HIGHER ORDER CONTRIBUTIONS TO THE 21 cm POWER SPECTRUM

Adam Lidz, 1 Oliver Zahn, 1, 2 Matthew McQuinn, 1, 3 Suvendra Dutta, 1 and Lars Hernquist 4

Received 2006 October 2; accepted 2006 November 30

ABSTRACT

We consider the contribution of third- and fourth-order terms to the 21 cm power spectrum during the epoch of reionization, which arise because the 21 cm brightness temperature involves a product of the hydrogenic neutral fraction and the gas density. The third-order terms vanish for Gaussian random fields and have been previously neglected or ignored. We measure these terms from radiative transfer simulations and estimate them using cosmological perturbation theory. In our simulated models, the higher order terms are significant, and neglecting them leads to inaccurate 21 cm power spectrum estimates. On small scales the higher order terms are produced by gravitational mode coupling. Small-scale structure grows more readily in large-scale overdense regions, but the same regions tend to be ionized and hence do not contribute to the 21 cm signal. This modifies an earlier intuition that the 21 cm power spectrum simply traces the density power spectrum on scales smaller than that of a typical bubble and implies that small-scale measurements contain more information about the ionizing sources than previously believed. On large scales, higher order moments are not directly related to gravity. They are nonzero because overdense regions tend to ionize first and are important in magnitude at late times, due to large fluctuations in the neutral fraction. Finally, we show that second-order Lagrangian perturbation theory approximately reproduces the statistics of the density field from full numerical simulations for all redshifts and scales of interest, including the mode-coupling effects mentioned above. It can, therefore, be used in conjunction with semianalytic models to explore the broad regions of parameter space relevant for future 21 cm surveys.

Subject headings: cosmology: theory — intergalactic medium — large-scale structure of universe

Online material: color figures

1. INTRODUCTION

A frontier in observational cosmology is the detection of 21 cm emission from neutral hydrogen gas in the high-redshift intergalactic medium (IGM; e.g., Scott & Rees 1990; Madau et al. 1997; Zaldarriaga et al. 2004; for a review, see Furlanetto et al. 2006b). These observations promise three-dimensional information regarding the epoch of reionization (EOR), constraining the nature of the first luminous objects and early structure formation. Indeed, several low-frequency radio telescopes (the Primeval Structure Telescope [PAST], Pen et al. 2004; the Milleura Wide-Field Array [MWA], Bowman et al. 2006; the Low Frequency Array [LOFAR]; and the Square Kilometer Array [SKA]) that are underway or in the planning stages aim at detecting this signal.

Detailed theoretical modeling is required to forecast constraints and eventually interpret the results of these observations and to understand their implications for early structure formation. The first generation of experiments lack the sensitivity required to make detailed 21 cm maps, and a statistical detection will be necessary (Zaldarriaga et al. 2004; Furlanetto et al. 2004b; Morales 2005; McQuinn et al. 2006). One statistic of choice is the power spectrum of 21 cm fluctuations, although other statistical measures should help in characterizing this non-Gaussian signal (e.g., Furlanetto et al. 2004c). It will be subtle to infer quantities such as the volume-filling factor and size distribution of H ii regions from the observed 21 cm power spectrum, and, more generally, to extract information regarding the ionizing sources.

In this paper, we consider an effect that, while important for accurate calculation and interpretation of the 21 cm power spectrum, has been neglected in many previous calculations. The 21 cm brightness temperature involves a product of the gas density and the hydrogenic neutral fraction, and so the 21 cm power spectrum involves third- and fourth-order terms. In Fourier space these contributions involve particular integrals of the three- and four-point functions, the bispectra and trispectra of the various fields. We thus loosely call these terms three- and four-point terms, even though in real space they involve only two points.

The usual intuition is that on scales much smaller than that of a typical H ii region, the 21 cm power spectrum should be proportional to the density power spectrum. This intuition ignores the coupling between large- and small-scale density fluctuations that arises naturally during the nonlinear growth of structure via gravitational instability (e.g., Bernardeau et al. 2002). Indeed, mode coupling should give rise to nonvanishing three-point terms, as we detail in later sections of this paper. Qualitatively, structure grows more rapidly in regions that are overdense on large scales: an overdense region acts like a closed universe with a boosted matter density. The same regions, however, contain more sources and are ionized before underdense regions in our models (Sokasian et al. 2003; Furlanetto et al. 2004a, 2004b; Iliev et al. 2006; Zahn et al. 2007). As the universe reionizes, the large-scale overdense regions quickly become “dark” in a 21 cm map. One can think of the 21 cm field as a “masked” density field, with the ionization field playing the role of the “mask.” Unlike in a typical galaxy survey, however, the mask is itself correlated with the density field, preferentially removing large-scale overdense regions that...
contain boosted levels of small-scale structure. The upshot of this is that, in models where overdense regions are ionized first, mode couplings should suppress the contribution of density fluctuations to the 21 cm power spectrum. The aim of the present paper is to demonstrate this effect and quantify its importance.

In § 2, we calculate the 21 cm power spectrum (for illustrative purposes, in real as opposed to redshift space) from radiative transfer simulations and demonstrate the significance of the three- and four-point terms. In § 3.1 we look at the small-scale effects and examine the importance of the higher order terms with analytic calculations based on second-order cosmological perturbation theory. In § 3.2 we study the large-scale limit of the higher order terms. We then illustrate (§ 4) the dependence of the higher order terms on the properties of the ionizing sources. Next, in § 5, we refine the fast numerical scheme of Zahn et al. (2005) to include the higher order effects studied here. In addition (§ 6), we examine how the results depend on redshift and ionization fraction. We provide results in redshift space, generalizing the illustrative calculations of the previous sections. Finally, we discuss our findings and conclude in § 7.

2. THE 21 cm POWER SPECTRUM

In this section, we define terms and measure separately the contribution of low- and high-order terms to the 21 cm power spectrum with radiative transfer simulations. For simplicity, we presently neglect the effect of peculiar velocities, which we incorporate subsequently in § 6. Ignoring peculiar velocities, the 21 cm brightness temperature, relative to the cosmic microwave background (CMB), at observed frequency $\nu$ and redshift $z$ is (e.g., Zaldarriaga et al. 2004)

$$\delta T(\nu) \approx 26x_H (1 + \delta_p) \frac{T_S - T_{CMB}}{T_S} \frac{\Omega_B h^2}{0.022} \times \left( \frac{0.15}{\Omega_m h^2} \frac{1 + z}{10} \right)^{1/2} \text{mK.}$$  \hspace{1cm} (1)

In this equation, $x_H$ is the hydrogenic neutral fraction, $1 + \delta_p$ is the gas density in units of the cosmic mean, $T_S$ is the spin temperature, and $T_{CMB}$ is the CMB temperature. The other symbols have their usual meanings. Throughout this work, we make the usual simplifying assumption that $T_S \gg T_{CMB}$ globally during reionization, implying that $\delta T \propto (1 + \delta_p) x_H$ (Ciardi & Madau 2003; Chen & Miralda-Escude 2004; Furlanetto 2006; Pritchard & Furlanetto 2007).

In the limit that $T_S \gg T_{CMB}$, and ignoring peculiar velocities, we can derive an exact formula for the 21 cm power spectrum, decomposed into the sum of several terms (generalizing the formula in Furlanetto et al. 2006a). Writing the brightness temperature at a point $x_1$, as $\delta T(x_1) = T_0(x_1) [1 + \delta_\phi (x_1)]$, and the brightness temperature two-point correlation function is then given by

$$\langle \delta T(x_1) \delta T(x_2) \rangle = T_0^2 (x_1)^2 \left[ \langle \delta_\phi (x_1) \delta_\phi (x_2) \rangle + 2 \langle \delta_\phi (x_1) \delta_\rho (x_2) \rangle + \langle \delta_\rho (x_1) \delta_\rho (x_2) \rangle \right] + \text{constant}.$$  \hspace{1cm} (2)

The 21 cm power spectrum is just the Fourier transform of this equation and is given by

$$\Delta^2_{21}(k) = T_0^2 \langle x_H \rangle^2 \left[ \Delta_{\delta_\phi}^2 (k) + 2 \Delta_{\delta_\phi \rho}^2 (k) + \Delta_{\delta_\rho}^2 (k) \right] + \text{constant}.$$  \hspace{1cm} (3)

In the two above equations, $\delta_\phi = (x_H - \langle x_H \rangle) / \langle x_H \rangle$ is the fractional fluctuation in the hydrogenic neutral fraction, and $T_0$ is the normalization factor from equation (1). Here and throughout, $\Delta_{\phi}^2(k)$ indicates the dimensionless cross-power spectrum between two random fields $a$ and $b$. The quantity $\Delta_{\phi \rho}^2(k) = k^2 P_{a \rho}(k) / (2\pi^2)$ is the contribution to the variance of field $a$ per ln $k$, and this relation defines a dimensional power spectrum, $P_{a \rho}(k)$, with our Fourier convention. The terms on the first line of equation (3) are the usual low-order terms, representing the power spectrum of neutral hydrogen fluctuations, the cross-power spectrum between neutral hydrogen and the gas overdensity, and the density power spectrum, respectively (e.g., Furlanetto et al. 2006a).

The terms on the following lines, which we refer to as “higher order,” are the focus of our present paper. Note that the term $\Delta_{\phi \phi}^2(k)$ indicates here the fully nonlinear density power spectrum. In spite of this, we loosely refer to it, as well as the other terms on the first line of equation (3), as “low-order” since they contain only two fields, and because previous analytic calculations included nonlinear effects for these terms using the halo model (e.g., Furlanetto et al. 2004b). Also note that the four-point term, $\Delta_{\phi \phi \rho \rho}^2(k)$, is nonvanishing even in the case that $\delta_p$ and $\delta_\phi$ are each Gaussian. In this sense it is perhaps misleading to refer to it as “higher order,” but we will do so throughout for convenience.

If we ignore the three-point terms and consider scales much smaller than that of a typical bubble, the dominant terms from equation (3) are $\Delta_{\phi \phi}^2(k)$ and $\Delta_{\phi \phi \rho}^2(k)$). In the Gaussian approximation, we will show in the next section (§ 3, eq. [10]) that the term $\Delta_{\phi \phi \rho \rho}^2(k)$ approaches $\Delta_{\phi \phi}^2(k) / f \Delta \ln k_3 \Delta_{\phi}^2(k)$ on small scales, i.e., the expression reduces to the variance of the field $\phi$ multiplied by the density power spectrum. Adding this four-point term to the density power spectrum piece, we expect the small-scale limit of equation (3) to approach $\Delta_{\phi}^2(k) \sim T_0^2 \langle x_H \rangle^2 \Delta_{\phi \phi \rho}^2(k)$. Further, to the extent that $x_H$ is either “1” or “0” at each point in the IGM, $\langle x_H \rangle = \langle x_H \rangle$, implying that $\Delta_{\phi}^2(k) \propto \langle x_{\rm HI} \rangle^2 \Delta_{\phi \phi}^2(k)$ on small scales. Note that if we had neglected the four-point term entirely, we would have obtained a different small-scale limit, $\Delta_{\phi}^2(k) \propto \langle x_{\rm HI} \rangle^2 \Delta_{\phi \phi}^2(k)$.

These expressions illustrate the usual intuition that, on sufficiently small scales, the 21 cm power spectrum should trace the density power spectrum. In fact, we will show that the three-point terms in equation (3) are generally substantial, resulting in large deviations from each of these small-scale limits.

2.1. Radiative Transfer Calculations

In order to check the effect of the higher order terms, we measure each term in equation (3) separately, using the reionization simulations of Zahn et al. (2007) and McQuinn et al. (2007). These simulations follow the growth of H I regions in a cubic box of comoving side length $L_{\rm box} = 65.6 \ h^{-1}$ Mpc. The Zahn et al. (2007) calculations start from an N-body simulation run with an enhanced version of Gadget-2 (Springel 2005), tracking 1024$^3$ dark matter particles and resolving dark matter halos with
mass $M \gtrsim 2 \times 10^9 M_\odot$. Ionizing sources are placed in simulated dark matter halos, using a simple prescription to connect ionizing luminosity and halo mass (Zahn et al. 2007). The simulated dark matter density field is then interpolated onto a 512$^3$ Cartesian grid, and we subsequently assume that the gas density closely tracks the simulated dark matter density field (see Zahn et al. 2007 for a discussion). Finally, radiative transfer is treated in a postprocessing stage using the code of McQuinn et al. (2007), a refinement of the Sokasian et al. (2001, 2003) code, which in turn uses the adaptive ray-tracing scheme of Abel & Wandelt (2002).

The result of these calculations is shown in Figure 1. The solid line shows the simulated 21 cm power spectrum in dimensionless units [i.e., it shows $\Delta_2^2(k)/T_0^2$ from eq. (3)], the dotted line shows the contribution from the low-order terms (i.e., it shows the sum of the terms on the first line of eq. [3]), and the dashed and dot-dashed lines indicate the higher order terms.

The bottom panel of Figure 1 further illustrates the importance of the three- and four-point terms for accurate predictions of the 21 cm power spectrum. The curve shows the fractional error one makes in neglecting the higher order terms: this error is at the $\sim 100\%$–$250\%$ level on scales of $k \sim 1$–$10 \, h \, \text{Mpc}^{-1}$. On still smaller scales, the simulation results are unreliable, due to our limited numerical resolution. As mentioned previously, we might instead have included the Gaussian part of the four-point function as a low-order term, in which case the low-order terms amount to $\Delta_2^2(k) \propto (\delta_{\text{c}})^3$. Our results differ from this limit by the even larger factor of $\sim 250\%$ at $k \sim 1 \, h \, \text{Mpc}^{-1}$.

Clearly, the three-point function terms are quite important in our simulations.

3. ANALYTIC ESTIMATES

3.1. Small Scales: Perturbative Estimates

In order to develop intuition regarding the three- and four-point terms, we estimate their form analytically, using second-order Eulerian perturbation theory (e.g., Scoccimarro 2000; Bernardeau et al. 2002). In this section, we restrict our analytic calculations to small scales ($k \gtrsim 1 \, h \, \text{Mpc}^{-1}$), where spatial fluctuations in the density field dominate over fluctuations in the neutral fraction, although we will demonstrate in the next subsection (§ 3.2) that the higher order terms are generally nonvanishing on larger scales as well. In the small-scale limit, we can ignore mode couplings between fluctuations in the hydrogenic fraction, $\delta_n$, at two different wavenumbers $k_1$ and $k_2$, which should damp out on scales smaller than the typical bubble size.

First, let us calculate the term $\Delta_2\delta_\text{c,}\delta_n(k)$. Writing $\delta_\text{c}(k) = \psi(k)$, and using the fact that the Fourier transform of a product is a convolution, one has

$$P_{\delta_\text{c},\delta_n}(k) = (2\pi)^3 \delta_\text{c}^2(k_1 + k_2) \langle \psi(k_1)\delta_n(k_2) \rangle$$

$$= \delta_\text{c}^2(k_1 + k_2) \int \frac{d^3k_3}{(2\pi)^3} \langle \delta_\text{c}(k_3)\delta_n(k_1 - k_3)\delta_n(k_2) \rangle. \quad (4)$$

To the lowest nonvanishing order, this expression receives contributions from expanding each of the density field terms to second order while leaving the remaining ionization field term at first order (see Fig. 3 for a check on the validity of this approximation). First let us expand $\delta_n(k_1 - k_3)$ to second order in the linear density field. The second-order density field in Fourier space, $\delta_\text{c}^2(k_1 - k_3)$, is given by perturbation theory as (e.g., Scoccimarro 2000)

$$\delta_\text{c}^2(k_1 - k_3) = \int \frac{d^3q_1}{(2\pi)^3} \frac{d^3q_2}{(2\pi)^3} \delta_\text{c}^2(q_1 - q_2)$$

$$\times F_2(q_1, q_2)\delta_\text{c}^{(1)}(q_1)\delta_\text{c}^{(1)}(q_2). \quad (5)$$

In this equation, $F_2(q_1, q_2)$ is the second-order kernel expressing mode coupling from nonlinear evolution, $\delta_\text{c}^{(1)}$ denotes the first-order density field, and $\delta_\text{c}^{(2)}$ denotes the second-order density field. The second-order mode-coupling kernel is given by (e.g., Scoccimarro 2000)

$$F_2(q_1, q_2) = \frac{5}{7} + \frac{q_1 \cdot q_2}{2q_1q_2} \left( \frac{q_1 + q_2}{q_1 + q_2} \right)^2 + \frac{2}{7} \left( \frac{q_1 \cdot q_2}{q_1q_2} \right)^2. \quad (6)$$

Inserting the second-order expansion into the integral of equation (4), the resulting integrand contains an expectation value of the form

$$\langle \delta_\text{c}(k_3)\delta_\text{c}^{(1)}(q_1)\delta_\text{c}^{(1)}(q_2)\delta_\text{c}^{(1)}(k_2) \rangle.$$

This can be rewritten as the sum of the product of two separate expectation values, with each of two terms yielding nonvanishing contributions:

$$\langle \delta_\text{c}(k_3)\delta_\text{c}^{(1)}(q_1) \rangle \langle \delta_\text{c}^{(1)}(q_2)\delta_\text{c}^{(1)}(k_2) \rangle$$

$$+ \langle \delta_\text{c}(k_3)\delta_\text{c}^{(1)}(q_2) \rangle \langle \delta_\text{c}^{(1)}(q_1)\delta_\text{c}^{(1)}(k_2) \rangle.$$
The contribution to the integral of equation (4) from expanding \( \delta_n(k_1 - k_1) \) to second order then simplifies to

\[
2 \delta P^2 \int \frac{d^3 k_1}{(2\pi)^3} F_2(-k_3, -k_3) P_{\delta \delta}(k_3).
\]

A second, similar term arises from expanding \( \delta_n(k_2) \) to second order. In total, our expression for this three-point term to second order in perturbation theory becomes

\[
P_{\delta \delta \delta}(k_1) = 2 \delta P^2 \int \frac{d^3 k_1}{(2\pi)^3} F_2(-k_3, -k_3) P_{\delta \delta}(k_3)
\]

This approximate expression has an illuminating form. The integral over \( \Delta_{\nu, \nu} \) is a measure of how well the ionized regions track the overdensities. This integral can be written as \( \langle \delta \delta \rangle = -1 + \langle x_{HI} / \rho \rangle \). Alternatively, it can be expressed in terms of the volume-weighted and mass-weighted ionization fractions, which we denote by \( x_i \) and \( x_m \), respectively, as \( \langle \delta \delta \rangle = (x_i - x_m) / (1 - x_i) \). This term is negative during reionization in our simulations: the ionizing sources lie in overdense regions and reionize their surroundings before eating out into underdense regions. Consequently, the mass-weighted ionization fraction always exceeds the volume-weighted ionization.

We illustrate this explicitly in Figure 2 (see also Zahn et al. 2007), where we show power and cross-power spectra for density and neutral hydrogen fluctuations, as well as the cross-correlation coefficient between neutral hydrogen and overdensity, which is defined by

\[
r_{\delta \nu}(k) = \frac{P_{\delta \nu}(k)}{\sqrt{P_{\delta \delta}(k)P_{\nu \nu}(k)}}.
\]

This approximate expression contains the linear density power spectrum rather than the fully nonlinear contribution.
density power spectrum. However, we expect to find an expression similar to equation (8) in the fully nonlinear regime, containing instead the fully nonlinear density power spectrum, and with a different, perhaps scale-dependent, coefficient. Indeed, integrating equation (7) numerically with the nonlinear density power spectrum as input provides a fairly good estimate of the small-scale three-point term in our simulation. We show this comparison in the bottom panel of Figure 3.\footnote{Note that the prefactor implied by our numerical integration is larger than the 47/21 of eq. (8), which is accurate only in the limit of very small scales. In other words, the three-point correction is even more important than is implied by this approximate expression.}

In our fiducial model at this redshift, the \( \delta_x \) mode couplings result only in a small correction to the large-scale 21 cm power spectrum (see eq. [3]), although we will illustrate in \S\,5 and 6 that their effect can be significant in other models and at different redshifts. On small scales, the perturbative calculations provide a fairly good match to the simulation results, except that they appear to mildly underestimate the strength of the three-point term at high values of \( k \). At any rate, our perturbative calculation clearly illustrates that the mode-coupling effect will be significant and demonstrates that its strength depends on how well the ionized regions trace overdensities.

Expressions for the other three-point term and the four-point term can be derived in a similar manner. The expression for the other three-point term is

\[
P_{\delta_x \delta_y \delta_z}(k_1) \sim \frac{34}{21} P_{\delta_x \delta_y}(k_1) \int d k_3 \Delta^2_{\delta_x \delta_y}(k_3).
\]

This is clearly less important than the above three-point term, since \( P_{\delta_x \delta_y \delta_z}(k_1) \ll P_{\delta_x \delta_y}(k_1) \) on small scales, although we find that this term is not completely negligible (it contributes at the \( \sim 10\% \) level on small scales). Finally, to the lowest nonvanishing order, the four-point term is given by

\[
P_{\delta_x \delta_y \delta_z \delta_w}(k_1) = \int \frac{d^3 k_3}{(2\pi)^3} P_{\delta_x \delta_y}(|k_1|)P_{\delta_x \delta_z}(|k_1 - k_3|)
+ \int \frac{d^3 k_3}{(2\pi)^3} P_{\delta_y \delta_z}(|k_1|)P_{\delta_x \delta_w}(|k_1 - k_3|).
\]

In the top panel of Figure 3 we compare the simulated four-point term and the results from equation (10), using the simulated values of \( P_{\delta_x \delta_y}(k) \), \( P_{\delta_x \delta_z}(k) \), and \( P_{\delta_x \delta_w}(k) \) as input. The agreement is comparable to, although slightly worse than, that for the three-point function. At this redshift, the four-point term works out to be comparable in magnitude to the dominant three-point term, except that the three-point terms come in with an additional factor of 2 (eq. [3]) and hence represent the dominant correction. Further, we have argued that this three-point correction will be comparable to the contribution from the density power spectrum, in good agreement with the simulation results of Figure 1.

3.2. Large Scales

What about large scales? For the specific case shown in Figure 1 (\( z = 6.89 \) and \( x_i = 0.48 \)), the higher order terms have only a small fractional effect. However, as we detail here and in \S\,6, the higher order terms are generally nonnegligible even on large scales. In general, it is challenging to calculate these terms analytically on scales where spatial fluctuations in the neutral hydrogen distribution are comparable in strength to density fluctuations. However, in this section we demonstrate that we can analytically estimate the higher order terms at high ionization fractions and on large scales, when fluctuations in the neutral hydrogen distribution strongly dominate over density fluctuations.

In order to gain insight into the properties of the higher order terms on large scales, we begin by calculating the cross-correlation coefficient between \( \delta_x \delta_y \) and each of \( \delta_y \) and \( \delta_z \).\footnote{We calculate cross-correlation coefficients here and throughout as follows. For two random fields \( x \) and \( y \), the cross-correlation coefficient is given by the cross-power spectrum of the two fields divided by the square root of the product of the fields’ auto power spectra: \( r_{x,y}(k) = \Delta^2_{x,y}(k)/[\Delta^2_x(k)\Delta^2_y(k)]^{1/2} \).} The results of this calculation are shown in Figure 4, where we examine a range of redshifts and corresponding ionization fractions. At \( z = 8.16 \), when the ionization fraction is \( x_i = 0.11 \) (left), the figure illustrates that \( \delta_x \delta_y \) is strongly correlated with fluctuations in the hydrogenic neutral fraction, \( \delta_x \), and strongly anticorrelated with the density field, \( \delta_y \). Further, examining the top left panel, one can see that the power spectrum of neutral hydrogenic fluctuations and the three-point terms each amount to a scale-independent bias factor multiplied by the density power spectrum on sufficiently large scales. At an intermediate ionization fraction (\( x_i = 0.48; \text{middle} \)), the cross-correlation coefficient between \( \delta_x \delta_y \) and each of \( \delta_x \) and \( \delta_y \) is reduced, and the three-point terms are correspondingly less important, as has been already illustrated in Figure 1.
Finally, at a high ionization fraction ($x_{H} = 0.70$; right), the correlation coefficients reverse sign and are again large in magnitude. The top right panel illustrates that the bias between neutral hydrogenic fluctuations and density fluctuations, $\Delta_{\delta_{0}/\delta_{p}}^2 / \Delta_{\delta_{0}/\delta_{p}}^2$, is large and has a strong scale dependence. The bias between $\delta_{0}/\delta_{p}$ and $\delta_{x}$, however, is relatively independent of scale. This occurs because, at this ionization fraction, fluctuations in the hydrogenic neutral fraction strongly dominate over density fluctuations, with $\Delta_{\delta_{0}/\delta_{p}}^2 / \Delta_{\delta_{0}/\delta_{p}}^2 \sim 30$ at $k \sim 0.1 \ h \ Mpc^{-1}$. In this case $\delta_{0}/\delta_{p}$ just directly tracks $\delta_{x}$, with a roughly scale-independent bias factor. The three-point term $\Delta_{\delta_{0}/\delta_{p}/\delta_{0}}^2$ is much greater than the other three-point term, $\Delta_{\delta_{0}/\delta_{x}/\delta_{0}}^2$, on large scales at this ionization fraction (the two terms differ in amplitude by a factor of $\sim 6$ near the fundamental mode of our simulation box). It is also significantly larger than the four-point term, $\Delta_{\delta_{0}/\delta_{0}/\delta_{0}^2}$, on the scales of interest, and hence represents the dominant higher order correction at this ionization fraction.

Can we understand analytically the weak scale dependence and strength of the bias between $\Delta_{\delta_{0}/\delta_{0}}$ and $\Delta_{\delta_{0}/\delta_{x}}$ at late times? The following calculation will be facilitated by considering the neutral hydrogenic field, $x$, rather than examining fluctuations in the neutral hydrogenic field, $\delta_{x}$. The relevant three-point term, $\Delta_{\delta_{0}/\delta_{0}/\delta_{x}}^2$, is related to our usual terms by the equality

$$
\Delta_{\delta_{0}/\delta_{0}/\delta_{x}}^2(k) = \langle \delta_{1} \rangle^2 \left[ \Delta_{\delta_{0}/\delta_{0}}^2(k) + \Delta_{\delta_{0}/\delta_{x}}^2(k) \right].
$$

We proceed to calculate $\Delta_{\delta_{0}/\delta_{0}/\delta_{x}}^2(k)$. It is simpler to understand what is going on by thinking about the correlation function rather than the power spectrum. Thus, we are looking for a formula for the correlation $\langle x(1) \delta_{0}(1) x(2) \rangle$, where “1” and “2” indicate two different points. We also recall that we are working in the regime in which the $x$ fluctuations are much larger than the density ones, so correlations will be determined by the structure of the $x$ field.
For simplicity, we consider the case when \( x \) can take only the values 0 or 1. We can then write

\[
\langle x(1)\delta(1)x(2) \rangle = \int d\delta(1)\delta(1)P[\delta(1), x(1) = 1, x(2) = 1] \\
= P[x(1) = 1, x(2) = 1] \\
\times \int d\delta(1)\delta(1)P[\delta(1)|x(1) = 1, x(2) = 1].
\]

We now note that \( P[x(1) = 1, x(2) = 1] \) is nothing other than \( \langle x(1)x(2) \rangle \). To approximate the integral, we make use of our assumption that it is the \( x \) field that dominates the correlations, so we can write

\[
P[\delta(1)|x(1) = 1, x(2) = 1] \approx P[\delta(1)|x(1) = 1].
\]

In other words, we are neglecting all correlations between the density and the neutral fraction at widely separated points other than the ones that originate in the correlations of \( x \). We thus obtain

\[
\langle x(1)\delta(1)x(2) \rangle \approx \langle x(1)x(2) \rangle \frac{\langle \delta(1) \rangle}{\langle x \rangle},
\]

where we have used the identity

\[
\int d\delta P[\delta|x = 1] = \frac{\langle \delta \rangle}{\langle x \rangle}.
\]

Thus, the correlation function \( \langle x(1)\delta(1)x(2) \rangle \) has the same shape as that of \( x \), \( \langle x(1)x(2) \rangle \).

The analytic prediction for the three-point term, in the limit of strong neutral hydrogenic fluctuations, is hence

\[
\Delta_{x,\delta}(k) \approx \langle \delta \delta \rangle \Delta_{x, \delta}(k).
\]

A very similar argument applies to the four-point function, yielding

\[
\Delta_{x,\delta, \delta, \delta}(k) \approx \langle \delta \delta \rangle^2 \Delta_{x, \delta}(k).
\]

In Figure 5, we compare the analytic predictions of equations (14) and (15) with simulation measurements. Our simple formulae capture the effect relatively well.

It becomes clear that in this regime the higher order terms have a very different origin: they are not related to gravity. They simply result from the large fluctuations in the neutral fraction and the fact that in our models a neutral point is more likely to be underdense, so that \( \langle \delta \rangle \langle x \rangle \) is nonzero.

We can also obtain formulae that are valid in the early regime, when density fluctuations dominate the correlations. The generic expectation value we have to calculate to compute the power spectrum involves the probability

\[
P[\delta(1), x(1) = 1, \delta(2), x(2) = 1].
\]

In the early regime we can approximate it by

\[
P[\delta(1), x(1) = 1, \delta(2), x(2) = 1] \\
\approx P[\delta(1), \delta(2)]P[x(1) = 1|\delta(1)]P[x(2) = 1|\delta(2)],
\]

which assumes that it is the \( \delta \) correlations that dominate. We can then write

\[
P[\delta(1), \delta(2)] \approx P[\delta(1)]P[\delta(2)] \left[ 1 + \xi(r) \frac{\delta(1)\delta(2)}{\sigma^2} + \ldots \right],
\]

where \( \xi(r) \) is the density correlation function and \( \sigma^2 \) is its variance. This approximation leads to all power spectra being proportional to that of the density. Again, this is a regime in which higher order moments do not depend on gravitational non-linearities (as we use only the lowest order form of the joint distribution function of the density). They are made relevant only by the large fluctuations of \( x \).

Finally, we note that the change in behavior of the correlation coefficients seen in Figure 4 as reionization proceeds can be understood as reflecting the transition between fluctuations being dominated by \( \delta \) at early times and being dominated by \( x \) at later stages. For example, equation (11) shows that \( \Delta_{x, \delta, \delta, \delta} \) has a contribution from \( \Delta_{x, \delta, \delta} \) and \( \Delta_{x, \delta, \delta} \). At early times \( \Delta_{x, \delta, \delta} \) dominates, but it becomes subdominant late during reionization. This transition leads to the change in sign of the cross-correlation coefficients. Similar arguments apply to \( \Delta_{x, \delta, \delta, \delta} \).

3.3. Convergence with Box Size

The mode-coupling effects described above imply that a rather large simulation volume is needed to accurately simulate the small-scale 21 cm power spectrum. Indeed, due to the significant transfer of power from large to small scales, one might question whether even our small-scale 21 cm power spectra results are reliable, given our limited box size of \( L = 65.6 \, h^{-1} \, \text{Mpc} \). Equations (8), (9), and (10) demonstrate that the higher order effects depend
on two integrals, $\int d\ln k \Delta^2_{\delta_i \delta_j}(k)$ and $\int d\ln k \Delta^2_{\delta_i \delta_j}(k)$, which represent the cross-correlation between $\delta_i$ and $\delta_j$, and the variance of $\delta_i$, respectively.

The convergence of our small-scale 21 cm results then depends on the convergence of these two integrals with increasing box size. We investigate the convergence of $\big< \delta_i^2 \big>$ and $\big< \delta_i \delta_j \big>$ using the analytic scheme of Zahn et al. (2005, 2007), which provides a quick and accurate check. More specifically, we apply the Zahn et al. (2005, 2007) methodology by generating a Gaussian random density field in a box of side length $250 \ h^{-1} \ Mpc$ and calculate the desired quantities. Although using a Gaussian random density field ignores the mode-coupling effects that are of present interest, it does yield an accurate calculation of $\big< \delta_i^2 \big>$ and $\big< \delta_i \delta_j \big>$ (Zahn et al. 2007), which determine the convergence of our results with increasing box size. To test convergence, we compare our calculations of these quantities in the $250 \ h^{-1} \ Mpc$ box to calculations done with smaller volume Gaussian realizations of the same density field.

The result of this test is shown in Figure 6 for ionization fractions of $x_{i,e} \simeq 0.5$ at $z = 6.89$ and $x_{i,e} \simeq 0.7$ at $z = 6.56$. With our current simulation box size of $L_{\text{box}} = 65.6 \ h^{-1} \ Mpc$, $\big< \delta_i \delta_j \big>$ and $\big< \delta_i^2 \big>$ have converged to 84% and 91%, respectively, at $x_{i,e} \simeq 0.5$, which implies that our predictions of the high-$k$ 21 cm power spectrum should be relatively free of errors due to missing large-scale power. For smaller box sizes the error increases, with a box size of $L_{\text{box}} \sim 30 \ h^{-1} \ Mpc$ resulting in a $\sim 50\%$ error. The sensitivity of $\big< \delta_i \delta_j \big>$ and $\big< \delta_i^2 \big>$ to large scales arises because H II regions around individual, highly clustered sources quickly merge into "superbubbles," which become quite large (Sokasian et al. 2003; Furlanetto et al. 2004a, 2004b; Zahn et al. 2007). Our point here is that this also impacts small-scale 21 cm power spectrum predictions. Naturally, the convergence properties will be worse at higher ionization fractions, when the H II regions are typically larger than they are at our fiducial ionization fraction of $x_{i,e} \simeq 0.5$. This is illustrated quantitatively by the bottom set of light gray lines in Figure 6.

The calculations in the previous section provide analytic understanding regarding the three-point functions and demonstrate that their strength depends on how closely the ionization field tracks large-scale overdensities. In this section, we illustrate that this provides additional leverage in constraining the nature of the ionizing sources and the topology of reionization from 21 cm observations. In particular, let us examine the higher order contribution to the 21 cm signal for three different models for the minimum host halo mass of the ionizing sources.

Specifically, we consider models in which the ionizing luminosity is proportional to the host halo mass, with sources residing in halos of mass larger than (1) the cooling mass ($M_{\text{min}} = 1.3 \times 10^8 \ M_\odot$ at $z \sim 7$; e.g., Barkana & Loeb 2001), (2) $M_{\text{min}} = 2 \times 10^8 \ M_\odot$, and (3) $M_{\text{min}} = 4 \times 10^{10} \ M_\odot$. These are toy models, but they span a plausible range of properties given our extremely limited observational knowledge regarding the sources that reionized the IGM. The first model assumes that all halos down to the cooling mass (i.e., halos with $T_{\text{vir}} < 10^4 \ K$) contribute to reionization. The source prescriptions in the second and third models might, for example, approximate models in which photo-heating has limited the efficiency of star formation in small-mass halos (e.g., Thoul & Weinberg 1996; Navarro & Steinmetz 1997; Dijkstra et al. 2004) and diminished their contribution to reionization. The formal halo mass resolution of our simulation is comparable to the minimum source mass in our second model (Zahn et al. 2007), but in our first model we use the results of McQuinn et al. (2007), which add lower mass sources into the simulation with the appropriate statistical properties.

In Figure 7, we show that the impact of the higher order terms differs significantly for these different models. In each
case the source efficiency is adjusted to yield $\langle x_{HI} \rangle \sim 0.5$ at $z \sim 7$.  

From the top panel it is clear that the effect depends significantly on the source properties. In the case that the minimum mass is $M_{\text{min}} = 4 \times 10^{10} M_\odot$, the effect is only at the $\sim 10\%$ level. For sources with a minimum mass of $M_{\text{min}} = 2 \times 10^{9} M_\odot$, as was already illustrated in Figure 1, the effect is at the $\approx 100\%$ level. Finally, with sources residing in halos down to the cooling mass, the effect is even larger, at the $\approx 200\%$ level.

The reason for this sensitivity is demonstrated in the bottom panel of the figure, which shows the cross-correlation coefficient between density and neutral fraction fluctuations as a function of scale. In models where small-mass halos contribute to reionization, the ionized regions track overdensities out to smaller scales. There are two reasons for this. First, when the ionizing sources reside in more massive halos, they are more biased and produce larger bubbles at a given ionization fraction (Furlanetto et al. 2006a), masking out neighboring voids, as well as their intermediate overdense environs. Next, Poisson fluctuations in the abundance of ionizing sources become increasingly important for rare, massive halos, limiting the cross-correlation between ionization and overdensity (Zahn et al. 2007). As a result, the three-point terms (eqs. [8] and [9]) become increasingly important when the ionizing sources are very abundant and more closely track overdensities.

We emphasize that each of these models already differs in its large-scale 21 cm power spectrum, due to the differences in $\Delta_{\delta,\delta}(k)$ and $\Delta_{\delta,\delta}(k)$ between these models. Our point here is merely that, due to mode coupling, the small-scale 21 cm power spectra give us an additional handle on distinguishing the different models. This is clearly demonstrated by Figure 7.

These effects might be offset somewhat if recombinations are more important than those simulated in our models. Since gas in overdense regions recombines faster, recombinations act to decrease the tendency for the overdense regions to reionize first. Further, in models where the voids reionize first, as might be the case if miniquasars reionize the IGM (Ricotti & Ostriker 2004; although see also Zhang et al. 2007), the three-point terms should be positive, since the volume-weighted ionization fraction will exceed the mass-weighted ionization fraction in these models.

Finally, note that the higher order terms contribute even on large scales, particularly in the cooling-mass model, where they amount to a 40% correction (see also § 6). In this model, the strongest large-scale contribution comes from the $\Delta_{\delta,\delta}(k)$ term, which is small and negative on small scales but becomes significant and positive near the bubble scale (see § 3.2 for comments on the impact of the higher order terms on large scales).

5. SECOND-ORDER LAGRANGIAN PERTURBATION THEORY AND A NUMERICAL REIONIZATION SCHEME

In order to forecast the ability of future 21 cm surveys to constrain reionization physics, we require fast and reasonably accurate predictions for the expected 21 cm signal, spanning a wide range of model parameters. For this purpose, rapid semianalytic calculations are extremely valuable. One such semianalytic scheme is that of Zahn et al. (2005), which is essentially a Monte Carlo implementation of the analytic model of Furlanetto et al. (2004b).

The original Zahn et al. (2005) scheme uses Gaussian random realizations of cosmological density fields and therefore neglects the mode-coupling effects that are the topic of our present paper. This semianalytic scheme can alternatively be applied using the density field and halo distribution from a full cosmological N-body simulation, as in Zahn et al. (2007). In this case, the approximate scheme includes the higher order effects discussed above, and the results agree well with more detailed radiative transfer calculations. Presently, we aim at still more rapid calculations that additionally remove the expense of performing an N-body simulation. More specifically, we refine the Gaussian random field scheme of Zahn et al. (2005) by generating cosmological density fields according to second-order Lagrangian perturbation theory (2LPT).

This ambition is plausible, given that even relatively small scales ($k \leq 10 h$ Mpc$^{-1}$) are still in the quasi-linear regime near $z \sim 6$. Because of this, we find that particle distributions set up using 2LPT accurately capture the dark matter density distribution at the redshifts and scales of interest.

In 2LPT, as in the Zel’dovich approximation, each particle is displaced from its initial Lagrangian position, $x$, to a final Eulerian position, $x$. The mapping between Lagrangian and Eulerian positions in 2LPT depends, however, on each of the first-order potential, $\phi^{(1)}(q)$, and the second-order potential, $\phi^{(2)}(q)$. Specifically, the mapping is described by (Scoccimarro 1998)

$$x = q - D_1 \nabla_q \phi^{(1)}(q) + D_2 \nabla_q \phi^{(2)}(q).$$

In this equation, $D_1$ and $D_2$ are the first- and second-order growth factors (Scoccimarro 1998), and $\nabla_q$ denotes the gradient with respect to the Lagrangian position. The particle peculiar velocities satisfy a similar equation (Scoccimarro 1998). The first-order potential $\phi^{(1)}(q)$ obeys the Poisson equation $\nabla^2 \phi^{(1)}(q) = \delta^{(1)}(q)$, while the second-order potential satisfies a separate Poisson equation (Buchert et al. 1994; Scoccimarro 1998),

$$\nabla^2 \phi^{(2)}(q) = \sum_{i,j} \left\{ \phi^{(1)}_{ij}(q) \phi^{(1)}_{ij}(q) - \left[ \phi^{(1)}_{ij} \right]^2 \right\}.$$

The procedure for generating particle realizations of a 2LPT density field is then straightforward. First, one generates a Gaussian random realization of the first-order density field with the appropriate linear power spectrum. Second, one solves the first-order Poisson equation for the potential, $\phi^{(1)}(q)$. From the first-order potential, one can calculate the source term in the second-order Poisson equation and subsequently solve this equation for the second-order potential, $\phi^{(2)}(q)$. Finally, one displaces each particle from its initial cell center, using equation (18) with the first- and second-order potentials as input. More specifically, we generate 2LPT displacements using the code of Scoccimarro (1998) and Crocce et al. (2006), which is now publicly available.\footnote{Although nonlinear contributions to the density power spectrum are relatively mild, higher order contributions to the 21 cm power spectrum are substantial, as we demonstrated previously. The comparatively larger importance of three-point terms for the 21 cm power spectrum arises because, on large scales, $P_{\delta,\delta}(q,k) \gg P_{\delta,\delta}(q,k)$.
\footnote{\textit{See \url{http://cosmo.nyu.edu/roman/2LPT/}.}}}

From a 2LPT particle realization, we simply interpolate to find the density field on a Cartesian grid. We can then calculate the 21 cm power spectrum, using the ionization field generated by applying the method of Zahn et al. (2005, 2007) to the 2LPT density field, or using the simulated ionization field. How well do these predictions agree with results from our full N-body simulation and radiative transfer calculation? We can test this by generating a 2LPT realization with precisely the same first-order displacements as in our N-body simulation.
Before presenting this comparison, we should make one caveat. The method of Zahn et al. (2005, 2007) provides a very good, but imperfect, match to the ionization field from more detailed radiative transfer simulations. Currently our aim is to test how well 2LPT predicts the higher order terms in the 21 cm power spectrum. We thus compare the simulated and 2LPT 21 cm fields, using in each case the ionization field calculated from the full radiative transfer simulations. We do this comparison, rather than using the ionization field from the radiative transfer calculation for our simulated 21 cm field and the analytic ionization field for our 2LPT calculation. In this way, any difference between our 2LPT and N-body calculations is attributable to differences in the density fields or the mode couplings that we study presently.

First we compare the simulated and 2LPT density power spectra. We use 512\(^3\) particles for our 2LPT particle realization, drawn from the same initial conditions used in our N-body simulation, and interpolate the results onto a 512\(^3\) mesh using cloud-in-cell (CIC) interpolation. We have explicitly tested that our results are relatively insensitive to the level of shell crossing in this calculation (e.g., Scoccimarro 1998) by filtering our initial conditions with several different low-pass filters. For our N-body calculation, we interpolate our 1024\(^3\) simulated particles onto a 512\(^3\) mesh. For each of the simulated and 2LPT density power spectra, we deconvolve the CIC smoothing window before calculating a binned, spherically averaged density power spectrum, and we present our results on scales only where aliased high-\(k\) power (e.g., Jing 2005) is insignificant. We do not attempt to subtract shot-noise power from our simulated results: we have run test simulations with varying particle numbers that indicate that the shot-noise power is significantly sub-Poissonian at these redshifts (see also Springel et al. 2005), which makes it difficult to estimate the precise level of the shot-noise power. Moreover, even in the Poisson case, shot-noise power would result in a very small correction to our 1024\(^3\) particle simulation results: in this case, the correction would be only \(\sim 1\%\) at \(k \sim 10 \, h \, \text{Mpc}^{-1}\), and smaller on larger scales.

This comparison is shown in Figure 8, demonstrating that 2LPT provides a reasonable match to the simulated density power spectrum, producing a \(\lesssim 20\%\) underestimate of the simulated power at \(k \leq 5 \, h \, \text{Mpc}^{-1}\) and a \(\lesssim 40\%\) underestimate at \(k \leq 10 \, h \, \text{Mpc}^{-1}\). As a further gauge of the level of agreement, we compare the simulated density power spectrum with the Peacock & Dodds (1996) fitting formula. The Peacock & Dodds (1996) power spectrum agrees closely with the 2LPT calculation, yet it appears to somewhat underestimate the simulated density power. We emphasize that the Peacock & Dodds (1996) fitting formula is calibrated at \(z = 0\) and is by no means guaranteed to match simulations at higher redshift. The figure demonstrates that 2LPT is, at any rate, just as good as this commonly used fitting formula at \(z \sim 6\) and \(k \leq 10 \, h \, \text{Mpc}^{-1}\), and it is a significant improvement over a purely linear calculation.

Next we compare calculations of the full 21 cm power spectrum, separating out contributions from the low-order and higher order terms as in equation (3). The results of this calculation are shown in Figure 9, demonstrating that the 21 cm power spectrum calculations agree well (to better than \(10\%\) at \(k \leq 10 \, h \, \text{Mpc}^{-1}\)). The agreement is hence even better than the agreement found in our density power spectrum calculations (Fig. 8). This superior agreement, however, is due in part to a cancellation that arises...
because the low-order terms in our 2LPT calculation are smaller than those in our $N$-body calculation, while the magnitude of the (negative) higher order terms is also smaller in the 2LPT calculation, as illustrated in Figure 9. The agreement might, therefore, be a little worse at different ionization fractions, or for different models, where this close cancellation may not occur. On still smaller scales, where the one-halo term in the density power spectrum is dominant (e.g., Cooray & Sheth 2002), 2LPT will break down further. In addition, our assumption that gas closely traces dark matter should break down (Gnedin & Hui 1998). However, even next-generation 21 cm experiments such as SKA will likely be limited to scales of $k \lesssim 10 h \text{Mpc}^{-1}$ (McQuinn et al. 2006; Bowman et al. 2006). In conclusion, 2LPT provides a significant improvement over the Gaussian random field scheme of Zahn et al. (2005), while requiring very little additional computational overhead.

6. REDSHIFT EVOLUTION AND RESULTS IN REDSHIFT SPACE

In the previous sections, we characterized the impact of the higher order terms, ignoring the effect of peculiar velocities and focusing on a single redshift for simplicity. In this section, we expand on these calculations by incorporating the effect of peculiar velocities (e.g., McQuinn et al. 2006) and by examining the dependence of our results on the ionization fraction.

In each case we calculate the spherically averaged 21 cm power spectrum, i.e., the redshift-space monopole, as in Zahn et al. (2007). In the case of the monopole, the sum of the low-order 21 cm power spectrum terms is given by (McQuinn et al. 2006; Zahn et al. 2007)

$$\Delta_{21, \text{low}}^2 = \frac{T_0}{c_1}(x_{\text{HI}})^2 \left[ \Delta_{\delta_x, \delta_x}^2 + \left( 8/3 \right) \Delta_{\delta_x, \delta_y}^2 + \frac{28/15}{\Delta_{\delta_x, \delta_z}^2} \right].$$

In principle, one can create an analog to equation (3) in redshift space, incorporating all of the relevant higher order terms. However, we instead simply calculate the full redshift-space 21 cm power spectrum and compare it with the decomposition above.

The results of this calculation are shown in Figure 10 for a range of different redshifts and ionization fractions. In the top panel we show the redshift-space monopole in units of mK$^2$, which can be more easily compared with observational noise estimates than the dimensionless 21 cm power, which we plotted previously for simplicity. The top panel shows the usual qualitative behavior for the 21 cm power spectrum redshift evolution (Furlanetto et al. 2004b; Zahn et al. 2007): spatial fluctuations in the hydrogenic neutral fraction imprint a knee in the 21 cm power spectrum on large scales when the H II regions become sufficiently large.

The bottom panel of the figure shows the fractional effect of the higher order terms on the redshift-space monopole. First, let us focus on the small-scale behavior. If we focus on the $z = 6.89$ curve for the moment and compare it with its real-space analog (Fig. 1), it seems that the effect is slightly enhanced in redshift space, resulting in a difference of up to a factor of $\sim 3$ from the low-order calculation. This presumably results because peculiar velocities introduce additional three-point terms, above and beyond the ones in equation (3), that are neglected in the usual decomposition.

At high redshift, $z = 8.16$, when the volume-weighted ionization fraction is $x_{\text{HI}} = 0.11$ in our model, the small-scale suppression is less significant than at $z = 6.89$. This results because $\langle \delta_x, \delta_y \rangle$ is smaller at this redshift than at our fiducial redshift ($\langle \delta_x, \delta_y \rangle = -0.12$, compared to $\langle \delta_x, \delta_y \rangle = -0.25$, amounting to a factor of $\sim 2$ less suppression (see eq. [8])). Finally, at the lowest redshift considered here, $z = 6.56$, where the volume-weighted ionization fraction is $x_{\text{HI}} = 0.70$, the small-scale suppression is less significant again. This occurs because the four-point function becomes more significant at low neutral fraction and partly compensates for the suppression of the three-point function. Roughly speaking, the four-point function term is generated by $\langle \delta_x \rangle^2$, while the three-point function term is generated by $\langle \delta_x \delta_y \rangle$ (see eqs. [10] and [8]). Since $\langle \delta_x \rangle$ grows more rapidly with decreasing neutral fraction than does $\langle \delta_x \delta_y \rangle$ (Zahn et al. 2007), the four-point function becomes more significant relative to the three-point term at $x_{\text{HI}} \gtrsim 0.5$, reducing the small-scale suppression, as seen in the figure.

What about the effect of the higher order terms on large scales? The figure clearly shows that the higher order terms are generally nonvanishing even on quite large scales, with the smallest effect occurring at our fiducial redshift of $z = 6.89$, when the ionization fraction is $x_{\text{HI}} \sim 0.5$. Second, note that the dependence on ionization fraction/redshift is not monotonic, with low ionization fractions resulting in a suppression of the 21 cm power spectrum signal, intermediate ionization fractions yielding an enhanced signal, and the high ionization fraction leading to a suppressed signal on large scales again. These large-scale effects are unrelated to gravitational instability and have their origin in the fact that in our models, high-density regions tend to ionize first. Just as in the small-scale case, their amplitude is relatively large because the fluctuations in the neutral fraction are large. The behavior of
the higher order terms on large scales depends on whether it is the density or $\chi$ that dominates the correlations. The cross terms have different signs in both limits, so they go through a minimum around the midpoint of reionization (see § 6).

7. CONCLUSIONS

In this paper, we demonstrated the significant impact of higher order terms on 21 cm power spectrum predictions. While on small scales the effect originates in the mode-mode coupling induced by gravitational instability, on large scales it is unrelated to gravity. It originates in the fact that high-density regions tend to ionize first. We showed that these effects can help distinguish between different models for the ionizing sources and can constrain how well ionized regions trace large-scale overdensities. Finally, we demonstrated that these effects can be captured in semianalytic calculations by using second-order Lagrangian perturbation theory. These techniques will be useful for exploring the large regions of parameter space that are relevant for upcoming 21 cm surveys.

How important are these effects for upcoming 21 cm surveys? The first generation of 21 cm experiments, such as MWA and LOFAR, will likely be sensitive only to modes with $k \lesssim 1 \ h \, \text{Mpc}^{-1}$ (Bowman et al. 2006; McQuinn et al. 2006), so only the large-scale effects that we discussed will be relevant. We showed that the higher order terms can be significant on larger scales to the extent that ionized regions trace large-scale overdensities, providing important information regarding the morphology of reionization. The subsequent generation of experiments, such as SKA, should extend power spectrum measurements to $k \sim 10 \ h \, \text{Mpc}^{-1}$ (Bowman et al. 2006; McQuinn et al. 2006), in which case our small-scale effect should be extremely important, unless the IGM is reionized by very rare sources.

Another natural question is: is there a statistic that isolates the mode-coupling effect described in this paper? As the 21 cm power spectrum is produced by several unknowns simultaneously, such a statistic would help to isolate the degree of correlation between the density and ionization fields. We examined higher order statistics in the vein of Zaldarriaga et al. (2001) to try and isolate our effect, but we find that the 21 cm three-point function involves terms $\propto |P_{\delta, \chi}(k)|_{\text{large}} |P_{\delta, \chi}(k)|_{\text{small}}$, where “large” and “small” refer to the large and small scales, respectively, that are nonvanishing even in the absence of correlations between the density and ionization fields. This makes it difficult to disentangle the effect of interest, but further work in this direction might be interesting.

In future work, we will forecast constraints for upcoming 21 cm surveys using the 2LPT scheme presented here (O. Zahn et al. 2007, in preparation). Finally, it might be interesting to investigate whether analogous three-point terms are important for accurate predictions of the kinetic Sunyaev-Zel’dovich effect.

We thank Steve Furlanetto for helpful comments on a draft, Roman Scoccimarro for providing us with his 2LPT code and for helpful discussions, and Volker Springel for discussions regarding the high-redshift density power spectrum. The authors are supported by the David and Lucile Packard Foundation, the Alfred P. Sloan Foundation, and NASA grants AST 05-06556 and NNG05GJ40G.

REFERENCES

McQuinn, M., Zahn, O., Zaldarriaga, M., Hernquist, L., & Furlanetto, S. R. 2006, ApJ, 653, 815
Morozevich, M. F. 2005, ApJ, 619, 678
Navarro, J. F., & Steinmetz, M. 1997, ApJ, 478, 13
Peacock, J. A., & Dodds, S. J. 1996, MNRAS, 280, L19
Pen, U.-L., Wu, X.-P., & Peterson, J. 2004, preprint (astro-ph/0404083)
Pritchard, J. R., & Furlanetto, S. R. 2007, MNRAS, in press (astro-ph/0607234)
Ricotti, M., & Ostriker, J. P. 2004, MNRAS, 352, 547
Scoccimarro, R. 1998, MNRAS, 299, 1097
———. 2000, ApJ, 544, 597
Scott, D., & Rees, M. J. 1990, MNRAS, 247, 510
Sokasian, A., Abel, T., & Hernquist, L. 2001, NewA, 6, 359
Sokasian, A., Abel, T., Hernquist, L., & Springel, V. 2003, MNRAS, 344, 607
Springel, V. 2005, MNRAS, 364, 1105
Springel, V., et al. 2005, Nature, 435, 629
Thoul, A. A., & Weinberg, D. H. 1996, ApJ, 465, 608
Zahn, O., Lidz, A., McQuinn, M., Dutta, S., Hernquist, L., Zaldarriaga, M., & Furlanetto, S. R. 2007, ApJ, 654, 12
Zahn, O., Zaldarriaga, M., Hernquist, L., & McQuinn, M. 2005, ApJ, 630, 657
Zaldarriaga, M., Furlanetto, S. R., & Hernquist, L. 2004, ApJ, 608, 622
Zaldarriaga, M., Seljak, U., & Hui, L. 2001, ApJ, 551, 48
Zhang, J., Hui, L., & Haiman, Z. 2007, MNRAS, 375, 324

Abel, T., & Walant, D. B. 2002, MNRAS, 330, L53
Barkana, R., & Loeb, A. 2001, Phys. Rep., 349, 125
Bernardeau, F., Colombi, S., Gaztañaga, E., & Scoccimarro, R. 2002, Phys. Rep., 367, 1
Bowman, J. D., Morales, M. F., & Hewitt, J. N. 2006, ApJ, 638, 20
Buchert, T., Melott, A. L., & Weiss, A. G. 1994, A&A, 288, 349
Chen, X., & Miralda-Escudé, J. 2004, ApJ, 602, 1
Ciardi, B., & Madau, P. 2003, ApJ, 596, 1
Cooray, A., & Sheth, R. 2002, Phys. Rep., 372, 1
Crocce, M., Pueblas, S., & Scoccimarro, R. 2006, MNRAS, 373, 369
Dijkstra, M., Haiman, Z., Rees, M. J., & Weinberg, D. H. 2004, ApJ, 601, 666
Furlaneto, S. R. 2006, MNRAS, 371, 867
Furlaneto, S. R., McQuinn, M., & Hernquist, L. 2006a, MNRAS, 365, 115
Furlaneto, S. R., Oh, S. P., & Briggs, F. 2006b, Phys. Rep., 433, 181
Furlaneto, S. R., Sokasian, A., & Hernquist, L. 2004a, MNRAS, 347, 187
Furlaneto, S. R., Zaldarriaga, M., & Hernquist, L. 2004b, ApJ, 613, 1
———. 2004c, ApJ, 613, 16
Gnedin, N. Y., & Hui, L. 1998, MNRAS, 296, 44
Iliev, I. T., Mellema, G., Pen, U.-L., Merz, H., Shapiro, P. R., & Alvarez, M. A. 2006, MNRAS, 369, 1625
Jing, Y. P. 2005, ApJ, 620, 559
Madau, P., Meiksin, A., & Rees, M. J. 1997, ApJ, 475, 429
McQuinn, M., Lidz, A., Zahn, O., Dutta, S., Hernquist, L., & Zaldarriaga, M. 2007, MNRAS, in press (astro-ph/0610094)