatterings even in a marginally neutral medium before it is sufficiently off line-centre to ‘free stream’. The scattering angle after each encounter is completely random and therefore the RT is often done in a Monte Carlo sense (Tasitsiomi 2006; Baek et al. 2009;...
Laursen, Razoumov & Sommer-Larsen 2009; Pierleoni, Maselli & Ciardi 2009) to capture this random nature of Lyα scatterings.

Unfortunately, these Monte Carlo RT schemes are computationally very expensive, especially if we need to simulate large fields of view necessary to generate mock data sets for next generation radio telescopes. In order to circumvent the need to perform such computer-intensive calculations to obtain \( T_s \), we develop an algorithm along the lines of BEARS (Thomas et al. 2009) as an approximation. In this paper we present an algorithm that follows the decoupling of \( T_s \) from \( T_{\text{CMB}} \) owing to Lyα photons, which couples the spin temperature to the colour/kinetic temperature via the Wouthuysen–Field effect (Wouthuysen 1952). Collisional excitation and heating caused by secondary electrons resulting from hard X-ray radiation are also included. The dominant source of Lyα flux is the background created by the redshifting of photons in the Lyman-band into Lyα. These photons are bluewards of Lyα and is injected into Lyα at some distance away from the source.

The amount of intrinsic Lyα, ionizing and ‘heating’ photons is a function of the source spectral energy distribution (SED). Thus, the evolution of the spin temperature critically depends on the source of reionization. Different reionization sources manifest themselves by influencing the IGM in markedly different ways. For example, deficiency of hard photons in the SEDs of ‘first stars’ limit the extent to which they heat the IGM (Zaroubi & Silk 2005; Zaroubi et al. 2007; Thomas & Zaroubi 2008), while mini-quasars (or mini-QSOs, characterized by central black hole masses less than a million solar), abundant in X-ray photons, cause considerable heating (Madau, Meiksin & Rees 1997; Furlanetto & Loeb 2002; Furlanetto, Zaldarriaga & Hernquist 2004; Ricotti & Ostriker 2004; Wyithe & Loeb 2004; Nusser 2005; Zaroubi et al. 2007; Thomas & Zaroubi 2008). Ionization profiles similarly have their characteristic source-dependent behaviour.

Although the question on which sources did the bulk of the reionization is up for debate, it is conceivable from observations of the local Universe up to redshifts around 6.5 that sources of reionization could have been a mixture of both stellar and quasar kinds (their respective roles again are uncertain). Implementing RT that includes both ionizing and hard X-ray photons has been difficult and as a result most 3D RT schemes restrict themselves to ionization due to stars (Ciardi et al. 2001; Gnedin & Abel 2001; Nakamoto, Umemura & Susa 2001; Ritzerveld, Icke & Rijkhorst 2003; Razoumov & Cardall 2005; Mellema et al. 2006; Rijkhorst et al. 2006; Susa 2006; Whalen & Norman 2006; Mesinger & Furlanetto 2007; Zahn et al. 2007; Pawlik & Schaye 2008). In Ricotti & Ostriker (2004), a ‘semi’ hybrid model of stars and mini-QSOs, like the one hinted above, has been used albeit in sequential order instead of a simultaneous implementation. That is, pre-ionization due to mini-QSOs was invoked between \( 7 < z < 20 \), after which stars reionize the Universe at redshift 7. We in this paper would like to address the issue of simulating the propagation of both the UV and hard X-ray photons, exactly in one dimension and as approximation in three dimensions.

The focus of this paper is therefore to introduce the algorithm that is used to implement IGM heating in BEARS along with the procedure to estimate the spin temperature of the IGM. As an application of this technique we explore the effects of heating due to mini-QSOs, stars and, for the first time, a mixed ‘hybrid population’. Subsequently, we provide quantitative and qualitative analysis of the differences in the 21-cm EoR signal with and without the usual assumption of \( T_s \) being always decoupled from \( T_{\text{CMB}} \).

The paper is organized as follows. Section 2 briefly describes the \( N \)-body and 1D RT codes used. In Section 3, we describe the adaptation of BEARS to include \( T_s \), followed by the calculation of the \( T_s \) and \( \Delta T_s \) within the simulation box. BEARS is then applied to three different scenarios of reionization in Section 4, viz. (1) the primary source being stars, (2) mini-QSOs and (3) a hybrid population of stars and mini-QSOs. Subsequently, observational cubes of \( \Delta T_s \) are generated for each of these scenarios and its properties discussed. In Section 5, we provide statistics on the simulated boxes and interpret the finding mainly from the point of view of the differences in \( \Delta T_s \) with and without the usual assumption that \( T_s \) is decoupled from \( T_{\text{CMB}} \). We also compare our work to that of Santos et al. (2008) in the same section. Conclusions and discussions of the results are presented in Section 6, along with a mention of a few topics that can be addressed using the data set simulated in this paper.

2 SIMULATIONS

In this section we briefly mention the dark-matter (DM)-only \( N \)-body simulations employed and the 1D RT code developed by Thomas & Zaroubi (2008) and provide an overview of the BEARS algorithm designed in Thomas et al. (2009).

2.1 \( N \)-body: dark matter only

The DM only \( N \)-body simulations are the same as in Thomas et al. (2009) and was performed by Joop Schaye and Andreas Pawlik at the Leiden observatory. The \( N \)-body/TREEPM/SFH code GADGET (Springel 2005) was used to perform a DM cosmological simulation containing 512\(^3 \) particles in a box of size 100\( h^{-1} \) comoving Mpc with each DM particle having a mass of 4.9 \( \times 10^8 \)\( h^{-1} \) M\(_\odot\). Initial conditions for the particle’s position and velocity were obtained from glass-like initial conditions using CMBFAST (version 4.1; Seljak & Zaldarriaga 1996) and the Zeldovich approximation was used to linearly evolve the particles down to redshift \( z = 127 \). A flat ΛCDM universe is assumed with the set of cosmological parameters \( \Omega_m = 0.238, \Omega_b = 0.0418, \Omega_\Lambda = 0.762, \sigma_8 = 0.74, n_s = 0.951 \) and \( h = 0.73 \) (Spergel et al. 2007). Snapshots were written out at 35 equally spaced redshifts between \( z = 12 \) and \( z = 6 \). Haloes were identified using the Friends-of-Friends algorithm (Davis et al. 1985), with linking length \( b = 0.2 \). The smallest mass haloes we can resolve are a few times \( 10^{10} h^{-1} \) M\(_\odot\). The density field was smoothed on the mesh with a Gaussian kernel with standard deviation \( \sigma_G = 2 \times 100/512 \) comoving Mpc\( h^{-1} \) (two grid cells).

2.2 1D radiative transfer code.

The implementation of the 1D radiative transfer code is modular and hence straightforward to include different spectra corresponding to different ionizing sources. Our 1D code can handle X-ray photons, the secondary ionization and heating it causes, and as a result perform well for both high (quasars/mini-QSOs) and low energy (stars) photons. Further details of the code can be found in Thomas & Zaroubi (2008). The parameter space simulated by the 1D RT scheme (Thomas & Zaroubi 2008) include (1) different SEDs (stars or mini-QSOs with different power-law indices), (2) duration of evolution (depending on the life-time of the source), (3) redshifts at which these sources turn on and (4) clumping factor or over-density around a given source. Information on the ionization and temperature profiles from these simulations was catalogued to be used later as in Thomas et al. (2009). Density profiles around sources are assumed to be

homogeneous although the code could be initialized using any given profile.

2.3 BEARS algorithm: overview

BEARS is a fast algorithm that simulates the underlying cosmological 21-cm signal from the EoR. It is implemented by using the $N$-body/sph simulation in conjunction with a 1D RT code; both discussed in the previous sections. The basic steps of the algorithm are as follows: first, a catalogue of 1D ionization profiles of all atomic hydrogen and helium species and the temperature profile that surround the source is calculated for different types of ionizing sources with varying masses, luminosities at different redshifts. Subsequently, photon rates emanating from DM haloes, identified in the $N$-body simulation, are calculated semi-analytically. Finally, given the spectrum, luminosity and the density around the source, a spherical ionization bubble is embedded around the source, whose radial profile is selected from the catalogue as generated above. In case of overlap between ionization bubbles, the excess ionized atoms in the overlap area is redistributed at the edge of the bubbles. For more details see Thomas et al. (2009). The outputs are data cubes (2D slices along the frequency/redshift direction) of density ($\delta$), radial velocity ($v_r$) and hydrogen and helium fractions ($x_\text{H}, x_\text{He}, x_\text{He}_2$ and $x_\text{He}_3$). Each data cube consists of a large number of slices each representing a certain redshift between 6 and 11.5. Because these slices are produced to simulate a mock data set for radio-interferometric sources, they are uniformly spaced in frequency (therefore, not uniform in redshift). Thus, the frequency resolution of the instrument dictates the scales over which structures in the Universe are averaged/smoothed along the redshift direction. The relation between frequency and redshift space $z$ is given by $z = \frac{v_21}{c} - 1$, where $v_21 = 1420$ MHz is the rest frequency that corresponds to the 21-cm line.

3 INCLUDING IGM HEATING IN BEARS

In Thomas et al. (2009), the BEARS algorithm was introduced and a special-purpose 3D RT scheme was used to simulate cosmological EoR signals. In that paper, we detailed the philosophy behind the code and its implementation to incorporate ionization due to a variety of sources. In this section, we extend the features of BEARS to include heating (on which the brightness temperature is sensitively dependent) due to hard photons within the same framework.

The algorithm to implement heating begins in a manner similar to that for ionization. The $T_k$-profile from the 1D RT code is used to embed a spherically symmetric ‘$T_k$ bubble’ at the locations of the centre-of-mass of DM haloes. The luminosity of the source is a function of the halo mass. The problem embedding a temperature profile in the simulation box is that the radius of the bubble is large ($>5$ Mpc) and results in extensive overlap, even at high redshifts; a problem encountered for ionization bubbles only towards the end of reionization. In a quasar-dominated part of the Universe this is particularly severe because of its large sphere-of-influence in heating the IGM.

3.1 Treating overlaps: energy conservation

Overlap in the spheres of ionized regions was treated by redistributing the excess ionizing photons in the overlapped region uniformly around the overlapping spheres (Thomas et al. 2009). Treating overlapped zones directly in terms of temperatures makes it difficult to come up with any ‘conserved quantity’. To elaborate, consider a pre-ionized zone in the simulation box close to the radiating source. Although at close proximity to the source, this region is not heated efficiently because of the absence of neutral hydrogen to capture the photons. On the other hand, the same source can dump more energy into an initially neutral zone that may be far away from it. Thus, embedding the $T_k$-profile directly from the catalogue (which assumes uniform IGM density) is not appropriate.

Here, we adopt a different approach where we estimate the total energy deposited in every region of the simulation box and invoke the conservation of energy deposited by the sources in the overlapped regions. We integrate the contribution to the energy budget, at a given location, from all sources whose sphere-of-influence extends to that location. This total energy is then redistributed equally to all the contributing sources, i.e. the energy output of each source is modified to account for the overlapping.

To illustrate, consider $N$ sources that overlap at a particular location $r$ and the total energy estimated at that location be $E_{\text{tot}} = \sum_{i=1}^{N} E_i$, where $E_i$ is the energy deposited by the $i$th source at location $r$. The fraction of ‘excess’ energy attributed to each of the $N$ sources is $\delta E_i = E_{\text{tot}}/N$. This energy $\delta E_i$ is then added to the total energy from the source to estimate a new normalization constant for the SED of the source. For example, in case of a power-law-type source, the SED includes a normalization term that is determined by the total energy of the source, $E_{\text{tot}}$. However, in the overlap case the total energy of the source is replaced by $E_{\text{tot}} + \delta E_i$. Now a new ‘bubble’ of kinetic temperature is embedded whose profile depends on a source whose output energy has gotten a $\delta E$ boost. In this manner $T_k(r)_{\text{est}}$ is estimated at every location in the simulation box. From this point on we need to estimate the coefficients that couple $T_k$ to $T_i$ that will eventually lead to the estimation of $\delta T_k$.

It is worthwhile also to note that the results are robust to variation in the exact algorithm used to treat the overlapped region. For example, if we choose to sum the energies deposited directly in a given region or choose $\max(E_1, E_2, \ldots, E_n)$, where $E_1, \ldots, E_n$ are energies deposited by sources 1, …, $n$ respectively, the final results are very similar.

This is obviously an approximation which assumes that the efficiency of the photons in heating the IGM does not depend on their frequency. For the case of power-law sources where most of the energy comes from hard photons this is probably a reasonable approximation. However, in the case of blackbody sources this is not a very good assumption because evidently the heating is done by a very small fraction of photons. But in these cases the overlap problem is not as severe as for the power-law sources since the extent of the heating is much more limited. In summary, despite the approximate nature of this approach, it provides an efficient and reasonable resolution for the issue of the overlapping of temperature bubbles. We note that self-consistent treatment of this problem requires taking into account the modification of each of sources’ SED in a different manner depending on the amplitude of its SED. Obviously, this is computationally very expensive.

3.2 Calculating $\delta T_k$ in the volume

Spin temperature can be thought of as a short-hand notation to represent the level population of the hyperfine states of the ground level of a hydrogen atom. Depending on the physical processes and background radiation that dominate a medium, $T_s$ is either coupled to the background CMB temperature or to the kinetic temperature of the hydrogen gas in the medium. Formally Field (1958) derived
\[ T_s^{-1} = \frac{T_{\text{CMB}}^{-1}(\nu) + y_o T_k^{-1} + y_{\text{coll}} T_k^{-1}}{1 + y_o + y_{\text{coll}}} \]  

where \( y_o \) and \( y_{\text{coll}} \) are parameters that reflect the coupling of \( T_s \) to \( T_k \) via Ly\( \alpha \) excitation and collisions, respectively. The efficiency of Ly\( \alpha \) coupling dominates over that of collisions, especially further away from the source (Chuzhoy et al. 2006; Thomas & Zaroubi 2008). In our treatment of calculating \( T_s \), we estimate both \( y_o \) and \( y_{\text{coll}} \).

The coefficient \( y_{\text{coll}} \) is a function of \( T_k \) and the ionized fraction of the medium, \( x_{\text{H}^0} \). This information on ionization and heating is available from the prescription outlined in the previous section. While simulating the 1D profiles we simultaneously calculate \( y_o \) as

\[ y_o = \frac{16\pi^2 k T_e^2 f_{\text{Ly} \alpha}(r)}{27 m_e c^2}, \]  

Here, \( f_{\text{Ly} \alpha}(r) \) is the Ly\( \alpha \) flux density at distance \( r \) from the source. For mini-QSOs with high energy photons, Ly\( \alpha \) coupling is mainly caused by collisional excitation due to secondary electrons (Chuzhoy et al. 2006). This process is accounted for by the following integral:

\[ J_{\text{Ly} \alpha}(r) = \frac{c}{4\pi H(z) v_o} n_{\text{H}_0}(r) \int_{2keV}^{\infty} \phi_{\text{H}}(E) \sigma(E) N(E; r, t) dE, \]  

where \( N(E; r, t) \) is the number of photons with energy \( 'E' \) at radius \( 'r' \) and time \( 't' \) per unit area (Zaroubi & Silk 2005). This number is obtained directly from the 1D RT by taking into account the absorption due to the optical depth along the line-of-sight to the source at a distance \( 'r' \). The 1D profiles generated are catalogued also as a function of time. Therefore the profiles that are embedded within the simulation are chosen to obey causality. \(^6\) The ionization cross-section of neutral hydrogen in the ground state is given by \( \sigma(\text{E})/f_{\text{Ly} \alpha} = 0.416 \) is the oscillator strength of the Ly\( \alpha \) transition, \( e \) and \( m_e \) are the electron’s charge and mass, respectively, \( \phi_{\text{H}} \) is the fraction of absorbed photo energy that goes into excitation (Shull & van Steenberg 1985; Dijkstra, Haiman & Loeb 2004). Note here that the fitting formula is a function of both ionization fraction and energy as given in the appendix of Dijkstra et al. (2004).

For the case of stars, the dominant source of Ly\( \alpha \) flux results from the redshifting of the source spectrum bluewards of Ly\( \alpha \) into the resonant line at different distances from the source. Frequency \( 'v' \) at the redshift of emission (or the source) \( 'z' \) is redshifted into \( v_{\text{Ly} \alpha} \) at redshift \( z(r) \) such that

\[ v = v_{\text{Ly} \alpha} \frac{1 + z}{1 + z(r)}. \]  

Thus, at every radius \( r \) away from the source the Ly\( \alpha \) flux \( J_{\text{Ly} \alpha}(r) \propto N(E; r, t)/r^2 \), where \( E' = 10.2 \frac{v_{\text{Ly} \alpha}}{2\text{cm}^{-3}} \) [eV].

Now, instead of embedding a bubble of Ly\( \alpha \) radiation, \( J_{\text{Ly} \alpha}(r) \), as estimated from equation (3). Since \( J_{\text{Ly} \alpha}(r) \) is basically the number of Ly\( \alpha \) photons at a given location, the overlap of two \( J_{\text{Ly} \alpha} \) ‘bubbles’ implies that the photons and hence the \( J_o \) have to be added, i.e. at a given spatial (pixel) location, \( x, y, z \) and time \( t \), the total Ly\( \alpha \) flux is given by

\[ J_{\text{Ly} \alpha}^M(x, y, z, t) = \sum_{i=0}^{N} J^i_{\text{Ly} \alpha}(x, y, z, t), \]  

where \( J^i_{\text{Ly} \alpha}(x, y, z, t) \) is the Ly\( \alpha \) flux contributed by \( i \) th source at the pixel location in the box, \( x, y, z \) and time \( t \). Equipped with the quantities \( T_s(r) \) and \( J_{\text{Ly} \alpha}(r) \), we can calculate \( y_o \) as in equation (2), and subsequently the spin temperature through equation (1). Now all terms required for the calculation of \( \delta T_b \), as in equation (6), are obtained.

\[ \delta T_b(r) = (20 \text{ mK}) (1 + \delta(r)) \left( \frac{x_{\text{H}_0}(r)}{h} \right) \left( 1 - \frac{T_{\text{CMB}}}{T_s(r)} \right) \times \left[ \frac{H(z)/1+z}{\text{d}z/\text{d}r} \right] \left( \Omega_m h^2 \right)^{-1} \left[ \frac{1+z}{10} \left( \frac{0.24}{\Omega_m} \right)^{1/2} \right]. \]  

4 EXAMPLE APPLICATIONS OF BEARS

In this section, we apply BEARS with its extended feature of including heating of the IGM to three different scenarios of reionization. The models described in this section are not ‘template’ reionization scenarios by any measure nor is any particular model favoured w.r.t the other. In fact, these models may be far from reality and only serve as examples of the potential of BEARS to provide a reasonable estimate of the 21-cm brightness temperature for widely different scenarios of reionization.

4.1 Heating due to stars

The first scenario explored using BEARS is the case in which the sources of reionization are only stars. In this section, we describe the model used to describe the stellar component and the prescription adopted to embed these stars into haloes of DM identified in an N-body simulation.

4.1.1 Modelling stellar radiation in BEARS

Most stars, to the first order, behave as blackbodies at a given temperature, although the detailed features in the SED depend on more complex physical processes, age, metallicity and mass of the star. This blackbody nature imprints characteristic signatures on the IGM, heating and ionization patterns (Thomas & Zaroubi 2008). Schaerer (2002) showed that the temperature of the star only weakly depends on its mass. The blackbody temperature of the stars in our simulation was thus fixed at \( 5 \times 10^4 \) K to perform the RT. We sample the parameter space of redshifts (12 to 6), density profiles around the source\(^7\) and masses (10 to 1000 M\(_\odot\)). The total luminosity is normalized depending on the mass of the star according to table 3 in Schaerer (2002).

For blackbody with a temperature around \( 10^5 \) K, similar to our adopted value, the spectrum peaks between \( \approx 20 \) to \( \approx 24 \) eV (Wien’s displacement law). Thus, from the form of the blackbody spectrum we can a priori expect, in the case of stars, that the ionization induced by these objects will be high, but the heating they cause will not be substantial given the exponential cut-off of the radiation towards higher frequencies.

Now, following the prescription in Thomas et al. (2009) we associate stellar spectra with DM haloes using the following procedure.

\(^7\) We can incorporate any given density profile like the homogeneous, isothermal or NFW profiles. For this paper, however, we ran all the simulations using a homogeneous background. Overdensities around sources can be corrected for by using the prescription in Thomas et al. (2009).
The global star formation rate density $\dot{\rho}_s(z)$ as a function of redshift was calculated using the empirical fit

$$\dot{\rho}_s(z) = \dot{\rho}_{0s} \frac{\beta \exp [\gamma(z - z_{0s})]}{\delta - \alpha + \alpha \exp [\beta(z - z_{0s})]} \left(\text{M}_\odot \, \text{yr}^{-1} \, \text{Mpc}^{-3}\right),$$

where $\alpha = 3/5$, $\beta = 14/15$, $z_{0s} = 5.4$ marks a break redshift, and $\dot{\rho}_{0s} = 0.15 \left(\text{M}_\odot \, \text{yr}^{-1} \, \text{Mpc}^{-3}\right)$ fixes the overall normalization (Springel & Hernquist 2003). Now, if $\delta t$ is the time-interval between two outputs in years, the total mass density of stars formed is

$$\rho_s(z) \approx \dot{\rho}_s(z) \delta t \left[\text{M}_\odot \, \text{Mpc}^{-3}\right].$$

Note that this approximation is valid only if the typical lifetime of the star is much smaller than $\delta t$, which indeed is the case in our model because the stellar mass we input ($100 \, \text{M}_\odot$) has a lifetime of about a few Myr (Schaefer 2002), compared to a typical time difference of few tens of Myr between simulation snapshots.

Therefore, the total mass in stars within the simulation box is $M_s(\text{box}) = L_s(\text{box}) \dot{\rho}_s \left(\text{M}_\odot\right)$. This mass in stars is then distributed among the haloes weighted by their mass,

$$m_s(\text{halo}) = \frac{m_{\text{halo}}}{M_{\text{halo} \,(\text{tot})}} M_s(\text{box}),$$

where $m_s(\text{halo})$ is the mass in stars in the DM ‘halo’, $m_{\text{halo}}$ the mass of the halo and $M_{\text{halo} \,(\text{tot})}$ the total mass in haloes within the simulation box.

We then assume that all of the mass in stars is distributed in stars of $100 \, \text{M}_\odot$, which implies that the number of stars in the halo is $N_{100} = 10^{-2} \times m_s(\text{halo})$. The luminosity of a $100 \, \text{M}_\odot$ star is obtained from fig. 1 of Schaefer (2002), assuming zero metallicity. The luminosity of $100 \, \text{M}_\odot$ star thus derived is in the range of $10^{38} \sim 10^{39} \, \text{L}_\odot$ and this value is multiplied by $N_{100}$ to get the total luminosity emanating from the ‘halo’ and the RT is done by normalizing the blackbody spectrum to this value. The escape fractions of ionizing photons from early galaxies are assumed to be 10 per cent.

### 4.1.2 Results: stellar sources

Results of the evolution of the $T_k$, $T_s$ and $\delta T_k$ of the IGM, when the sources of reionization comprise only of stars is shown in Figs 1, 2 and 3, respectively.

Fig. 1 shows the kinetic temperature for stellar sources at redshifts 10, 8, 7 and 6 at which their ionized fractions are 0.12, 0.5, 0.83 and 0.98, respectively. The blackbody-type stellar spectra do not have sufficient high energy photons to heat the IGM substantially far away from the source. Thus, we see compact regions (bubbles) of high temperature in the immediate vicinity of the source. In the inner parts, where the ionized fraction is high ($X_{\text{H}_2} > 0.95$), the temperatures are of the order of $10^4 \, \text{K}$ and drops sharply in the transition zone to neutral IGM. The ionized region is restricted to about 100 kpc in physical coordinates around a halo (Thomas & Zaroubi 2008).

Fig. 2 shows $T_s$ at four different redshifts. Collisional coupling (by coll) is important close to the radiating source ($< 200 \, \text{kpc}$). The primary source of coupling between $T_s$ and $T_k$ is the redshifting of photons bluewards of the Ly$\alpha$ line into the Ly$\alpha$ frequency. It has to be emphasized here that the Ly$\alpha$ photons are produced only due to the source and secondary processes. Thus we see that stellar sources are efficient in building up a significant background of $J_o$ far away from the source which is sufficient to couple $T_s$ to $T_k$ during reionization (Ciardi & Madau 2003). As an example, in Fig. 12 we show the reionization history ($\delta T_k$) assuming a high background $J_o$, in other words, assuming perfect $T_k$-$T_s$ coupling.

In Fig. 3, $\delta T_k$ corresponding to the same redshifts as in the previous figures is shown. In this particular model $\delta T_k$ values are not very high ($|\delta T_k| < 10 \, \text{mK}$). At early epochs (top-left) at $z \approx 10$, there are only a few sources and the heating of the IGM or the secondary $J_o$ is not high enough to cause substantial differential brightness temperatures. At later times, the ionized bubbles overlap significantly driving the brightness temperature to zero. Thus, there is only a small portion of the Universe (in volume) that has sufficient Ly$\alpha$ coupling and neutral hydrogen density to cause large
number of plausible SEDs that can be considered is numerous and serves as a reminder of the extent of ‘unexplored parameter space’ even while considering the case of mini-QSOs alone, and argues for an extremely quick RT code like BEARS.

The mini-QSOs are assumed to accrete at a constant fraction $\epsilon$ (normally 10 per cent) of the Eddington rate. Therefore, the luminosity is given by

$$L = \epsilon L_{\text{Edd}}(M)$$

$$= 1.38 \times 10^{37} \left( \frac{\epsilon}{0.1} \right) \left( \frac{M}{M_\odot} \right) \text{ erg s}^{-1}. \quad (12)$$

The luminosity derived from the equation above is used to normalize the relation in equation (10) according to equation (11). The energy range considered is between 10.4 and 10 keV. Simulations were carried out for a range of masses between $10^5$ and $10^9 M_\odot$. To justify comparing the case of stars and mini-QSOs we argue that, although the number of photons at different energies is a function of the total luminosity and spectral index in the case of mini-QSOs, if we assume that all photons from the mini-QSO are at the hydrogen ionization threshold, then the number of ionizing photons obtained, for the mass range fixed above, is about $10^{50}$ to $10^{55}$; the same order of magnitude as the number of ionizing photons in the case of stars and it also matches the numbers being employed for simulations by various other authors like Mellema et al. (2006) and Kuhlen & Madau (2005).

The mini-QSOs are embedded into an N-body output following the prescription in Thomas et al. (2009). DM haloes are identified using the friends-of-friends (FoF) algorithm and masses of black holes assigned according to

$$M_{\text{BH}} = 10^{-4} \frac{\Omega_h}{\Omega_m} M_{\text{halo}}, \quad (14)$$

where the factor $10^{-4}$ reflects the Magorrian relation (Magorrian et al. 1998) between the halo mass ($M_{\text{halo}}$) and black hole mass ($M_{\text{BH}}$) multiplied with the radiative efficiency assumed to be 10 per cent, and the fraction $\frac{\Omega_h}{\Omega_m}$ gives the baryon ratio (Ferrarese 2002).

### 4.2 Heating due to mini-QSOs

In this section, we will consider heating due to high-energy X-ray photons emanating from power-law-type sources (e.g. mini-QSOs). Because of their large mean-free path ($\propto E^3$), it has been difficult to incorporate the effect of heating by power-law sources self-consistently in a 3D RT simulation.

#### 4.2.1 Modelling mini-QSOs in BEARS

Observations reveal the energy spectrum of quasar-type sources typically follows a power law of the form $E^{-\alpha}$ (Elvis et al. 1994; Laor et al. 1997; Vanden Berk et al. 2001; Vignali, Brandt & Schneider 2003). Here, we assume $\alpha = 1$ and thus the SED of the mini-QSOs is given by

$$I(E) = A_\text{g} \times E^{-\alpha} \quad 10.4 \text{ eV} < E < 10^4 \text{ eV}, \quad (10)$$

with the normalization constant,

$$A_\text{g} = \frac{E_{\text{total}}}{\int_{E_{\text{range}}} I(E) dE}, \quad (11)$$

where $E_{\text{total}}$ is the total energy output of the mini-QSO within the energy range, $E_{\text{range}}$. Any complex, multi-slope spectral templates as in Sazonov, Ostriker & Sunyaev (2004) can be adopted. The
Spin-temperature evolution during the EoR

Figure 4. Kinetic temperature for mini-QSO sources. Slices correspond to that in Fig. 1 with temperatures indicated on a log T [K] scale. Here, we see the striking difference between mini-QSOS and stars in the extent of heating. The amplitude is about \( \approx 10^{6.5} \) K towards the centre and spatial extent of the heating is about a few Mpc. Already at redshift 10 (top-left) the average temperature is of the order \( 10^3 \) K.

Figure 5. Spin temperature for mini-QSO sources. Slices correspond to that in Fig. 1 with the temperatures indicated on a log T [K] scale. Spin temperatures show an interesting ring-like behaviour (easily visible in the top-left panel). The reason for this is discussed in the text.

Fig. 5 shows the evolution of \( T_s \) as a function of redshift. Owing to a high secondary \( J_o \) produced due to X-ray photons, \( T_s \) is coupled to \( T_k \) for the large part. The snapshots of \( T_s \) show a peculiar ring-like behaviour (Fig. 5). This is because towards the central part of the bubble around the source, the IGM is highly ionized and \( J_o \propto x_{HII} \) obtains an extremely low value. On the other hand \( J_o \) progressively gets lower away from the source, regions (>5Mpc). Therefore, only a relatively narrow zone (a few hundred kpc) in between the ionizing front and regions further out has \( J_o \) high enough to decouple \( T_s \) from \( T_{CMB} \).

Figure 6. Differential brightness temperature for mini-QSO sources. Slices correspond to that in Fig. 1. Note here that the brightness temperature (mK) is plotted on a linear scale with values as indicated on the colour bar. We see again from the top-left panel that although the number of sources in the field are few, they were efficient in both increasing \( T_k \) dramatically and providing sufficient \( J_o \) to ‘light-up’ the Universe in 21-cm around them. The spheres in the top-left panel have \( \delta T_b \) of zero because they are highly ionized.

Fig. 6 shows \( \delta T_b \) for redshifts 10, 9, 8 and 7 in panels top-left to bottom-right, respectively. The \( \delta T_b \) plotted in this figure are high enough to be detectable by upcoming telescope’s like LOFAR and MWA, whose sensitivities should reach \( \delta T_b > 5 \) mK (Labropoulos et al. 2009). We see in the top-left panel of this figure that even though the number of sources in the field is small, they are efficient in both increasing \( T_k \) dramatically and providing sufficient \( J_o \) to ‘light-up’ the Universe in the 21-cm differential brightness temperature. The \( \delta T_b \) inside the spheres are zero because they are highly ionized \((x_{HII} > 0.99)\).

4.3 Modelling co-evolution of stars and mini-QSOs

In the observable Universe we know that stars and quasars do co-exist. Although, there are indications of the quasar number-density peaking around redshift two (Nusser & Silk 1993) and declining thereof, there are also measurements by Fan et al. (2006) of high-mass (>\(10^8 \)M\(_\odot\)) quasars at \( z > 6 \). This allows us to envisage a scenario of reionization in which stars and quasars (or mini-QSOS) contributed to the ionization and heating of the IGM in a combined fashion. As a final example-application of BEARS, we present our model of a ‘hybrid’ star-mini-QSO SED and examine its results on the ionization and heating of the IGM.

4.3.1 The ‘hybrid’ SED

The uncertainty regarding the properties and distributions of objects during the dark ages allows us to come up with strikingly different ways of incorporating the co-existence of stars and mini-QSOS. For example, consider that there are \( N \) different haloes within our simulation box. One approach would be to suppose that each of these haloes hosts both a mini-QSO and stars, whose masses/luminosity is derived according to the previous two examples. The other approach would be to place one or two massive mini-QSOS (almost
quasars), still conforming to the black hole mass density predictions of Volonteri, Lodato & Natarajan (2008), and the rest of the haloes in the simulation box with populations of stars. For this example, given the minimum mass halo our simulation can resolve, we have chosen to adopt the former approach, i.e. a mini-QSO and stars in every halo.

In our approach, given the halo mass we embed them with stellar sources as described in Section 4.1.1. Then, the black hole mass is set as \(10^{-4}\) times the stellar mass. RT is performed using this hybrid SED, i.e. a superposition of power-law-type mini-QSO SED and blackbody spectrum normalized according to the criterion in the previous sections. The results of ionization and heating are presented below.

### 4.3.2 Results: hybrid model

The hybrid model proposed does have large amounts of high-energy X-ray photons from mini-QSOS that influence the temperature and ionization of the IGM prior to full reionization. The X-ray photons have larger mean-free paths than their UV counterparts, and their secondary electrons have significant influence on the thermal and ionization balance. The UV photons on the other hand are efficient at keeping the IGM in the vicinity of the halo highly ionized. For the redshifts 10, 8, 7 and 6 we plot the ionization due to the hybrid model in Fig. 7 and the ionized fraction at these redshifts are 0.01, 0.38, 0.86 and 0.995, respectively.

For this hybrid model the number of UV photons was not high enough to ionize the Universe completely by redshift 6 (the ionized fraction reaches 0.95). Full reionization thus could be achieved either by increasing the mass of the black hole and/or by changing the ratio between the black hole and stellar masses.

The hybrid model considered here yielded \(T_k\), \(T_s\) and \(\delta T_b\) as in Figs 8, 9 and 10, respectively.

The hybrid model produces heating patterns that interpolate between the results for the previous two cases and thus is qualitatively different (Fig. 8). The power-law components take over the role of heating an extended region and the stellar component maintains a very high temperature in the central parts.

The spin temperature (Fig. 9) again shows the characteristic ring-like structure around the source. The amount of secondary Ly\(\alpha\) radiation produced due to the mini-QSO results in an efficient coupling of the spin temperature and the kinetic temperature.

The brightness temperature for the hybrid model is plotted in Fig. 10. The secondary \(J_{\nu}\) produced due to the power-law component efficiently couples the high ambient \(T_k\) of the IGM to \(T_s\) and this...
4.4 Reionization histories: a comparison

In this section, we compare the reionization histories for the three scenarios explored above. To create a contiguous observational cube or ‘frequency cube’ (right ascension (RA) × declination (Dec.) × redshift), we adopt the procedure described in Thomas et al. (2009). The procedure involves the stacking of RA and Dec. slices, taken from individual snapshots at different redshifts (or frequency), interpolated smoothly to create a reionization history. This data cube is then convolved with the point spread function (PSF) of the LOFAR telescope to simulate the mock data cube of the redshifted 21-cm signal as seen by LOFAR. For further details on creating this cube refer to Thomas et al. (2009).

As expected the signatures (both visually and in the rms) of the three scenarios (Fig. 11) are markedly different. In the mini-QSO-only scenario, reionization proceeds extremely quickly and the Universe is almost completely ($\langle x_{\text{H}II} \rangle = 0.95$) reionized by around redshift 7. Reionization ends at redshift 6 in the case of stars as the only source of radiation. Also in this case, compared to the previous one, reionization proceeds in a rather gradual manner. The hybrid model, as explained previously, interpolates between the previous two scenarios.

The $\delta T_b$ in Fig. 11 is calculated based on the effectiveness of $J_o$, produced by the source, to decouple the CMB temperature ($T_{\text{CMB}}$) from the spin temperature ($T_s$). This flux, both in spatial extent and in amplitude, is obviously much larger in the case of mini-QSOs compared to that of stars resulting in a markedly higher brightness temperatures in both the mini-QSO-only and hybrid models when compared to that of the stars. However, we know that stars themselves produce Ly$\alpha$ radiation in their spectrum. Apart from providing sufficient Ly$\alpha$ flux to their immediate
surrounding, this radiation builds up, as the Universe evolves, into a strong background $J_0$ (Ciardi & Madau 2003), potentially filling the Universe with sufficient Lyα photons to couple the spin temperature to the kinetic temperature everywhere. Thus, we plot in Fig. 12 the same set of reionization histories as in Fig. 11 but now assuming that $T_s$ coupled to $T_k$. Clearly, the ‘cold’ regions in the Universe show up as regions with large negative brightness temperature. This assumption though is not strictly applicable towards the beginning of reionization. In Section 5, we quantify the differences in the brightness temperature evolution when this assumption is made.

It has to be noted that the results we are discussing here are extremely model dependent and any changes to the parameters can influence the results significantly. This on the other is the demonstration of the capability and the need for a ‘BEARS-like’ algorithm to span the enormous parameter space of the astrophysical unknowns in reionization studies.

4.5 Looking through LOFAR

To test the feasibility of 21-cm telescopes (specifically LOFAR) in distinguishing observational signatures of different sources of reionization, we need to propagate the cosmological 21-cm maps generated in Section 4.4 using LOFAR’s telescope response. The PSF of the LOFAR array was constructed according to the latest configuration of the antenna layouts for the LOFAR-EoR experiment.

The LOFAR telescope will consist of up to 48 stations in The Netherlands of which approximately 22 will be located in the core region (Labropoulos et al. 2009). The core marks an area of $1.7 \times 2.3$ km and is essentially the most important part of the telescope for an EoR experiment. The core station consists of two sets of antennas, the Low Band (LBA; 30–90 MHz) and the High Band Antenna (HBA; 110–240 MHz). The HBA in the core stations is further split into two ‘half-stations’ of half the collecting area (35-m diameter), separated by $\approx 130$ m. This split further improves the uv-coverage. For details on the antenna layout and the synthesis of the antenna beam pattern refer to upcoming paper by Labropoulos et al. (2009).

In its current configuration, the resolution of the LOFAR core is expected to be around 3 arcmin. Thus, as an example at redshift 10, all scales below $\approx 800$ kpc will be filtered out. Fig. 13 shows this effect for the reionization histories corresponding to Fig. 11. The corresponding changes in the rms of the brightness temperature are also plotted. We see that, although smoothed to a large extent, there still exists qualitative differences between the different scenarios. This of course is a reflection of the vastly contrasting models of reionization compared in this paper, and difference will disappear if the models investigated are more similar to each another.

5 STATISTICAL ANALYSIS OF THE SIMULATIONS

The previous section provided a qualitative description of the differences in the 21-cm $\delta T_b$ fluctuations for two cases i.e. with and without the assumption that $T_s = T_k$. In this section, a number of statistical tests are performed to quantify these differences. For this purpose, we focus on the scenario with the mini-QSOs. This exercise can be repeated for the other two scenarios as well.

First, Fig. 14 shows the 3D power spectra of $\delta T_b$ at redshifts 12, 10, 8 and 6. In our model, reionization begins at around redshift 12.7
and thus $z = 12$ can be considered the onset of reionization. The dashed curve reflects the assumption that $T_s = T_k$ while the solid curve takes into account the evolution of $T_s$ self-consistently. At the initial stages of reionization, only regions at close proximity to the source have been ionized and heated, and the volume filling by ‘spheres of ionization’ has just begun, leaving large portions of the Universe neutral and cooler than the CMB. Here, we assume that after the epoch of recombination the Universe cools adiabatically, i.e. $T_k \propto 1/(1 + z)^2$ and $T_{\text{CMB}} \propto 1/(1 + z)$, which results in $T_k \ll T_{\text{CMB}}$ at the onset of reionization. Thus, we have a situation in which $T_s = T_k$, with $T_k \ll T_{\text{CMB}}$, resulting in an artificial decoupling of $T_s$ and $T_{\text{CMB}}$, and is manifested as increased 21-cm power. The discrepancy quickly (by $z = 10$) disappears as the ‘spheres of Ly$\alpha$’ overlap to volume fill the simulation box and hence increase the $T_s$–$T_k$ coupling efficiency. Therefore, in our model, it is safe to make the assumption that $T_s$ follows $T_k$ after about $z = 10$.

From equation (6) it follows that $\delta T_s$ attains large negative values when two conditions are satisfied, $T_s \ll T_{\text{CMB}}$ and a high neutral hydrogen overdensity. We therefore plot the mean, minimum and maximum values of $\delta T_s$ as a function of redshift in Fig. 15. As expected, the mean and minimum values of $\delta T_s$ are much lower for the case in which the spin temperature has been set to the kinetic temperature, because the Universe has cooled substantially below the CMB and coupling $T_k$ everywhere in the Universe to $T_s$ enforces the conditions required for large negative $\delta T_s$ as stated above. The maximum positive values though do not differ because a positive $\delta T_s$ indicates that $T_s > T_{\text{CMB}}$ and hence has to be heated by the radiating source. In regions where the source has heated the IGM, the presence of Ly$\alpha$ flux and collisional coupling almost always guarantees the coupling of $T_s$ to $T_k$ anyway.

As another simple diagnostic of the efficiency of $T_s$–$T_k$ coupling we plot (i) the differential temperature, i.e. $1 - T_{\text{CMB}}/T_s$, (ii) their ratio, $T_k/T_s$, as a function of redshift (Fig. 16). Note here that if the spin temperature was artificially set to the kinetic temperature, the differential temperature would be saturated at unity. But the coupling ensures that the spin temperature remains below that of the CMB till about a redshift of 10. Although significantly different at the early phases of reionization, in the model we have assumed, $T_s$ catches up with $T_k$ at a redshift of about 8, when the coupling due to Ly$\alpha$ and collisions become significant enough to tie $T_s$ to the local $T_k$.

As an alternative probe to investigate the influence of Ly$\alpha$ coupling, in Fig. 17 we plot the power spectra, now of the kinetic (solid line) and the spin (dashed line) temperatures at four different redshifts. There are a few interesting attributes to this figure. First we see that at all scales $T_s$ is considerably lower than $T_k$ at the onset of reionization ($z \approx 12$). This scenario changes rapidly as $T_s$ approaches $T_k$. Note that it is only towards the end of reionization ($z = 6$) that $T_s$ is identical to $T_k$ at all scales. The peculiarity observed is that all scales in $T_s$ do not approach $T_k$ simultaneously. As seen from the top two panels of the figure at $z = 10$ and $z = 8$, $T_s$ approaches $T_k$ at large scales (small $k$ values), and then subsequently at small scales towards the end of reionization. This is because the central parts of the ionized bubble around the source was highly ionized and because $J_\alpha \propto x_{\text{H}_2}$, the spin temperature obtains extremely low values. Now, as you go further away from the source, the IGM becomes neutral, but $J_\alpha$ from the source and the secondary Ly$\alpha$ photons are high enough to couple the spin temperature to the kinetic temperature. Thus, the large scales (large volumes outside the ionized bubble) get ‘matched’ first followed by the small scales, when the IGM is hot and collisions become important.
Figure 14. The 3D power spectra of $\delta T_b$ at four different redshifts (as indicated on the panels) are plotted. The solid curves indicate the power spectra resulting from the self-consistent inclusion of $T_s$ and the dashed curve, under the assumption $T_s = T_k$. At the onset of reionization, $z \approx 12$ in our model, $\delta T_b$ is larger at all scales under this assumption because we have enforced, in effect, an artificial decoupling of $T_s$ from $T_{\text{CMB}}$ in regions of the simulated Universe where $T_k \ll T_{\text{CMB}}$. But by redshift 10 the power spectra match exactly as the Ly$\alpha$ becomes efficient everywhere in the box to couple $T_s$ to $T_k$. Note that the power keeps dropping as $x_{\text{HI}} \to 0$ and Universe gets reionized at lower redshifts.

5.1 Comparison to similar work

Here, we briefly compare the output of our simulation with that of Santos et al. (2008), wherein a semi-analytical scheme is developed to look at ionization and heating during the EoR. Fig. 18 shows the comparison between our simulations which has now been performed for the case of a power-law source starting at 100eV to facilitate a balanced comparison with the 100 eV case of Santos et al. (2008). Plotted in this figure are the average gas temperature (solid line and crosses) and volume filling factor of X-ray radiation (dashed line and filled hexagons). The lines correspond to our simulation and points to Santos et al. (2008). Their case with the normalization factor $f_x = 10$, and photon energies of 100.0 eV, shows similar trends. Because we start reionization a bit later ($z = 12$) the temperature is a bit lower initially.

Their model is qualitatively different because the X-ray emissivity is tied to their star formation rate. Otherwise, the manner in which heating is implemented is similar to the one described in our case albeit without terms involving Compton heating/cooling. These effects though are important towards the central regions of the source (Thomas & Zaroubi 2008).

6 CONCLUSIONS AND OUTLOOK

The focus of this paper was threefold: (1) to introduce an extension to BEARS in order to incorporate heating (including X-ray heating) and discuss its application to two cases of reionization and heating, i.e. for blackbody (stellar) and power-law (mini-QSO) type sources, (2) to monitor the evolution of spin temperature ($T_s$) self-consistently and contrast its influence against the usual assumption made in most reionization simulation that $T_s \gg T_{\text{CMB}}$ and (3) to use the extended BEARS code to study reionization due to a hybrid population of stars and mini-QSOs as reionizing sources.

Santos et al. (2008) normalized their spectrum assuming a total integrated power density to be $3.4 \times 10^{40} f_x$ erg s$^{-1}$ Mpc$^{-3}$.
At four different redshifts are plotted the power spectra of the kinetic temperature (solid) and the spin temperature (dashed) within the simulation box. Note how the $T_k$ is considerably lower than the $T_b$ initially and then merges with $T_k$ as reionization proceeds. Refer text for more details.

Figure 18. Plotted here are the evolution of the gas temperature $T_k$ (solid line) and the volume filling factor (dashed line) of the X-ray radiation as a function of redshift for the case of the mini-QSOs. For comparison, points from Santos et al. (2008) are shown for $T_k$ (crosses) and filling factor (filled hexagons) with their case of $T_k = 10$ and photon energies 100.0 eV.

To incorporate heating into BEARS, we embedded spheres of ‘kinetic temperature’ around the sources of radiation, much like in the algorithm used to obtain the ionized fraction (Thomas et al. 2009). The BEARS algorithm implemented is extremely fast, in that it takes $\approx 5\ h\ (2\ GHz,\ 16\ core,\ 32\ GB\ shared\ RAM)$ to perform the RT (including heating) on about 35 different boxes ($512^3$ and $100\ h^{-1}\ comoving\ Mpc$) between redshifts 12 and 6. These snapshots are interpolated between redshifts to produce a contiguous data cube spanning redshifts $z \approx 6$–12, i.e. the observational range of the LOFAR-EoR experiment. The efficiency of the code facilitates the simulation of many different scenarios of reionization and test their observational signatures. Apart from predicting the nature of the underlying cosmological signal, these simulations can be used in conjunction with other probes of reionization to enhance the detectability and/or constrain parameters concerning reionization. In Jelic et al. (2010), these simulations were cross-correlated with the simulations of the CMB anisotropy (mainly the kinetic and thermal Sunyaev-Zeldovich effect) to probe reionization. In the same paper, Jelic et al. repeated the same exercise by using reionization simulations from Mellema et al. (2006) and found similar results, further emphasizing the validity of the approximate manner in which we solve the evolution of the kinetic temperature in our simulations.

The improved BEARS code was used to simulate three distinct reionization scenarios, i.e. mini-QSOs, stellar and a mixture of both. These simulations further emphasized that mini-QSOs were not only very efficient in increasing $T_k$ of the IGM but the secondary Ly$\alpha$ flux produced by these sources was enough to drive $T_k$ away from $T_{CMB}$ in an extended region around the source thereby rendering the IGM around the source ‘bright’ in $\delta T_b$. This implies, if a mini-QSO hosting a black hole in the mass range $>10^7\ M_\odot$ is within the observing window of LOFAR, the value of $\delta T_b$ and its spatial extent would be conducive to a possible detection. The code was also applied to simulate reionization with a hybrid population of stars and mini-QSOs. Every DM halo was embedded with both a quasar and a stellar component. The relation between the two was set according to the ‘Magorrian relation’ we observe today. The total mass in quasars was constrained following black hole mass density estimates by Volonteri et al. (2008). The effect of the hybrid population on the IGM was an interpolation between the scenarios of stars and mini-QSOs, i.e. although the heating (and ionization) was not as extended as in the case of mini-QSOs, it was definitely larger than that for stars.

Our ultimate goal is to simulate mock data sets for the LOFAR-EoR experiment. Towards this end, reionization simulations performed on 35 different snapshots between redshifts 6 and 12 were combined to form ‘frequency cubes’ (reionization histories; Thomas et al. 2009) for all three scenarios, i.e. stars, mini-QSOs and the hybrid case. To fold-in the effect of the instrument we smoothed these frequency cubes according to the LOFAR beam-scale. Notwithstanding the convolution by the LOFAR beam, stark differences between the scenarios clearly persist. The rms $\delta T_b$ clearly shows this difference between scenarios.

All three scenarios of reionization discussed above were performed for two different cases: (i) assuming that $T_k$ is always coupled to $T_k$ and (ii) following the evolution of $T_k$ self-consistently in the simulation. Figs 11 and 12 reflect the differences between the two cases. To further quantify the influence of the self-consistent evolution of $T_b$, especially at the beginning of reionization, a suite of statistical analyses was performed. First, the 3D power spectra of $\delta T_b$, (Fig. 14) for the two cases was calculated at four redshifts (12, 10, 8 and 6). We see that although there is a considerable difference at the onset ($z = 12$) of reionization, the power spectra of the brightness temperature match-up by a redshift of 8. This is attributed to the filling volume nature of the spin-temperature coupling induced by mini-QSOs. The minimum, maximum and mean values of $\delta T_b$ as a function of redshift reveal similar differences between the two cases. The maximum value of $\delta T_b$ is the same in both cases because...
regions where the IGM is considerably heated also correspond to regions with a large supply of Ly\textalpha\ photons and they are also regions where collisional coupling is effective. The minimum and average values reveal a difference since under the assumption that $T_s = T_i$, regions much below $T_{\text{CMB}}$ are artificially coupled to $T_c$. As a final statistic we compute the 3D power spectra of $T_s$ and $T_c$ and compare them (Fig. 17). Vast differences do exist between the two almost till the end of reionization, when they become identical. An interesting result of this comparison is that the large scales of the two spectra get matched before the small scales in the box. The interpretation of this behaviour is given in Section 5. We also compared our results to that of Santos et al. (2008) and found good match for the evolution of gas temperature and the volume filling factor of X-ray radiation.

In the near future calibration errors expected from a LOFAR-EoR observational run will be added to these simulations along with the effects of the ionosphere and expected radio frequency interference (RFI). Subsequently, Galactic and extra-galactic foregrounds modelled as in Jelić et al. (2008) will be merged with these simulations to create the final ‘realistic’ data cube. These data cubes will be processed using the LOFAR signal extraction and calibration schemes being developed to retrieve the underlying cosmological signal in preparation for the actual LOFAR-EoR experiment which has already begun.

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