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COSMIC REIONIZATION ON COMPUTERS. MEAN AND FLUCTUATING REDSHIFTED 21 cm SIGNAL

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ABSTRACT

We explore the mean and fluctuating redshifted 21 cm signal in numerical simulations from the Cosmic Reionization On Computers project. We find that the mean signal varies between about ±25 mK. Most significantly, we find that the negative pre-reionization dip at z ~ 10–15 only extends to ~25 mK, requiring substantially higher sensitivity from global signal experiments that operate in this redshift range (EDGES-II, LEDA, SCI-HI, and DARE) than has often been assumed previously. We also explore the role of dense substructure (filaments and embedded galaxies) in the formation of the 21 cm power spectrum. We find that by neglecting a neutral substructure inside ionized bubbles, the power spectrum can be misestimated by 25–50% at scales k ~ 0.1–1 h Mpc^{-1}. This scale range is of particular interest, because the upcoming 21 cm experiments (Murchison Widefield Array, Precision Array for Probing the Epoch of Reionization, Hydrogen Epoch of Reionization Array) are expected to be most sensitive within it.

Key words: cosmology: theory – intergalactic medium – methods: numerical

1. INTRODUCTION

The redshifted 21 cm signal from the epoch of reionization has been considered as an extremely powerful but highly futuristic probe of the spatial distribution of neutral hydrogen in the intergalactic medium (IGM) for a long time. Commonly, the redshifted 21 cm signal is split into a global (or mean) signal averaged over the whole sky ⟨ΔT⟩ and the fluctuating component; the latter can be characterized by the power spectrum P_k or by some other statistical technique (and, eventually, with direct imaging). Observations of these two components rely on very different instrumental techniques and can be treated as effectively two different (but related) observational probes of cosmic reionization.

The time may be approaching, however, when the actual signal is finally detected: recent constraints from the Murchison Widefield Array (Dillon et al. 2014, 2015) and Donald C. Backer Precision Array for Probing the Epoch of Reionization (Parsons et al. 2014; Ali et al. 2015; Jacobs et al. 2015; Pober et al. 2015) are steadily edging toward the predicted cosmological signal. While no detection has been made so far, the current progress was deemed sufficient by NSF to start funding the next-generation experiment, Hydrogen Epoch of Reionization Array, that is expected to achieve a robust detection before the end of this decade (Pober et al. 2014).

While the observational detection remained distant, simple analytical and semi-numerical techniques were sufficient for modeling the cosmological signal theoretically, and for making an order-of-magnitude estimate of the expected signal. An excellent recent review of these methods is given by Pritchard & Loeb (2012), so we mention only two of them: a widely cited prediction of the mean signal by Pritchard & Loeb (2008) and a publicly available code 21CMFAST (Mesinger et al. 2011) for making maps of the fluctuating 21 cm signal.

As the whole field matures and the detection of the cosmological signal appears to become increasingly likely, it is important to continuously refine and improve theoretical modeling, making sure that all crucial physical processes are adequately included. The recognition of this need resulted in a field-wide effort to develop “next generation” modeling capabilities, both with full cosmological numerical simulations and with advanced semi-numerical techniques. Projects like “DRAGONS” (Duffy et al. 2014), “Renaissance Simulations” (O’Shea et al. 2015), “Cosmic Dawn” (Ocvirk et al. 2015), and “Emma” (Aubert et al. 2015) form a certainly incomplete list.

In this paper, we rely on numerical simulations from the Cosmic Reionization On Computers (CROC) project (Gnedin 2014; Gnedin & Kaurow 2014) as our theoretical model. Of course, for a given simulation to serve as a test of a simple model, the physical realism of the simulation should be sufficiently high. CROC simulations are useful in this regard, since they include most of the physical effects thought to be important for modeling cosmic reionization (such as star formation and feedback, spatially inhomogeneous and time-dependent radiative transfer, non-equilibrium, radiation-field-dependent ionization and cooling, etc.) in a fully coupled manner, in simulation volumes exceeding 100 comoving Mpc in size and with proper spatial resolution approaching 100 pc.

Another useful feature of CROC simulations is the availability of simulation boxes of various sizes and resolutions, which allows one to test the dependence of physical predictions from the simulations on these numerical parameters.

In this paper we model redshifted 21 cm emission with two sets of simulations: a set of three 40 h^{-1} Mpc runs labeled as B40.sf1.uv2.2w10 in Gnedin (2014) and a single new 80 h^{-1} Mpc simulation (B80.sf1.uv15.2w10). In each simulation volume, we compute a 1024^3 2D × 1D (sky × frequency) grid of 21 cm brightness temperature at each simulation snapshot, accounting for all relevant physical effects (coupling of kinetic and spin temperatures by Lyα radiation and collisions with electrons and neutral atoms, redshift space distortions, line cone effects, etc.); since CROC simulations include full 3D radiative transfer at native resolution, we have access to the full spatially and temporally resolved radiation spectrum at each simulation location. We then use the gridded values to compute various observational quantities, like the mean signal and the power spectrum.
2. MEAN 21 cm SIGNAL

The mean, or "global," 21 cm signal in CROC simulations is shown in Figure 1. Our results are reasonably consistent in boxes of various sizes, although variations between sets of simulations of the order of 5 mK remain, which should be considered as an estimate of our theoretical error. These predictions are substantially different from the most widely used model of Pritchard & Loeb (2008, see also Pritchard & Loeb 2012). Most significantly, the negative pre-reionization dip at \( z \sim 10-15 \) only reaches down to \( \Delta T_B \approx -25 \) mK, rather than \(-100\) mK as predicted by Pritchard & Loeb (2008).

Following the notation of Pritchard & Loeb (2008), we can derive the parameters \( f_s \) and \( f_x \) that correspond to the production efficiency of \( \text{Ly}\alpha \) photons and X-rays per baryon in stars (see Pritchard & Loeb 2008 for the details). In our fiducial model the values are 1 and 9 respectively.

In fact, earlier simulations of Gnedin & Shaver (2004) found a similarly low value for the dip, and interpreted the difference from (a similar earlier work to) Pritchard & Loeb (2012) as a new and dominant mechanism of heating cosmic gas before a sufficient \( \text{Ly}\alpha \) background is built up: shock heating by small-scale structure. They showed that without shock heating (or, more precisely, with the \( P_{dV} \) term in the energy balance equation artificially switched off) the pre-reionization dip indeed extends to \( \Delta T_B \sim -100 \) mK, in agreement Pritchard & Loeb (2008). That claim was challenged by McQuinn & O’Leary (2012), who showed that shock heating due to structure formation caused only a small amount of heating. However, their simulation boxes (0.2 \( h^{-1} \) Mpc and 0.5 \( h^{-1} \) Mpc) were far too small to account for the bulk of power in the velocity field (which, for Planck cosmology, peaks at a scale of about \( 80 \) \( h^{-1} \) Mpc), and hence are not guaranteed to be representative of the mean universe.

Our full simulation results are consistent with Gnedin & Shaver (2004), so their actual results are confirmed; however, their interpretation can and should be challenged. To that end, we repeated and extended the tests performed by Gnedin & Shaver (2004). Such an extensive parameter study would be unfeasible for any except our smallest, 20 \( h^{-1} \) Mpc boxes, and only for one simulation rather than all six. Therefore, we selected one realization (box A) that has its mean signal most closely matched to the average over all six boxes, and ran several modifications of that simulation with varied physical assumptions. The results of such exploration are shown in Figure 2.

The single physical component with the largest effect on the pre-reionization dip is the intensity of cosmic \( \text{Ly}\alpha \) background: setting it to zero removes any mean signal altogether (we do not show such a line, since it would be trivial), while increasing it 10-fold deepens the dip to the values (\(-100\) mK) quoted by Pritchard & Loeb (2008). Removing X-rays (all radiation above 4 Rydberg units) extends the dip by almost a factor of 2, while excluding in addition the \( P_{dV} \) term from the energy equation makes only a modest further increase in the depth of the dip. Hence, we do not confirm the claim made by Gnedin & Shaver (2004) about the dominance of the \( P_{dV} \) term, although their claim is not completely wrong (just quantitatively off by a factor of 2–3), since the \( P_{dV} \) term does matter somewhat.

There are many causes that can produce such a discrepancy, from different models of cosmology and star formation/feedback to the lower quality of the numerical hydrodynamic scheme used by Gnedin & Shaver (2004); it does not seem fruitful to explore this discrepancy further since CROC simulations are far superior to those of Gnedin & Shaver (2004) in any imaginable respect.

Conversely, increasing the strength of the X-ray emission from our modeled stars (which is dominated by Wolf–Rayet stars, and hence may be deemed somewhat uncertain) by a factor of 10 substantially reduces the depth of the dip, and pumping the X-ray emission by a factor of 100 erases the dip altogether. Thus, we also confirm the conclusions of Pritchard & Loeb (2008), who emphasized the critical role of the interplay between the X-ray heating of the gas and the \( \text{Ly}\alpha \) coupling between the gas temperature and the cosmic microwave background. The large difference between our prediction for the depth of the dip (\(-25\) mK) and the value of \(-100\) mK quoted by Pritchard & Loeb (2008) is in the assumptions about the strengths of these two contributions. Naturally, we would like to think that our results are more realistic, since CROC simulations treat all relevant physical
processes in a “self-consistent” manner, in a sense that the full spectral shape of stellar radiation, from UV to X-rays, is taken from Starburst99 models (Leitherer et al. 1999), and therefore the relationships between Lyα, ionizing, and X-ray backgrounds are as realistic as Starburst99 models are. Since CROC simulations match essentially all existing observational constraints on reionization, including observed UV luminosity functions of galaxies at all redshifts \( z \gtrsim 6 \), they reproduce correct star formation histories of individual galactic halos. They thus provide a complete model of the reionization process, and our results cannot be adjusted or tuned to modify the depth of the dip by more than a modest amount allowed by the current uncertainties on various observational constraints.

Of course, no model is complete, and some of the physical processes that CROC simulations do not include may provide important contributions to X-ray or Lyα backgrounds. Unfortunately, most plausible enhancements to our models, such as X-rays from stellar binaries or miniquasars, would only reduce the depth of the pre-reionization dip even further. The only reasonable possibility to increase the depth would be if Starburst99 models were underestimating stellar UV and Lyα emission significantly (by a factor of several). At present, though, that seems unlikely.

Our results may bring bad news to several planned global signal experiments that rely on the deep pre-reionization dip to detect the signal, such as low-frequency EDGES-II (Bowman & Rogers 2010), LEDA (Greenhill & Bernardi 2012), and SCILHI (Voytek et al. 2014), as they should aim at a sensitivity that is factor of 5 higher to be certain to detect the signal. On the other hand, for a more sensitive experiment such as DARE (Burns et al. 2012), there will be a high enough signal-to-noise ratio to clearly confirm or rule out our predictions. We also confirm the expected reionization signal of about 20 mK for global experiments that focus on the redshift range \( z < 10 \), like the high-frequency window of EDGES-II, BIGHORNs (Sokolowski et al. 2015), or SARAS (Patra et al. 2013, 2015).

Finally, we have also explored the question of the role of shock heating, in order to resolve the apparent conflict between Gnedin & Shaver (2004) and McQuinn & O’Leary (2012). Since, as we showed above, we find the contribution of the \( P_{D}V \) term to be modest, the question by itself is not particularly relevant. Nevertheless, we performed several simulations with smaller box sizes, all the way to 0.5 \( h^{-1} \) Mpc, the size of the largest boxes of McQuinn & O’Leary (2012). One challenge with such tests is that the box size is too small to be even a qualitatively representative volume, and such boxes would have very different reionization history (and boxes below a few Mpc would fail to reionize themselves at all). Thus, in order to maintain consistency, we imposed on such small boxes the Lyα background taken from our 20 \( h^{-1} \) Mpc box A. With this setup, we find negligible dependence on the box size, and hence confirm the conclusions of McQuinn & O’Leary (2012) (we do not show this in a figure because it would be trivial, all lines roughly coinciding with each other). The interpretation of Gnedin & Shaver (2004)—that the main role of the \( P_{D}V \) term is in shock heating—is therefore incorrect (shock heating would be strongly dependent on the box size, since, as we mentioned above, most of the power in the velocity field is on scales around 80 \( h^{-1} \) Mpc). Rather, the contribution of the \( P_{D}V \) term seems to be more involved, a combination of adiabatic heating/cooling in the over/underdense gas and the local variation in the strength of the Lyα background.

3. ROLE OF SUBSTRUCTURE

The dense substructure, namely filaments and galaxies embedded in them, may remain partially neutral even after the surrounding IGM is fully ionized due to the higher recombination rate (Miralda-Escudé et al. 2000). These neutral patches occupy a small volume but are very dense and hence biased; therefore, they may contribute significantly to the 21 cm power spectrum. Since the substructure is largely resolved in CROC simulations (Kaurov & Gnedin 2015), we can estimate the significance of its contribution to the 21 cm signal.

In order to test the contribution from the substructure, we spatially separate the 21 cm brightness temperature field \( \Delta T_B \) into “ionized bubbles with semi-neutral filaments” \( \Delta T_B^{\text{SUB}} \) and “neutral IGM” \( \Delta T_B^{\text{IGM}} \). For this analysis we use our largest \( 80 h^{-1} \) Mpc run. The separation is performed using the phase space for the ionization parameter that was introduced in Kaurov & Gnedin (2015), and the details are presented in Appendix A. The result of such spatial separation is shown in Figure 3. The regions colored in white are assumed to contribute zero signal.

The \( \Delta T_B^{\text{IGM}} \) field is interesting because it mimics the commonly used analytical models that do not account for the substructure. By studying the effect of adding \( \Delta T_B^{\text{SUB}} \) to \( \Delta T_B^{\text{IGM}} \), we will see how the power spectrum simulated by the analytical approach systematically diverges from the one calculated using the full numerical simulations with hydrodynamics and radiation transfer.

We directly compute the power spectrum of the 21 cm brightness temperature of each component separately. The result is plotted in Figure 4. Immediately we see that the power spectra \( \Delta T_B^{\text{SUB}} \) and \( \Delta T_B^{\text{IGM}} \) do not simply add up, because they are not independent quantities.

We can describe the discrepancy between the full power spectrum, \( P_k^{\text{TOT}} \), and the sum of the power spectra of individual components with the cross-correlation coefficient,

\[
r(k) \equiv \frac{P_k^{\text{TOT}} - P_k^{\text{IGM}} - P_k^{\text{SUB}}}{2 \sqrt{P_k^{\text{IGM}} P_k^{\text{SUB}}}}.
\]

The value of \( r(k) \) quantifies the correlation between \( \Delta T_B^{\text{SUB}} \) and \( \Delta T_B^{\text{IGM}} \) fields. A negative sign corresponds to anticorrelation. The value of \( r(k) \) is plotted in the left panel of Figure 8. In the right panel of Figure 5 we plot the ratio \( P_k^{\text{IGM}} / P_k^{\text{TOT}} \) that explicitly shows how far off \( P_k^{\text{IGM}} \) is from the true 21 cm power spectrum \( P_k^{\text{TOT}} \).

During reionization the direct contribution from the neutral substructure, \( P_k^{\text{SUB}} \), remains small compared to the IGM contribution, \( P_k^{\text{SUB}} \sim (0.05–0.2) P_k^{\text{IGM}} \). Hence, the effect of neutral substructure is entirely determined by the behavior of the correlation coefficient \( r \). When \( |r| \sim 1 \), neutral substructure contributes somewhere in the vicinity of 25%–50%.

At the highest redshifts (\( z \gtrsim 10 \), \( x_{HI} > 0.85 \)) contributions from \( \Delta T_B^{\text{IGM}} \) and \( \Delta T_B^{\text{SUB}} \) are highly correlated, because the \( \Delta T_B^{\text{IGM}} \) component closely traces the overall density field, and the \( \Delta T_B^{\text{SUB}} \) component is its biased representation. Because reionization proceeds inside out at the beginning, in time the \( \Delta T_B^{\text{IGM}} \) field becomes less and less correlated with the \( \Delta T_B^{\text{SUB}} \) field, until at \( x_{HI} \sim 0.82 \) the two fields become uncorrelated and the contribution of the \( \Delta T_B^{\text{SUB}} \) field vanishes. At later times, i.e., during most of the duration of reionization, the two
Figure 3. Spatial separation of the simulation snapshot (left panel) at redshift 8.0 ($x_{\text{HI}} = 0.82$) into a “neutral IGM” component (middle panel) and “ionized regions including semi-neutral substructure” (right panel).

Figure 4. 21 cm power spectra of separate components normalized to the power spectrum of the baryon overdensity at different global ionization fractions. Solid red curves correspond to the full observable emission; dashed green lines show the component without semi-neutral substructure in ionized regions; finally, dotted blue lines mark the semi-neutral substructure within ionized regions only.

Figure 5. Correlation coefficient $r(k)$ (left panel) and the ratio of the power spectrum for the neutral IGM component to the total power spectrum $P_{\text{IGM}}/P_{\text{TOT}}$ (right panel).
fields become strongly anticorrelated, and the contribution of the $\Delta T_B^{\text{SUB}}$ field again becomes significant (and negative), reducing the overall 21 cm power spectrum by up to 50%.

Finally, after reionization is complete at $z \sim 6$, the $\Delta T_B^{\text{SUB}}$ component becomes the only one. Overall, the $\Delta T_B^{\text{SUB}}$ component affects the 21 cm power spectrum in a non-trivial way at all redshifts and scales.

This behavior of the correlation coefficient $r$ can be understood analytically. Indeed, Furlanetto et al. (2004) derived an analytical expression for the correlation function of the quantity $\psi = \tilde{x}_{\text{HI}}(1 + \delta)$. On large scales, where the effect of peculiar velocity becomes trivial, the actual brightness temperature of 21 cm emission is $\Delta T_B \propto \psi(T_5 - T_{\text{CMB}})/T_5$, where $T_5$ is the spin temperature. The second factor may, in principle, invalidate the model of Furlanetto et al. (2004); however, as we show in Appendix B, that factor is not important as soon as $\tilde{x}_{\text{HI}}$ deviates even slightly from unity, so the approximation $\Delta T_B \propto \psi$ is a very good one.

In that approximation Furlanetto et al. (2004) show that the correlation function for the $\Delta T_B^{\text{IGM}}$ component is (their Equation (11))

$$\xi_\psi = \xi_{xx} (1 + \xi_{\delta\delta}) + \bar{x}_{\text{HI}}^2 \xi_{\delta\delta} + \xi_{xx} (2\bar{x}_{\text{HI}} + \xi_{\delta\delta}),$$

where $\xi_{xx} = \langle x_{\text{HI}}(1)x_{\text{HI}}(2) \rangle - \bar{x}_{\text{HI}}^2$ is the autocorrelation function of the neutral hydrogen fraction, $\xi_{\delta\delta}$ is the autocorrelation function of density, and $\xi_{\delta\delta}$ is their cross-correlation. On large scales, where the correlation function is small, this equation can be simplified by retaining only terms that are linear in $\xi$,

$$\xi_\psi = \xi_{xx} + \bar{x}_{\text{HI}}^2 \xi_{\delta\delta} + 2\bar{x}_{\text{HI}} \xi_{\delta\delta}. \quad (2)$$

With our definitions, we identify $\xi_\psi$ with $\xi_{\text{IGM}}$. Including neutral substructure is equivalent (on large scales) to adding a biased density tracer to $\psi$,

$$\psi = x_{\text{HI}}(1 + \delta) + b_f f_{\text{HI}}(1 + \delta),$$

where $b_f$ is the filament bias factor and $f_{\text{HI}} \ll 1$ is the fraction of neutral hydrogen remaining neutral within the ionized bubbles. With this definition for $\psi$, the total correlation function of neutral hydrogen becomes

$$\xi_{\text{TOT}} = \xi_{xx} + 2b_f f_{\text{HI}} \xi_{\delta\delta} + b_f^2 f_{\text{HI}}^2 \xi_{\delta\delta} + \bar{x}_{\text{HI}}^2 \xi_{\delta\delta} + 2\bar{x}_{\text{HI}} (\xi_{\delta\delta} + b_f f_{\text{HI}} \xi_{\delta\delta}). \quad (3)$$

With $\xi_{\text{SUB}} = b_f^2 f_{\text{HI}}^2 \xi_{\delta\delta}$, we find

$$\xi_{\text{TOT}} - \xi_{\text{IGM}} - \xi_{\text{SUB}} = 2b_f f_{\text{HI}} (\xi_{\delta\delta} + \bar{x}_{\text{HI}} \xi_{\delta\delta}).$$

Under the assumption that each halo of mass $M$ drives an ionized bubble of volume $V(M)$ around it, Furlanetto et al. (2004) derived an expressions for $\xi_{\delta\delta} = -\bar{x}_{\text{HI}} b_h b_f Q \xi_{\delta\delta}$, where $b_h = \int dM b(M) dn/dM$ is the average halo bias, $b_f = Q^{-1} \int dM b(M) V(M) dn/dM$ is the halo bias weighted by bubble volume, and $Q = \int dM V(M) dn/dM$ is the porosity of the IGM.

It is not possible to derive an expression for $\xi_{xx}$ in a closed form, but from the Schwartz inequality it can be written as $\xi_{xx} = w b_h^2 b_f^2 b_f^2 Q^2 \xi_{\delta\delta}$, where $w \geq 1$. With these expressions we find

$$\xi_{\text{TOT}} - \xi_{\text{IGM}} - \xi_{\text{SUB}} = 2b_f f_{\text{HI}} \bar{x}_{\text{HI}} \xi_{\delta\delta} (1 - b_h b_f Q)$$

and

$$r = \frac{2b_f f_{\text{HI}} \bar{x}_{\text{HI}} \xi_{\delta\delta} (1 - b_h b_f Q)}{2(\bar{x}_{\text{IGM}} \xi_{\text{SUB}})^{1/2}} = \left(1 - b_h b_f Q \right)^{1/2} \left(1 + w b_h b_f^2 Q^2 - 2b_h b_f Q \right)^{1/2}. \quad (4)$$

This expression for $r$ has the correct limiting behavior: $r \rightarrow 1$ for $Q \rightarrow 0$, $r$ changes sign at $\bar{x}_{\text{HI}} \approx Q = 1/(b_h b_f) \approx 0.82$ if $b_h b_f \approx 5.5$, which is a very reasonable value, and $r \rightarrow -1$ for $Q \rightarrow \infty$, if the fudge factor $w$ goes to 1 in that limit.

## 4. CONCLUSIONS

In this study we check two commonly used (semi-)analytical approximations for modeling redshifted 21 cm emission against the fully self-consistent numerical simulations. We highlight two effects that are important for analyzing observational data or generating mock data for the present and future 21 cm experiments.

First, we show that the global 21 cm signal is limited to within a range of $\pm (20-25)$ mK, in agreement with previous simulation studies (Gnedin & Shaver 2004) and in apparent disagreement with the analytical prediction of Pritchard & Loeb (2008). That disagreement, however, is not substantive, but merely due to different assumptions about the relative strengths of the X-ray and Lyα backgrounds. We expect our results, as based on fully self-consistent and observationally consistent modeling of the whole process of cosmic reionization, to be more accurate. This conclusion implies that observational efforts aimed at detecting the pre-reionization negative dip in the global signal will need to reach a sensitivity that is a factor of 4 to 5 higher than is currently planned.

Second, we show that the signal from neutral hydrogen remaining in galaxies and filaments within ionized regions of the IGM should not be neglected. Even though this substructure gives a negligible contribution to the global 21 cm signal throughout the epoch of reionization, it changes the 21 cm power spectrum by 25%–50% at scales $k \sim 0.1-1$ h Mpc$^{-1}$. This range of scales is expected to be the most foreground-free in the observations (Datta et al. 2010; Trott et al. 2012; Dillon et al. 2014; Pober et al. 2014). However, it is unlikely that the first measurements will be capable of determining the shape of the power spectrum with very high accuracy. Therefore, the first measurements is likely to be limited to the overall amplitude of the 21 cm signal only. The amplitude mostly depends on the heating mechanism, discussed in the first part of the paper, and also, as we show in the second part of the paper, on the often neglected substructure. Hence, models that do not intrinsically account for the neutral substructure due to their limited resolution or adopted approximations need either to add semi-neutral filaments explicitly in their modeled volumes or to include corrections to the predicted 21 cm power spectrum in post-processing.

However, other physical and numerical effects may influence theoretical predictions by much larger factors. In order to illustrate that, we compare in Figure 6 our predictions for the 21 cm power spectrum with the previous result from Lidz et al. (2008), which is widely used as a target signal by experimental
groups (Bowman et al. 2013; Ali et al. 2015). For $x_{\text{HI}} < 0.5$ the power at $k \sim 0.1 h \text{Mpc}^{-1}$ in our run is about five times lower. One potential reason for the discrepancy is purely numerical—our largest box size is only $80 h^{-1} \text{Mpc}$, whereas Lidz et al. (2008) used a box of $130 h^{-1} \text{Mpc}$. In order to test the effect of the box size, we also show in Figure 6 a blue band that encompasses $2\sigma$ scatter estimated from three independent realizations of a $40 h^{-1} \text{Mpc}$ box. The box size seems to matter little for our simulations, but since we are not yet able to reach the $130 h^{-1} \text{Mpc}$ scale, a purely numerical source of the discrepancy can not yet be excluded.

Another potential source of the difference is actually physical: the modeled physics is very different in our simulations and in Lidz et al. (2008). In particular, CROC simulations fully account for the limited photon mean free path due to Lyman Limit systems, while the models of Lidz et al. (2008) allow photons to extend to arbitrarily large distance. A limited photon mean free path may also limit the sizes of the largest bubbles (although the connection between the photon mean free path and the bubble size is not that direct, since bubbles around individual sources are clustered). The actual value of the mean free path due to Lyman Limit systems in the CROC simulations is taken from Songaila & Cowie (2010) and is also shown in Figure 6. It is in the same range as the scales on which our results deviate significantly from Lidz et al. (2008), but whether this is indeed a reason for the discrepancy or just a coincidence cannot, of course, be deduced from Figure 6 alone, and would require a much more comprehensive and involved investigation, which goes well beyond the scope of this paper.

It thus appears that theoretical predictions for the $21 \text{cm}$ power spectrum still differ by factors as large as 5 even at the same $x_{\text{HI}}$ (and would differ even more at the same redshift, due to variations in the reionization history). Obviously, theorists still have some work to do before one can analyze and interpret any future observational measurement.

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APPENDIX A

SPATIAL CLASSIFICATION OF REGIONS

The “ionization state indicator” $\kappa$ is defined as

$$\kappa = (1 + \delta) \frac{x_{\text{HI}}}{\bar{x}_{\text{HI}}}, \quad (5)$$
Figure 8. Correlation coefficient $r$ (Equation (1)) as a function of the wavenumber $k$ and redshift for the actual brightness temperature $\Delta T_B$ (left panel—identical to the left panel of Figure 5) and for the approximate quantity $\psi = x_{\text{HI}}(1 + \delta)$, commonly used in analytical models (right panel). The approximate quantity $\psi$ provides a very good approximation to the actual brightness temperature.

and its properties are described in detail in Kaurov & Gnedin (2015). In Figure 7 the phase space diagram is plotted, along with the dashed line that is used to distinguish between ionized bubbles with embedded semi-neutral substructure ($\Delta T_B^{\text{SUB}}$) and yet-to-be-ionized IGM ($\Delta T_B^{\text{IGM}}$). Here we had a choice to assign ionized voids to either $\Delta T_B^{\text{IGM}}$ or $\Delta T_B^{\text{SUB}}$. Since the contribution from the ionized voids is minimal (they are more than 99.9% ionized and underdense), it is not important whether they belong to one or the other. Therefore, we assign them to $\Delta T_B^{\text{SUB}}$ for simplicity.

In this paper we use downsampled snapshots of our simulations, rebinned into a $1024^2 \times 2D$ (sky and frequency) grid; therefore, the information about the finest structure (galaxies and filaments) is degraded. That is why the phase plot in Figure 7 looks less detailed than those shown in Kaurov & Gnedin (2015). Nevertheless, the resolution is still sufficient to observe the main features, which allow us to separate neutral IGM from neutral substructure.

APPENDIX B

APPROXIMATION FOR THE BRIGHTNESS TEMPERATURE

On large scales, where the effects of peculiar velocity can be neglected, the brightness temperature of the 21 cm line is $\Delta T_B \propto x_{\text{HI}}(1 + \delta)(T_S - T_{\text{CMB}})/T_S$. Analytical models, including the model of Furlanetto et al. (2004), often operate with the quantity $\psi = x_{\text{HI}}(1 + \delta)$, ignoring the last temperature factor. In two panels of Figure 8 we show the correlation coefficient $r$ (Equation (1)) both for the actual brightness temperature $\Delta T_B$ and for $\psi$. The two panels are very similar, demonstrating that the spin temperature factor $(T_S - T_{\text{CMB}})/T_S$ can indeed be neglected at $z \lesssim 10$.

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