RECONSTRUCTING THE INITIAL DENSITY FIELD OF THE LOCAL UNIVERSE: METHODS AND TESTS WITH MOCK CATALOGS

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ABSTRACT

Our research objective in this paper is to reconstruct an initial linear density field, which follows the multivariate Gaussian distribution with variances given by the linear power spectrum of the current cold dark matter model and evolves through gravitational instabilities to the present-day density field in the local universe. For this purpose, we develop a Hamiltonian Markov Chain Monte Carlo method to obtain the linear density field from a posterior probability function that consists of two components: a prior of a Gaussian density field with a given linear spectrum and a likelihood term that is given by the current density field. The present-day density field can be reconstructed from galaxy groups using the method developed in Wang et al. Using a realistic mock Sloan Digital Sky Survey DR7, obtained by populating dark matter halos in the Millennium simulation (MS) with galaxies, we show that our method can effectively and accurately recover both the amplitudes and phases of the initial, linear density field. To examine the accuracy of our method, we use N-body simulations to evolve these reconstructed initial conditions to the present day. The remodeled density field thus obtained accurately matches the original density field of the MS in the density range $0.3 \lesssim \rho/\bar{\rho} \lesssim 20$ without any significant bias. In particular, the Fourier phases of the remodeled density fields are tightly correlated with those of the original simulation down to a scale corresponding to a wavenumber of $\sim 1 h \, \text{Mpc}^{-1}$, much smaller than the translinear scale, which corresponds to a wavenumber of $\sim 0.15 h \, \text{Mpc}^{-1}$.

Key words: dark matter – galaxies: halos – large-scale structure of universe – methods: statistical

Online-only material: color figures

1. INTRODUCTION

In the current cold dark matter (CDM) cosmogony, a key concept in the buildup of structure is the formation of dark matter halos. These are quasi-equilibrium systems of dark matter, formed through nonlinear gravitational collapse. In a CDM-like hierarchical scenario, most of the mass is bound within halos; galaxies and other luminous objects are assumed to form in these halos because of cooling and condensation of baryonic gas (see Mo et al. 2010). With N-body simulations, the properties of the halo population, such as the spatial clustering properties, the mass function, the assembly histories, and the internal structures, are well understood. Nevertheless, how galaxies form in dark matter halos in the cosmic density field remains an unsolved problem. A long-standing problem in current galaxy formation theory is explaining the low efficiency with which baryonic gas is converted into stars: the observed mass in stars at the present time is less than 10% of the total baryonic mass in the universe (Bell et al. 2003). Including cold gas associated with galaxies only increases this fraction to $\sim 12\%$. This low efficiency of star formation and gas assembly into galaxies is not a natural consequence of hierarchical formation, in which the gas is expected to cool rapidly at high redshift in low-mass dark matter halos. A number of physical processes have been proposed to suppress gas cooling and the star formation efficiency. These include photoionization heating by the UV background (e.g., Efstathiou 1992; Thoul & Weinberg 1996; Somerville 2002; Gnedin 2000; Hoeft et al. 2006), feedback from supernova explosions (e.g., White & Rees 1978; Dekel & Silk 1986) and active galactic nuclei (AGNs; e.g., Tabor & Binney 1993; Ciotti & Ostriker 1997; Hopkins et al. 2006, and references therein; Wang et al. 2012b), pre-heating by star formation/AGNs (e.g., Mo & Mao 2002), and pre-heating by pre-virialization (Mo et al. 2005). Unfortunately, our understanding of all these processes is still poor, making it difficult to test the predictions of these scenarios with observations.

In order to understand the galaxy formation processes throughout the cosmic density field, a key step is to study the distributions and properties of galaxies and the intergalactic medium (IGM) and their interactions with each other and with dark matter. In the local universe, detailed observations of the galaxy population are now available from large redshift surveys, for example, the Sloan Digital Sky Survey (SDSS; York et al. 2000). These surveys not only allow us to study the large-scale structure in the local universe, but they can also be used to derive a large number of physical quantities characterizing the intrinsic properties of individual galaxies, such as luminosity, stellar mass, color, morphology, size, star formation rate, and nuclear activity. There have also been observational programs dedicated to the various aspects of the IGM. Extensive X-ray observations have been conducted to study the hot gas associated with clusters and rich groups of galaxies but the total gas mass associated with these systems is expected to be small.
With the advent of accurate measurements of the cosmic microwave background from observations, such as the South Pole Telescope, the Atacama Cosmology Telescope, and the Planck satellite, one can also probe the hot, diffuse gas outside clusters and groups through the Sunyaev–Zel’dovich (SZ) effect. However, at low redshift, about 70% of all the mass is in virialized halos with virial temperatures below $10^6$ K (see Mo & White 2002), too cold to be studied with X-ray data and/or the SZ effect. A promising way to study the diffuse IGM at such low temperatures is through quasar absorption lines. With the installation of the Cosmic Origins Spectrograph on the Hubble Space Telescope, the sample of UV absorption systems at low redshift is expected to increase by an order of magnitude or more, allowing a much more detailed examination of the warm component of the local IGM.

These observational programs together provide an unprecedented database to study how galaxies form and evolve in the cosmic density field. However, in order to make full use of the potential of the observational data to test models, one has to develop an optimal strategy. Conventionally, one starts with a cosmological model, e.g., the current $\Lambda$CDM model, and uses computer simulations to follow the evolution of the cosmic density field. These simulation results are then compared with observational data in a statistical way. However, such a comparison can be made directly only under the assumption that the observational sample and simulation are fair representations of the universe, so that cosmic variance is not an issue. Unfortunately, this assumption is almost always violated in reality. Simulations are limited by the dynamic ranges they can cover. In order to resolve processes on the scale of galaxies, the simulation volume has often to be much smaller than a fair sample of the large-scale structure. Observationally, finite sample volumes also lead to a biased representation of the statistical properties of the cosmic density field and the galaxy population in the universe.

It is thus imperative to have theoretical and empirical inputs to optimize an observational strategy and to help interpret the limited observations in an unbiased way. The uncertainties can be minimized if comparisons between observations and model predictions are made for systems that have both the same environments and the same formation histories. Ideally, if we can accurately reconstruct the initial conditions for the formation of the structures in which the observed galaxy population resides and from which the actual gas emissions and absorptions are produced, then we will be able to compare observations and simulations (i.e., data and theory) in a way that is free of cosmic variance, thereby greatly enhancing the constraining power of the observational data.

The goal of this paper is to develop a method that can be used to reconstruct the initial (linear) density field that forms the large-scale structure in the local universe. In this first paper in a series, we describe our reconstruction method and test its performance with realistic mock galaxy catalogs. The structure of the paper is arranged as follows. In Section 2, we describe our reconstruction method. In Section 3, we test our method using a simulated density field. In Section 4, we present our mock catalog that is used to test our method and our results of the linear density field reconstructed from it. In Section 5, we use $N$-body simulations to follow the structure formation seeded by the reconstructed initial density field and compare the final density field with the original one used to construct the mock catalogs. Finally, Section 6 contains a summary of the main results and some further discussions.

In order to avoid confusion, we list here the various matter density fields used in the text. (1) The final density field, $\rho(x)$: the true present-day (final) density field, either in the real universe or in an original $N$-body simulation. (2) The reconstructed density field, $\rho_{\text{rec}}(x)$: the present-day density field reconstructed from the mock catalog. (3) The reconstructed initial (linear) density field: the initial linear density reconstructed from a present-day density field. (4) The resimulated density field, $\rho_{\text{resim}}(x)$: the present-day density field obtained from numerical $N$-body simulations using the reconstructed initial density field as initial conditions. (5) The modeled density field, $\rho_{\text{mod}}(x)$: a model prediction for the present-day density field obtained from the initial density field using the modified Zel’dovich approximation (MZA) introduced by Tassev & Zaldarriaga (2012b, hereafter TZ12). This model density field is used in the reconstruction method to link the initial and final density fields.

2. METHOD

Our reconstruction consists of the following several steps: (1) use galaxy groups$^6$ selected from the SDSS, to represent dark matter halos; (2) use halos above a certain mass to reconstruct the cosmic density field at the present day; and (3) reconstruct the initial density field that best matches the final density field under the constraint of current cosmology and a linear perturbation spectrum. The galaxy group finder used is described and tested in detail in Yang et al. (2005, 2007). The method for reconstructing the density field starting from dark matter halos (i.e., galaxy groups) above a given mass threshold is described and tested in Wang et al. (2009b, 2012a). In what follows, we describe how we reconstruct the initial linear density field from a given present-day density field.

2.1. Objectives and the Posterior Probability Distribution

Our goal is to obtain the linear density field that can reproduce a given present-day density field. We work in Fourier space, so that the initial density field is specified by $\delta(k)$, the Fourier modes of the initial density field. Two constraints are used in the reconstruction. First, according to the standard cosmology, we assume the linear density field to be Gaussian, so that the Fourier modes obey the following probability distribution:

$$P[\delta_j(k)] = \prod_{k} \frac{1}{\pi P_{\text{lin}}(k)}^{1/2} \exp\left[-\frac{[\delta_j(k)]^2}{P_{\text{lin}}(k)}\right],$$

where $P_{\text{lin}}(k)$ is the (analytical) linear power spectrum and the subscripts $j = 0, 1$ denote the real and imaginary parts, respectively. Because $\delta(k)$ is the Fourier transform of a real field, $\delta(k) = \delta^*(-k)$ so that only the Fourier modes in the upper half-space (i.e., with $k_z \geq 0$) are needed. Second, the density field, $\rho_{\text{mod}}(x)$, evolved from this linear density field according to a chosen model of structure formation, should best match a present-day density field, $\rho_{\text{f}}(x)$. In other words, we seek the appropriate $\delta(k)$ to minimize a “cost parameter” that we define as

$$\chi^2 = \sum_x \frac{[\rho_{\text{mod}}(x) - \rho_{\text{f}}(x)]^2}{2\sigma_x^2},$$

where $\sigma_x$ is the error on the density.

$^6$ We use “galaxy group” to refer a galaxy system (a cluster or a group) without regard to its richness.
where $\sigma_p(x)$ is the statistical uncertainty in $\rho_p(x)$ and $\omega(x)$ is a weight function used to account for the survey geometry. The present-day density field, $\rho_p$, may either be the original simulated density field ($\rho_p$; Section 3) or the density field reconstructed from a galaxy redshift survey ($\rho_r$; Section 4). The uncertainties $\sigma_p(x)$ are found to be roughly proportional to $\rho_p(x)$ (see Section 4.2), and so we set $\sigma_p(x) = \mu \rho_p(x)$, with $\mu$ being a constant parameter. In order to obtain the model prediction for the final density field, we need a model to link $\rho_{mod}(x)$ with $\delta(k)$. This model should not only be accurate, but should also be efficient so that the computation can be achieved in a reasonable amount of time, as discussed in Section 2.3.

In practice, all these fields are to be sampled in a periodic box of length $L$ on a side, divided into $N_c$ grids in each dimension, so that the number of Fourier modes to be dealt with is finite.

Because of the statistical uncertainties in $\rho_p(x)$ and the finite survey volume, the solution for $\delta(k)$ under the two constraints described above is not unique, but should obey the posterior probability distribution of $\delta(k)$. Assuming that the likelihood of $\rho_{mod}(x)$ given $\rho_p(x)$ is $\exp(-\chi^2)$, the posterior probability distribution for $\delta(k)$ given $\rho_p(x)$ can be written as

$$Q(\delta(k)|\rho_p(x)) = e^{-\sum_k[r_{mod}(x) - \rho_{mod}(x)]^2/2\sigma^2_k} \times \prod_k \frac{1}{\sqrt{2\pi}P_{lin}(k)} e^{-[\delta(k)]^2/P_{lin}(k)}.$$

(3)

For our purpose, we seek the solutions for $\delta(k)$ that maximize this posterior probability distribution function.

We use the Hamiltonian Markov Chain (HMC) Monte Carlo technique to achieve our goal. The HMC method was originally developed to sample a posterior distribution (Duane et al. 1987; Neal 1996) and has proven to be effective for exploring large, multi-dimensional posterior spaces (e.g., Hanson 2001). Different from the conventional Markov Chain Monte Carlo technique, the HMC method introduces a persistent motion of the Markov Chain when exploring the parameter space so that the random walk is greatly suppressed and the efficiency is much improved (Duane et al. 1987). This method has already been widely used in astrophysics and cosmology (see Hajian 2007; Taylor et al. 2008; Jasche & Kitaura 2010; Kitaura et al. 2012b; Jasche & Wandelt 2013, hereafter JW13; Kitaura 2013). For example, both JW13 and Kitaura (2013) developed methods incorporating the HMC to reconstruct the initial density field from a galaxy distribution. In particular, JW13 used a posterior distribution function composed of a Poissonian likelihood based directly on galaxy distribution and a prior distribution of the initial density field. They successfully drew a sample of the initial density field from their posterior distribution, demonstrating that HMC is a powerful method for reconstructing the initial density field. In principle, such a sample can be used to inspect the statistical uncertainties in the reconstruction. However, this kind of analysis requires a careful design of the likelihood function to take into account in detail the statistical uncertainties in the constraining data and in the model of the cosmic density field. Our basic idea is similar to that of JW13, but for our purpose described above we restrict ourselves to seeking the maximum posterior estimates of $\delta(k)$ instead of obtaining the posterior distribution of $\delta(k)$. As we will demonstrate below using realistic mock catalogs constructed from a cosmological $N$-body simulation, our HMC method based on the likelihood function defined above is sufficient for this research objective.

### 2.2. The Hamiltonian Monte Carlo Method

In this subsection, we briefly outline the HMC method (see Hanson 2001; Taylor et al. 2008; JW13, for more detailed descriptions). The method is itself based on an analogy to solving a physical system in Hamiltonian dynamics. As a first step, we define the potential of the system to be the negative of the logarithm of the target probability distribution,

$$\psi[\delta_j(k)] = -\ln[Q(\delta_j(k)|\rho_p(x))] = \sum_k \ln[\pi P_{lin}(k)] + \sum_k \frac{1}{2} \frac{[\delta_j(k)]^2}{P_{lin}(k)} + \sum_x \frac{[\rho_{mod}(x) - \rho_p(x)]^2}{2\sigma^2_p(x)}.$$

(4)

For each $\delta_j(k)$, a momentum variable, $p_j(k)$, and a mass variable, $m_j(k)$, are introduced. The Hamiltonian of the fictitious system can then be written as

$$H = \sum_k \frac{1}{2} \frac{p_j^2(k)}{m_j(k)} + \psi[\delta_j(k)].$$

(5)

The statistical properties of the system are given by the partition function, $\exp(-H)$, which can be separated into a Gaussian distribution in momenta $p_j(k)$ multiplied by the target distribution,

$$\exp(-H) = Q(\delta_j(k)|\rho_p(x)) \prod_k \frac{1}{\sqrt{2\pi}m_j(k)} e^{-p_j^2(k)/2m_j(k)}.$$  

(6)

Thus, the target probability distribution can be obtained by first sampling this partition function and then marginalizing over momenta (i.e., setting all the momenta to zero).

In order to sample from the partition function, we first pick a set of momenta $p_j(k)$ randomly from the multi-dimensional uncorrelated Gaussian distribution with variances $m_j(k)$. We describe how to pick the mass variables in Section 2.4. We then evolve the system from the starting point $[\delta_j(k), p_j(k)]$ in phase space to some pseudotime $T$ according to the Hamilton equations,

$$\frac{d\delta_j(k)}{dt} = \frac{\partial H}{\partial p_j(k)} = \frac{p_j(k)}{m_j(k)};$$

$$\frac{dp_j(k)}{dt} = -\frac{\partial H}{\partial \delta_j(k)} = -\frac{2\delta_j(k)}{P_{lin}(k)} - F_j(k),$$

(7)

(8)

where $F_j(k) = \partial \chi^2/\partial \delta_j(k)$ is the likelihood term of the Hamiltonian force discussed below. The integrated trajectory finally reaches a point $[\delta_j(k), p_j(k)]$ in phase space and we accept this state with a probability

$$p = \min \left\{ 1, e^{-[H(\delta_j(k), p_j(k)) - H(\delta_j(k), p_j(k))]} \right\}. $$

(9)

The procedure is repeated by randomly picking a new set of momenta.

Since the Hamiltonian of a physical system is conserved, the acceptance rate should in principle be unity, which is one of the main advantages of working with the partition function,
exp(\(-H\)), instead of the target distribution function itself. However, rejection may occur because of numerical errors. In order to optimize the acceptance rate, it is common practice to integrate the “equations of motion” using the leapfrog technique,

\[
p_j(k, t + \tau / 2) = p_j(k, t) - \frac{\tau}{2} \frac{\partial H}{\partial \delta_j(k)} \bigg|_t
\]

\[
\delta_j(k, t + \tau) = \delta_j(k, t) + \frac{\tau}{m_j(k)} p_j(k, t + \tau / 2); \tag{11}
\]

\[
p_j(k, t + \tau) = p_j(k, t + \tau / 2) - \frac{\tau}{2} \frac{\partial H}{\partial \delta_j(k)} \bigg|_{t+\tau}, \tag{12}
\]

where \(\tau\) represents the time increment for the leapfrog step. The leapfrog technique uses half-time steps in Equations (10) and (12) so that the scheme is accurate to the second order in \(\tau\). The equations are integrated for \(n\) steps so that \(n\tau = T\). The value of \(T\) must be randomized to avoid resonance trajectories. We thus randomly pick \(n\) and \(\tau\) from two uniform distributions in the range of \([1, n_{\text{max}}]\) and \([0, \tau_{\text{max}}]\), respectively. We will discuss our choices of \(n_{\text{max}}\) and \(\tau_{\text{max}}\) below. The \(n\) leapfrog steps are referred to as one chain step.

### 2.3. The Hamiltonian Force and the Structure Formation Model

As shown in Equation (8), the Hamiltonian force consists of two components, the prior term, 2\(\delta_j(k)/\rho_{\text{mod}}(k)\), and the likelihood term, \(F_j(k)\). The latter can be rewritten as

\[
F_j(k) = \sum_x \left[ \rho_{\text{mod}}(x) - \rho_p(x) \right] \omega(x) \frac{\partial \rho_{\text{mod}}(x)}{\partial \delta_j(k)} = \sum_x \rho_d(x) \frac{\partial \rho_{\text{mod}}(x)}{\partial \delta_j(k)} = \sum_{k_2} \rho_d(k_2) e^{i k_2 \cdot x} \frac{\partial}{\partial \delta_j(k)} \sum_{k_1} \rho_{\text{mod}}(k_1) e^{i k_1 \cdot x} = N^3 \sum_{k_1} \rho_d(k_1) \frac{\partial \rho_{\text{mod}}(k_1)}{\partial \delta_j(k)}, \tag{13}
\]

For the sake of simplicity, we have introduced in this equation a new quantity, \(\rho_d(x)\), which is directly related to \(\rho_{\text{mod}}(x)\), as defined in the second equation.

To derive the solution of the Hamiltonian force, we need a model of structure formation to connect \(\rho_{\text{mod}}(k)\) and \(\delta(k)\). In this work, we adopt the model developed in TZ12. According to TZ12, the present-day density field can be written in terms of the modeled density field, \(\rho_{\text{mod}}\), as \(\rho_p(k) = \rho_{\text{mod}}(k) + \rho_{\text{res}}(k)\). Here, \(\rho_{\text{res}}(k)\), a random mode-coupling residual, is generally small on mildly nonlinear scales and can be neglected. The modeled density can be obtained via \(\rho_{\text{mod}}(k) = R_N(k) \rho_{\text{MZ}}(k)\), where \(\rho_{\text{MZ}}\) is the density field predicted by the MZA developed by TZ12 and \(R_N(k)\) is a density transfer function. The transfer function is obtained by comparing the prediction of the Zel’dovich approximation (Zel’dovich 1970) with \(N\)-body simulations and can suppress the effects of shell crossing. Using numerical simulations as a reference, TZ12 found that the prediction of MZA is better (worse) than that of the second-order Lagrangian perturbation theory (2LPT) on small (large) scales. Because the MZA is computationally faster than the 2LPT, we choose the MZA to predict the present-day density field. Following TZ12, we use the MZA to derive the displacement field, \(s(q)\),

\[
s(q) = \sum_{k_2} s(k_2) e^{i k_2 \cdot q} = \sum_{k_2} R_c(k_2) s_2(k_2) e^{i k_2 \cdot q} = \sum_{k_2} R_c(k_2) \frac{i k_2}{k_2^2} \delta(k_2) e^{i k_2 \cdot q}, \tag{14}
\]

where \(q\) is a Lagrangian coordinate, \(s_2(k_2)\) is the Zel’dovich displacement field, and \(R_c(k_2) = \exp(-0.085k_2 / k_{NL}^2)\) is the transfer function for the Zel’dovich displacement field, with \(k_{NL}\) being the nonlinear scale at redshift zero. We move particles, which are initially located on uniform grids of positions \(q\), to \(x(q) = q + s(q)\) to sample the density field. We then utilize a clouds-in-cells (CIC) assignment (Hockney & Eastwood 1981) to construct the MZA density field on grids from the particle population. We Fourier transform the MZA density, and multiply it by the density transfer function \(R_N(k) = \exp(0.58d)\), where \(d \equiv \delta^2(k/2)\), and the Gaussian kernel \(w_{\text{CIC}}(R, k)\) characterized by a smoothing scale \(R_s\). We then deconvolve the CIC kernel by dividing the resulting density field in Fourier space by the Fourier transform of the CIC kernel, \(w_{\text{CIC}}(k) = \text{sinc}(kL/2N) \text{sinc}(kL/2N) \text{sinc}(kL/2N)\), where \(k_s, k_v, k_e\) are the \(x, y, z\) components of the wavevector \(k\), respectively. Finally, we obtain the modeled density field as

\[
\rho_{\text{mod}}(k_1) = \frac{R_s(k_1) w_{\text{CIC}}(R_s)}{N_c^3} \sum_q e^{-i k_1 \cdot x_q}. \tag{15}
\]

Inserting Equations (14) and (15) together with \(x(q) = q + s(q)\) into Equation (13) then yields the likelihood term of the Hamiltonian force:

\[
F_j(k) = \sum_{k_1} \rho_d(k_1) R_s(k_1) w_{\text{CIC}}(R_s) \sum_q e^{-i k_1 \cdot x_q} \frac{\partial}{\partial \delta_j(k)} (q) = \sum_{k_2} R_c(k_2) \frac{i k_2}{k_2^2} \sum_q e^{i k_2 \cdot q} \sum_{k_1} (-i k_1) \rho_d(k_1) R_s(k_1) w_{\text{CIC}}(R_s) e^{-i k_1 \cdot x_q}. \tag{16}
\]

Note that \(\partial x / \partial \delta_j(k) = \partial s / \partial \delta_j(k)\) is used in the derivation. For convenience, we introduce a density-vector field,

\[
\Psi(q) = \sum_{k_1} (-i k_1) \rho_d(k_1) R_s(k_1) w_{\text{CIC}}(R_s) e^{-i k_1 \cdot x_q}. \tag{17}
\]

It is important to note that \(\Psi(q)\) cannot be directly derived with a Fourier transformation because \(x(q)\) are not regularly spaced. To bypass this problem, we introduce a transitional field in Fourier space, \(\Gamma(k_1) = N^3 \sum_{k_1} (-i k_1) \rho_d(k_1) R_s(k_1) w_{\text{CIC}}(R_s)\), which is related to the density vector through \(\Psi(q) = \Gamma[-x(q)] = \Gamma(L - x(q))\), with \(\Gamma(x)\) being the Fourier transform of \(\Gamma(k_1)\) and the vector \(L = (L, L, L)\). One might think that the density-vector field can be derived straightforwardly via interpolation. Unfortunately, interpolation can cause smoothing and serious errors in the final estimation of the Hamiltonian force. In order to correct for these effects, we proceed as follows. We first divide \(\Gamma(k_1)\) by \(w_{\text{CIC}}(k_1)\) to deconvolve the CIC interpolation

7 Both \(k_{NL}\) and \(\delta^2\) can be read off from Equation (3.9) in TZ12. The detailed form of the density transfer function for the MZA was communicated to us by Svetlin Tassev.
that is applied later. We then Fourier transform the deconvolved \( \Gamma(k_1) \) into real space to obtain \( \Gamma(x) \). Finally, we interpolate \( \Gamma'(x) \) to the position \( L - x(q) \) to obtain \( \Psi(q) \) via a CIC scheme. We emphasize again that deconvolving the CIC kernel is crucial for obtaining an accurate estimate of the Hamiltonian force (see Section 3). With \( \Psi(q) \), we obtained, we can rewrite the Hamiltonian force as

\[
F_j(k) = \sum_{k_2} R_z(k_2) \frac{\partial \delta(k_2)}{\partial \delta_j(k)} (i k_2) \sum_q 1_N q e^{i k_2 q} \Psi(q)
\]

\[
= \sum_{k_2} R_z(k_2) \frac{\partial \delta(k_2)}{\partial \delta_j(k)} (i k_2) \Psi^*(k_2),
\]

where \( \Psi(k_2) \) is the Fourier transform of \( \Psi(q) \). Again, the last equation cannot be obtained directly from Fourier transforms since the signs in the exponents are not negative; it is obtained using the fact that \( e^{i k_2 q} = e^{-i(k_2 q)} \) and \( \Psi(-k_2) = \Psi^*(k_2) \).

Since \( \delta(k_2)/\delta_j(k) \) is nonzero only when \( k_2 = \pm k \), the likelihood term of the Hamiltonian force for the real part of \( \delta(k) \) can be obtained as

\[
F_0(k) = \frac{2 R_z(k)}{k^2} k \cdot \Psi_1(k),
\]

and for the imaginary part as

\[
F_1(k) = -\frac{2 R_z(k)}{k^2} k \cdot \Psi_0(k),
\]

where \( \Psi_0(k) \) and \( \Psi_1(k) \) are the real and imaginary parts of \( \Psi(k) \), respectively. It is interesting to note that the formulae for the Hamiltonian force are very similar to the gravitational force respectively. It is interesting to note that the formulae for the Hamiltonian force are very similar to the gravitational force equation in Fourier space if we consider \( \Psi^*(k) \) as the mass density field.

### 2.4. The Hamiltonian Mass and Other Adjustable Parameters

The method described above has two free parameters: the Hamiltonian masses \( m_j(k) \) and the pseudotime \( T \). The efficiency of the HMC method is strongly dependent on the choices of these parameters. Taylor et al. (2008) suggested that a variable’s Hamiltonian mass is inversely proportional to the width of the target probability distribution; Hanson (2001) suggested almost the opposite. In this paper, we take a different and much simpler approach.

When the Hamilton equations are evolved to a pseudotime \( T \), the change in \( \delta_j(k) \) is, to a first-order approximation

\[
\Delta \delta_j(k) \approx \frac{T}{m_j(k)} P_{lin}(k) - \left[ \frac{2 \delta_j(k)}{P_{lin}(k)} + F_j(k) \right] \frac{T^2}{m_j(k)}.
\]

To ensure the convergence of the Hamiltonian system, \( \Delta \delta_j(k) \) cannot be much larger than \( \delta_j(k) \). We thus require that both the first and second terms of \( \Delta \delta_j(k) \) be of the same order as or less than \( \sqrt{P_{lin}(k)/2} \), the root mean square (rms) of \( \delta_j(k) \). Let us first consider the second term. Supposing \( T \sim 1 \), one can deduce that the mass is of the same order as (or less than) \( \delta_j(k)/(P_{lin}(k)/2)^{1/2} + F_j(k)/\sqrt{P_{lin}(k)/2} \). We therefore define the Hamiltonian mass as

\[
m_j(k) \equiv m(k) = \frac{2}{P_{lin}(k)} + \sqrt{\sum_{q=0}^{l=\infty} \langle \Omega_q^2(k) \rangle_k},
\]

where \( \langle \cdots \rangle_k \) denotes the average over the phase of \( k \). Note that the first and second terms in the mass equation are actually the rms of \( \delta_j(k)/(P_{lin}(k)/2)^{1/2} \) and \( F_j(k)/\sqrt{P_{lin}(k)/2} \), respectively. Since the momentum \( p_j(k) \) follows a Gaussian distribution with a variance \( m_j(k) \), i.e., \( p_j(k) \sim \sqrt{m_j(k)} \), our mass definition also ensures that the first term in Equation (21) is comparable to or less than \( \sqrt{P_{lin}(k)/2} \). For consistency, we set \( n_{\text{max}} = 13 \) and choose \( \tau_{\text{max}} \) around 0.1 to guarantee that \( T \) is of order unity.

The quantities \( \langle F_j^2(k) \rangle_k \) vary significantly before the HMC chain converges and so it is not necessary to compute the masses at every step. In practice, we only calculate the masses twice during the whole sampling. The first calculation is before the generation of the first sample. After proceeding \( n_m \) accepted chain steps, we use the new Hamiltonian forces to update the mass variables and then retain the masses all the way to the end of the sampling. In the next section, we will show that the parameters \( \tau_{\text{max}} \) and \( N_m \) have no important impact on our final results.

### 2.5. Summary of the Method

Given the complicated, technical nature of the method described above, this subsection gives a step-by-step description of the Hamiltonian Monte Carlo method used to reconstruct the linear density field, given a present-day density field, \( \rho_p(x) \). This summary serves as a "road map" for anyone who wishes to implement this powerful method.

1. Pick a cosmology, which sets the analytical, linear power spectrum, \( P_{lin}(k) \).
2. Randomly pick an initial guess for the modes \( \delta(k) \) of the initial density field by specifying the corresponding real and imaginary parts.
3. Pick a set of Hamiltonian masses, \( m_j(k) \), using Equation (22).
4. Randomly draw a set of momenta, \( p_j(k) \), from multidimensional, uncorrelated Gaussian distributions with variances \( m_j(k) \).
5. Randomly pick values for the number of time steps, \( n \), and the leapfrog time steps \( \tau \), from uniform distributions in the range \([1, n_{\text{max}}]\) and \([0, \tau_{\text{max}}]\), respectively. In this paper, we set \( n_{\text{max}} = 13 \) and \( \tau_{\text{max}} = 0.1 \), unless otherwise specified.
6. Integrate the Hamiltonian “equations of motion” using the leapfrog technique (Equations (10)–(12)) for a total pseudotime \( T = n \tau \), starting from \( [\delta_j(k), p_j(k)] \). The detailed numerical operations performed for each time step \( \tau \) are listed below.
7. Accept the new “state” \( [\delta_j'(k), p_j'(k)] \), to which the system has evolved, with a probability given by Equation (9).
8. Go back to step 4 and repeat until the Markov Chain has converged and accumulated the required number of chain elements.

Finally, we list the numerical operations performed in each leapfrog time step \( \tau \) as the following.

1. Starting from the modes \( \delta_j(k) \), use Equation (14) to compute the displacement field, \( s(q) \), and move particles initially located on a uniform rectangular grid with positions \( q \) to \( x(q) = q + s(q) \).
2. Construct the MZA density field utilizing the CIC assignment method of Hockney & Eastwood (1981).
3. Fourier transform this density field using the fast Fourier transform method, and multiply the result by the density
transfer function \( R_g(k) = \exp[0.58\delta^2(k/2)] \) and the Gaussian kernel \( u_{\text{CIC}}(R_g,k) \). Divide the result by the Fourier transform of the CIC kernel to obtain the modeled density field, \( \rho_{\text{mod}}(k) \).

4. Use \( \rho_{\text{mod}}(k) \) to compute \( \rho_\mu(k) \) as described in Equation (13) and use the method described in the paragraph below Equation (17) to compute the density-vector field \( \Psi(q) \).

5. Fourier transform \( \Psi(q) \) to get \( \Psi(k) \) and compute the likelihood term of the Hamiltonian forces using Equations (19) and (20) for the real and imaginary parts, respectively.

6. Use the Hamiltonian forces to evolve the system according to Equations (10)–(12).

The main purpose of using the Gaussian kernel is to suppress noise on the grid size \( L/N_c \) that affects the efficiency of the HMC. We find that using \( R_c \leq 2L/N_c \) results in a quite low acceptance rate, so we adopt \( R_c \geq 3L/N_c \) throughout the paper. The efficiency of our HMC method depends also on the value of \( \mu \), in the sense that a smaller \( \mu \) leads to a lower acceptance rate. In fact, the value of \( \mu \) affects the HMC in a similar way as the smoothing scale \( R_c \), as we will see in the next section. Moreover, in order to achieve good performance, the mass variables and the pseudotime \( T = n \tau \) should not be specified independently, but instead specified according to their combinations in Equation (21). In this paper, we always choose \( T \) to be of order unity and derive the mass variables accordingly.

Finally, we note that our method is very fast. The computations shown below were all performed using one single processor (AMD Opteron 8380, 2.5 GHz). Each chain step took about 21, 2080 s for \( N_c = 128, 256, 512 \), respectively (see Table 1).

### 3. TEST WITH N-BODY SIMULATIONS

In this section, we use the Millennium simulation (MS; Springel et al. 2005) to test our method and tune the adjustable parameters when necessary. This simulation adopts a spatially flat ΛCDM model, with \( \Omega_m = 0.25, \Omega_{\Lambda} = 0.045, h = 0.73, \) and \( \sigma_8 = 0.9 \), where \( h \) is the Hubble constant and \( \sigma_8 \) is the rms amplitude of linear mass fluctuations in a sphere of radius \( 8 h^{-1} \) Mpc. The simulation follows the evolution of the density field with \( 2160^3 \) particles, each having a mass of \( 8.6 \times 10^8 h^{-1} M_{\odot} \), in a cubic box of \( L = 500 h^{-1} \) Mpc. We divide the simulation box into \( N_c^3 \) grid cells and use a Gaussian kernel with a smoothing scale of \( R_c \) to smooth the particle distribution on to the grid (see Table 1 for the values of \( N_c \) and \( R_c \) used). The method used to sample the density field on the grid is the same as that used to calculate \( \rho_{\text{mod}}(x) \) except that now we do not include the density transfer function. The resultant density field, denoted by \( \rho_t(x) \), is what we want to match in the reconstruction (\( \rho_t \equiv \rho_t(x) \)), and we assume \( \sigma_p(x) = \mu \rho_t(x) \) as discussed in Section 2.1.

As discussed in Section 2.1, moreover, \( \omega(x) \) is always set to be unity and the nonlinear scale \( k_{NL} \) used in the transfer function for the Zel'dovich approximation is chosen to be 0.28 h Mpc\(^{-1}\). Before showing the test results, we verify the accuracy of our estimation of the Hamiltonian forces. To this end, let us start with how the forces should be calculated based on their definitions. Suppose we want to calculate the Hamiltonian force for a chosen variable \( \delta_j(k) \). We alter \( \delta_j(k) \) by a small amount, \( \Delta \delta_j(k) \), with all other variables held fixed. This leads to a small variation, \( \Delta \chi^2 \), in the parameter \( \chi^2 \). Consequently, we can obtain the corresponding force numerically, \( F_j(x) = \Delta \chi^2 / \Delta \delta_j(k) \). This is what we would like to have. Unfortunately, this method is very time-consuming and cannot be used to evolve the Hamiltonian system. The left panel of Figure 1 shows a plot of \( F_j(k) \), obtained using Equations (19) and (20), versus \( F_j^\text{IC}(k) \). There is almost no visible difference between these two quantities. We also present a probability distribution of \( F_j(k) / F_j^\text{IC}(k) \) in the right panel of Figure 1. The distribution exhibits a high peak at unity with a shallow, but broad, wing. A further investigation finds that the Hamiltonian forces in the broad wing are very small, which explains why we do not see any scatter in the left panel. We also show the Hamiltonian forces without deconvolving the CIC kernel in deriving the density-vector field \( \Psi(q) \). The resultant \( F_j(k) \) is systematically smaller than \( F_j^\text{IC}(k) \) due to the smoothing with the CIC kernel. This demonstrates that our estimates of the Hamiltonian forces based on Equations (19) and (20) are accurate, and that deconvolution of the CIC kernel is essential.

Now we apply our Hamiltonian method to the MS simulation. We first perform a test with the following parameters: \( N_c = 128, R_c = 11.7 h^{-1} \) Mpc, \( \mu = 0.5 \), and \( \sigma_{\Delta} = 0.1 \). In what follows, this test is referred to as the “primary test.” The initial set of \( \delta_j(k) \) is randomly drawn from the prior probability distribution given by Equation (1). We make calculations of 2000 HMC steps and the average acceptance rate is \( A_r = 72\% \). Figure 2 shows \( \chi^2 = \chi^2 / \sum_{\omega(x)} \omega(x) \) (here, \( \sum_{\omega(x)} = N_c^3 \)) as a function of the chain step. One can see that \( \chi^2 \) drops sharply at the beginning (the burn-in phase), then remains almost constant after about 150 chain steps (the convergence phase). The density field of a converged chain step matches well the original input density field, with an rms difference between the two of about \( \mu \sqrt{2 \chi^2} \approx 4.6\% \). For reference, the important parameters and characteristics of the primary test are listed in Table 1.

In Figure 3, we show the power spectra measured from different chain steps. We refer to these power spectra as the Hamiltonian power spectra \( \{P_h(k)\} \), to distinguish them from the input linear power spectrum and the analytic linear power spectrum. The “two-phase” behavior can be clearly seen in the evolution of the power spectra. For the first 150 steps, one sees an obvious tuning process: on large scales, the Hamiltonian spectrum first decreases and then increases, while on small

### Table 1

| HMC                  | Resimulation |
|----------------------|--------------|
| \( L \) | \( N_c \) | \( R_c \) | \( \chi^2 \) | \( t_c \) | \( A_r \) | \( N_p \) | \( m_p \) | \( \epsilon \) | \( z_i \) |
|----------------------|--------------|
| Primary test         | 500          | 128         | 11.7         | 4.2       | 21          | 72\%       | 1283         | 414          | 80           | 20          |
| LRR                  | 726          | 512         | 5.67         | 2.9       | 2080        | 35\%       | 5123         | 19.8         | 28           | 30          |
| HRR                  | 181.5        | 256         | 2.84         | 3.8       | 222         | 58\%       | 2563         | 2.47         | 15           | 36          |

Notes. Here, \( L \) and \( R_c \) have units of \( h^{-1} \) Mpc, while the softening length \( \epsilon \) has units of \( h^{-1} \) kpc. The mean consumption time \( t_c \) for each chain step is measured in seconds. \( A_r \) is the acceptance rate. The particle mass \( m_p \) for resimulation has units of \( 10^{10} h^{-1} M_{\odot} \).
The Astrophysical Journal, 772:63 (19pp), 2013 July 20

Wang et al.

Figure 1. Comparison between the Hamiltonian forces $F_{0,1}(k)$ and $F_{n,n}(k)$. $F_{0,1}(k)$ is calculated using Equations (19) and (20), while $F_{n,n}(k)$ is obtained using the numerical method presented in Section 3. The subscripts 0 and 1 denote the real and imaginary parts, respectively.

(A color version of this figure is available in the online journal.)

Figure 2. Evolution of $\chi^2_w$ for various tests. See the text (Section 3) for the definition of $\chi^2_w$. The black lines in the four panels are the same: the result of the primary test with parameters $N_c = 128$, $R_s = 11.7 \, h^{-1} \, \text{Mpc}$, $\mu = 0.5$, and $\tau_{\text{max}} = 0.1$. The labels in each panel show the parameters different from those of the primary test.

In order to show the burn-in phase clearly, we omitted the last 500 steps.

(A color version of this figure is available in the online journal.)

scales, the behavior is the opposite. The first (starting) spectrum is very similar to the analytic linear power spectrum, because the initial $\delta_j(k)$ are drawn from Equation (1). After about 150 steps, the Hamiltonian spectra settle close to the initial spectrum used in the simulation, implying the convergence of the chain. Both the $\chi^2$ and the power spectrum results demonstrate that our method ensures quick convergence.

Such two-phase behavior is common in HMC runs (e.g., Hanson 2001; Taylor et al. 2008) and can be understood in terms of the behavior of a physical system. The system initially has a very large potential and a large $\chi^2$ because its initial configuration, represented by the randomly generated initial $\delta_j(k)$, is unstable and tends to fall rapidly into the deep potential well, which reduces $\chi^2$ and the potential of the system but increases its kinetic energy. Since the kinetic energy is directly related to the current momenta that are reset to lower values before each chain step, the system is “cooled” so that it continuously falls toward the potential well (burn-in phase). Once the changes in the potential and the kinetic energy become insignificant within one chain step, the “cooling process” can be neglected and the total energy of the system becomes stable and so the value of $\chi^2$ remains more or less constant. In this convergence phase, the accepted states reach the bottom region of the potential well around the posterior peak we are searching.

Recall again that we want to generate a linear density field that obeys the prior Gaussian probability function specified by a linear power spectrum and evolves to a nonlinear density field that matches the input density field. In what follows, we will examine our results in two different aspects. One is whether or not our reconstructed $\delta_j(k)$ matches the prior constraints. The other is how well the predicted (or modeled) density field (from the MZA), $\rho_{\text{mod}}$, and the original simulated density field,
In order to clearly compare \( P \) spectra, well, we measure the phase correlation between the two density fields. Such a sharp transition is due to the fact that small-scale structures are severely suppressed by our Gaussian smoothing. However, for our purpose we are not trying to sample the whole posterior distribution; it is not necessary to perform the correlation analysis any longer.

The very small \( \chi^2 \) for the converged chain states demonstrates that our method can recover the input density field with high accuracy. To further quantify at which scales \( \rho_{\text{mod}} \) matches \( \rho_{\text{t}} \) well, we measure the phase correlation between the two density fields. We define a phase correlation coefficient between the two fields \( X(\mathbf{k}) \) and \( Y(\mathbf{k}) \) as

\[
C_p(k) = \frac{(X_0(\mathbf{k})Y_0(\mathbf{k}) + X_1(\mathbf{k})Y_1(\mathbf{k}))}{\sqrt{\langle |X(\mathbf{k})|^2 \rangle k \langle |Y(\mathbf{k})|^2 \rangle k}},
\]

where the subscripts 0 and 1 indicate the real and imaginary parts, respectively. Note that \( C_p(k) = 1 \) means that two quantities have exactly the same phase, while \( C_p(k) = 0 \) indicates no correlation. We show the phase correlation between \( \rho_{\text{t}} \) and \( \rho_{\text{mod}} \) at the 1700th chain step for our primary test in Figure 4. The correlation coefficient is close to one at large scales \((k < 0.17 h\ Mpc^{-1})\) and declines quickly toward smaller scales. Such a sharp transition is due to the fact that small-scale structures are severely suppressed by our Gaussian smoothing and so contribute little to \( \chi^2 \) and to the Hamiltonian force. As a result, the transition scale should be related to the smoothing scale.

To understand the origin of this discrepancy on intermediate scales, we perform a series of tests with smoothing scales ranging from \( 3 h^{-1} \) Mpc to \( 23 h^{-1} \) Mpc. In each case, we find that the input linear power spectrum is well recovered at both large and small scales, but that noticeable discrepancies are apparent on intermediate scales. The discrepancies move gradually from small to large wavenumbers as the smoothing scale decreases (see, e.g., the lower right panel of Figure 6). We define a wavenumber \( k_c = \frac{\sum_k k(1 - r(k)) / \sum_k (1 - r(k))}{\sqrt{\langle X(\mathbf{k})^2 \rangle k}} \) with \( r(k) = \rho_{\text{mod}}(k)/\rho_{\text{lin}}(k) \) to quantify this scale, and find that the \( k_c - R_s \) relation can be well fit by \( k_c = 1.88/R_s^{0.94} \). Note that the phase correlation between \( \rho_{\text{mod}} \) and \( \rho_{\text{t}} \) also depends on the smoothing scale. We show \( k_c \) so defined as the dashed lines in the phase correlation plot (Figure 4), which clearly shows that \( k_c \) also characterizes the transition scale in the phase correlation. The question is why the reconstructed linear power spectrum deviates from the analytical linear power spectrum just around \( k_c \). According to Equation (8), the Hamiltonian force has two components, the prior term and the likelihood term. The phase can be well recovered only when the likelihood term dominates the force because the prior term actually generates...
random phases. The mean ratio of these two terms is

$$R_F(k) = \frac{P_{lin}(k)}{2} \sqrt{\frac{\sum_j (F_j^2(k))_k}{\sum_j (\delta_j^2(k))_k}}.$$  \hspace{1cm} \text{(24)}$$

We find that $R_F(k)$ decreases continuously with $k$ and is about unity around $k_c$. This implies that $\chi^2$ is more sensitive to $\delta(k)$ at smaller $k$ and is almost completely independent of $\delta(k)$ at $k \gg k_c$. At $k \gg k_c$, the trajectories of $\delta(k)$ in the HMC are dominated by the prior so that the Hamiltonian spectra match the linear power spectrum but the Fourier phases are not constrained. At $k \ll k_c$, on the other hand, the trajectories of $\delta(k)$ are governed by the likelihood term so that they try to trace the original linear density field of the MS simulation, consequently leading to a small $\chi^2$ and a strong phase correlation between the reconstructed and original density fields. However, on scales around $k_c$, $\delta(k)$ has a reduced contribution to $\chi^2$ and the posterior distribution is partly regulated by the prior. Consequently, the final result is a compromise between the prior constraint and the likelihood. Since the likelihood term decreases with an increasing smoothing scale (see Equations (17), (19), and (20)) while the prior term does not, it explains why both $k_c$ and the transition scale of the phase correlation depend linearly on the smoothing scale.

Although the discrepancy between the reconstructed and original linear power spectra is not large, we may want to correct it using a “renormalization” process. First, we visually identify the region where the discrepancy is significant ($0.12 < k < 0.21 \, h \, \text{Mpc}^{-1}$ for the primary test), and then we use $\sqrt{P_{lin}(k)/P_H(k)}$ to scale the amplitude of $\delta_j(k)$ without changing its phase. Since the $\delta_j(k)$ values in this region are still well described by a Gaussian distribution (see Figure 5), and since rescaling preserves the shape of the distribution, the distribution of the scaled $\delta_j(k)$ is still close to Gaussian. Because the discrepancy to be corrected is fairly small and the contribution of $\delta(k)$ around $k_c$ to $\chi^2$ is not large, the scaling does not cause any significant change in $\chi^2$ and in the phase correlation.
Section 5, we will use the renormalized $\delta(k)$ to generate initial conditions at high redshift, then use an N-body simulation to evolve the initial conditions to the present day and compare the resimulated density fields with the original simulated density field.

Finally, we discuss the effects of changing $\tau_{\text{max}}$, $N_m$, and $\mu$ on our results. We perform several tests with different $\tau_{\text{max}}$, $N_m$, and $\mu$ values. Similar to the primary test, all these tests exhibit a two-phase behavior and a final convergence with a low $\chi^2_w$ is always achieved (see Figure 2). Inspecting the results in detail, one can see that the values of $\tau_{\text{max}}$ and $N_m$ affect the number of steps required for burn-in: larger $\tau_{\text{max}}$ and smaller $N_m$ both result in a quick burn-in phase. Similar to $R_s$, the value of $\mu$ also affects the difference between the converged $\rho_{\text{mod}}$ and $\rho_t$, in the sense that a smaller $\mu$ results in a smaller $\mu \sqrt{2\chi^2_w}$, as shown in the lower left panel of Figure 2. Furthermore, the value of $k_s$ decreases with increasing $\mu$ (see the lower left panel of Figure 6), because a larger $\mu$ suppresses the contribution of small-scale structures to $\chi^2$ more. Thus, $\mu$ affects the accuracy of the final result in a similar way as $R_s$ does. On the other hand, since the MZA becomes increasingly inaccurate on small scales, a smaller $\mu$ value also leads to a lower acceptance rate. As a compromise between efficiency and accuracy, and because the effects of changes in $\mu$ and $R_s$ are degenerate, we fix $\mu = 0.5$ and only test the impact of changing $R_s$. We have also checked the Hamiltonian power spectra and the probability distribution of $\delta(k) / \sqrt{P(k)}$ in these tests and found that they are very similar to those in the primary test (Figure 6).

4. APPLICATION TO THE RECONSTRUCTED DENSITY FIELD

As we discussed above, the HMC method needs a present-day density field, $\rho_p$, as an input. Therefore, the HMC method is useful only when we have a reliable method to obtain the present-day density field from observations. In Wang et al. (2009b), we developed a method to reconstruct the present-day density field based on the distribution of galaxy groups (halos). In this section, we apply this method to a mock galaxy catalog to reconstruct the density field and then apply our HMC method to the reconstructed density field to obtain the initial linear density field ($\rho_{\text{mod}} \equiv \rho_{\text{rc}}$). In the first subsection, we briefly describe how we construct the mock galaxy and group catalogs, and the method to correct for redshift-space distortions of the groups. The two mock catalogs are exactly the same as those used in Wang et al. (2012a) and are constructed from the MS with the use of the SDSS DR7 sky coverage and selection functions. We refer the interested reader to Wang et al. (2009b, 2012a) and references therein for further details.

4.1. The Mock Galaxy and Group Catalogs

The construction of the mock galaxy catalog is similar to that described in Yang et al. (2007, hereafter Y07). First, we populate galaxies inside dark matter halos according to the conditional luminosity function (Yang et al. 2003) model of van den Bosch et al. (2007). These halos are identified from the MS with a friends-of-friends algorithm (hereafter FOF; Davis et al. 1985) employing a linking length of $b = 0.2$. Next, we assign phase-space parameters to these galaxies following Yang et al. (2004; see also More et al. 2009). Briefly, in each halo, the brightest galaxy is regarded as the central galaxy and assumed to be located at the halo center, while the other galaxies are satellites and distributed spherically following an NFW (Navarro et al. 1997) density profile, with the concentration–mass relation given by Macciò et al. (2007). The peculiar velocity of the central galaxy is set equal to the mean velocity of the corresponding halo, while satellites have additional velocity components to account for the virial motions within the host halo. These component velocities are drawn from a Gaussian probability function with a dispersion computed from the Jeans equation (see More et al. 2009). Then, we stack $3 \times 3 \times 3$ galaxy-populated simulation boxes together and place a virtual observer at the center of the stack. We assign each galaxy a redshift and $(\alpha, \delta)$ coordinates with respect to the observer. Note that the redshift of a galaxy is a combination of its cosmological redshift and peculiar velocity. The mock galaxy catalog is constructed by mimicking the sky coverage of the SDSS DR7, taking into account the angular variation of the magnitude limit and the survey completeness (see Li et al. 2007).

Mock galaxy groups are identified with a halo-based group finder developed by Yang et al. (2005). This group finder has already been successfully applied to the SDSS DR4 (Y07). The application to our mock galaxy catalog is the same, except that a different cosmology and a larger sky coverage are adopted. Groups are selected in the survey region that has a redshift completeness criterion of $C_z > 0.7$. The masses of groups are estimated based on the ranking of the characteristic luminosities of groups. The characteristic luminosity of a group is determined from the luminous group members with $M_r > -19.5$. To take into account the survey edge effect, the group finder calculates the fraction of each group’s volume that falls inside the survey region and then uses this fraction to correct for the group luminosity and mass. In this paper, we use all groups with an assigned mass $M_h \geq M_{h0} = 10^{12} h^{-1} M_\odot$ and we restrict our reconstruction of the present-day density field to the cosmic volume covering the redshift range $0.01 \leq z \leq 0.12$, which we call the survey volume.

In order to reconstruct the density field in real space, we have to correct for redshift-space distortions. To do that, we follow exactly the procedure described in Wang et al. (2012a; see also Wang et al. 2009b). First, we embed the survey volume in a periodic cubic box of side length $726 h^{-1}$ Mpc, which is referred to as the survey box in the following. We divide the survey box into $1024^3$ grids and assign the masses of groups (with $M_h \geq M_{h0}$) on the grids according to their redshift-space coordinates. The grids outside of the survey volume are assigned the mean mass density of the groups ($M_h \geq M_{h0}$) in the survey volume. Then, we calculate the overdensity field of the groups and smooth it using a Gaussian kernel with a large smoothing scale of $8 h^{-1}$ Mpc. In the linear regime, the peculiar velocities induced by density perturbations are proportional to the amplitudes of the density fluctuations, hence we can use this smoothed overdensity field to derive the peculiar velocities. Adopting a relatively large smoothing scale can effectively suppress nonlinear velocities that cannot be predicted accurately. As shown in Wang et al. (2009b), the resultant velocities based on the halo (group) population are biased but are tightly proportional to the real velocities. We thus can predict the peculiar velocity of each group by simply taking into account the bias factor of the overdensity field represented by the groups and we use Equation (10) in Wang et al. (2009b) to calculate the bias factor. Finally, we use the line-of-sight component of the predicted velocity to correct for the redshift-space distortions. Since the velocity field is obtained from the groups distributed in redshift space, this method requires iteration.
According to the results obtained by Wang et al. (2009b) and the results from our further tests, the average offset between the real and predicted positions of groups is between 1.1 and 1.4 h⁻¹ Mpc. Using the 2LPT to correct for the redshift distortion can produce a higher accuracy than the simple linear model (Kitaura et al. 2012a). However, in our case it is not necessary to adopt the more accurate 2LPT because the density field reconstructed from the mock groups is smoothed on a scale of at least 2.84 h⁻¹ Mpc (see below). This smoothing scale is larger than the typical offset, so the linear theory and the 2LPT lead to very similar results. Another important issue related to redshift distortion is the finger-of-God effect. This effect is mainly due to the virial motion within individual groups, especially massive groups, and thus cannot be handled by a method based on a linear or quasi-linear model. Such an effect, if not properly corrected for, can lead to artifacts in the reconstructed density field. An advantage of our reconstruction is that it is based on galaxy groups rather than on galaxies. The redshift of a group is estimated using the luminosity-weighted average of all member galaxies so that the finger-of-God effect within the group is largely mitigated (see Figure 8 in Yo7 for a comparison between the distributions of groups and galaxies). However, some small groups that are close to massive groups may have significant nonlinear motions (see Wang et al. 2009a), and such motions cannot be corrected for properly with any linear or quasi-linear model. Fortunately, the total mass contained in such groups is very small and their effect is expected to be small.

4.2. Density Reconstruction from the Mock Group Catalog

In Wang et al. (2009b), we developed a method to reconstruct the present-day density field starting from the distribution of galaxy groups (halos). We tested this method using FOF halos but did not apply it to mock groups to examine its reliability against uncertainties due to false identification of group members and the survey boundary effect. Survey boundaries have no direct impact on our reconstruction, but can affect the correction for redshift-space distortions. In this subsection, we reconstruct the density field using the mock group catalog corrected for redshift-space distortions as described above and compare our reconstruction with the original simulation.

As in Wang et al. (2009b), we first calculate the density profiles in “domains” using the MS. For a given population of FOF halos with mass of \( M_h \geq M_{th} \), we partition the cosmic space into a set of domains in such a way that each domain contains one and only one halo. Any point in the domain of a halo is closer (according to a distance proximity defined below) to this halo than to any other halos. The proximity of a point to a halo with a virial radius of \( R_h \) is defined as

\[
r_p = \frac{r_h}{R_h},
\]

where \( r_h \) is the physical distance from the point to the halo center. We calculate the average density profile around halos of the same mass in the corresponding domains. Figure 7 shows the results in six different mass bins. Despite using a different cosmology, these profiles are very similar to those shown in Wang et al. (2009b). Then, we “convolve” our mock groups with these density profiles to reconstruct the cosmic density in the following way. For a mock group of mass above the mass threshold \( M_{th} \), we pick a density profile shown in Figure 7 according to the mass of this group. Using a Monte Carlo method, we put particles around this group at distances up to \( \sim 32 \) times the virial radius regardless of the domain. We remove particles outside of the domain of the group. We repeat the above three steps for all groups with masses larger than \( M_{th} \). Eventually, we get a present-day density field embedded in the survey box.

One advantage of our reconstruction method is that we define a very special cross-correlation function (i.e., the average density profile in domain). It is different from the conventional cross correlation, which does not use domains. In the conventional one, all halos contribute to the average density profiles at all scales, especially on large scales. This has the effect of smoothing halo masses over very large scales. On the other hand, in our cross correlation based on domains, massive halos \( (M_h > M_{th}) \) contribute only to the density profiles within the virial radii, while the diffuse-mass and low-mass halos with \( M_h < M_{th} \) contribute to the large scale. Another advantage of our method is that we use galaxy groups (halos) instead of galaxies. While the bias of galaxy distribution relative to the underlying density field may depend on various galaxy properties, such as luminosity and color, the exact form of the bias is not well established; the use of galaxy groups (halos) automatically takes into account the bias of the galaxy distribution through the connection between galaxies and halos.

In order to compare our reconstructed density field with the simulated density field, we divide the survey box into \( 1024^3 \) grids with size of 0.71 h⁻¹ Mpc and smooth the sample particles on the grids using a Gaussian kernel with \( R_s = 2.84 h^{-1} \) Mpc. Since the peculiar velocities are predicted more accurately in the inner region than near the boundary of survey volume (Wang et al. 2012a) and we use these velocities to correct for the redshift-space distortions, one may expect that the reconstruction is more reliable in the inner region. To check whether or not this is the case, we need to compute the distance of any point in the survey volume to the boundary. Following Wang et al. (2012a), we define a filling factor \( p_f \) to characterize the closeness of a grid to the boundary. For a grid \( g \) in the survey volume, \( p_f \) is the fraction of a spherical volume of radius \( 80 h^{-1} \) Mpc centered on the grid \( g \) that falls inside the

![Figure 7. Density profiles of mass in and around the halos in various mass bins. Here, the mass threshold for the halo population is \( M_{th} = 10^{12} \) M\(_\odot\). The radius \( r \) is scaled by the halo virial radius \( R_h \) and the density is scaled by \( \bar{\rho} \), the mean density of the universe.](image-url)

(A color version of this figure is available in the online journal.)
survey volume. Therefore, \( p_l \simeq 1 \) for grids located more than \( 80 h^{-1} \text{Mpc} \) from any survey boundary, while \( p_l \) is much less than unity for grids close to the boundary.

In Figure 8, we present a comparison between the simulated density field \( \rho_l \) and the reconstructed density field \( \rho_{\text{rc}} \) in the inner region with \( p_l \geq 0.6 \), which is about 66\% of the survey volume. The solid line shows the mean relation and the error bars indicate the standard deviation in \( \rho_l \) for a given \( \rho_{\text{rc}} \). The bias is very small and the uncertainties are about 30\%–50\% of \( \rho_{\text{rc}} \) in most bins. At the two largest density bins, there is a significant deviation from the one-to-one relation. The volume of the grids in these two bins is tiny and their presence does not affect our reconstruction significantly. We then show the same comparison for grids near the boundary, i.e., with \( p_l < 0.6 \). As one can see, the result is as good as that in the inner region.

![Figure 8](image)

**Figure 8.** Comparison of density between the original simulation and the reconstruction. The reconstruction here is obtained by using mock groups with \( M_\text{sh} = 10^{12} h^{-1} M_\odot \) and the density profiles shown in Figure 7. The two density fields are smoothed with a Gaussian kernel with a smoothing scale of \( 2.84 h^{-1} \text{Mpc} \). The black and red lines show the results for the grids with a different filling factor, \( p_l \) (see the text for the definition).

A color version of this figure is available in the online journal.

Apparentely, the smoothing used is able to partly remedy the problem of correcting for the redshift-space distortions near the survey boundary. Overall, with an appropriate choice of the smoothing radius, our method is able to reconstruct the density field accurately and the effects due to survey boundary and group contamination do not introduce any significant biases.

In the next subsection, we will apply the HMC method to the reconstructed density field in two volumes, one that is the entire survey volume and the other that is a cubic volume well inside the survey volume (see below for details). Before doing that, we show in Figure 9 the phase correlation between our reconstructed and simulation fields in these two volumes. These correlations set an upper limit on the accuracy we can achieve for our reconstruction of the linear density field. As one can see, the correlation coefficient is almost unity on large scales, and declines gradually with increasing wavenumber. At \( k \sim 1 h \text{Mpc}^{-1} \), the coefficient drops to \( \sim 0.5 \), demonstrating that our method is successful well into the nonlinear regime (the translinear scale is \( k \sim 0.15 h \text{Mpc}^{-1} \)). The phase correlation at \( k > 0.2 h \text{Mpc}^{-1} \) obtained for the inner cube is slightly stronger than that for the total volume, indicating that boundary effects indeed have a non-negligible impact on the reconstruction.

### 4.3. Reconstruction of the Linear Density Field

We first apply our HMC method to the reconstructed density field in the entire survey volume, which is embedded in the survey box with size \( L = 726 h^{-1} \text{Mpc} \) on a side. In order to examine the ability of our method over a large dynamic range, we divide the survey box into \( N = 512 \) grids in each dimension so that our reconstruction deals with more than \( N^3 \sim 10^8 \) free parameters. We adopt a smoothing radius of \( R = 5.67 h^{-1} \text{Mpc} \), on which our reconstructed density field is quite similar to the original density field. In order to derive the weight \( w(x) \), we divide each grid into \( 2^3 \) subgrids. If more (fewer) than six subgrids of a grid are located inside the survey volume, this grid is assigned a weight of unity (zero). The other parameters are chosen as \( \tau_{\text{max}} = 0.1, \mu = 0.5, \) and \( N_\text{m} = 50 \), similar to those in the primary test. This application is referred to as the “low-resolution run” or LRR in the following. As shown in Table 1, on average it takes \( \sim 2080 s \) for each HMC step and

![Figure 9](image)

**Figure 9.** Phase correlation among modeled density \( \rho_{\text{mod}} \), resimulated density \( \rho_l \), reconstructed density \( \rho_{\text{rc}} \), and original density \( \rho_f \). The left panel shows the results for the LRR. The right panel shows the results for the HRR. The vertical dashed lines denote the characteristic wavenumber, \( k_c \).

(A color version of this figure is available in the online journal.)
Figure 10. Black lines show the analytic linear power spectrum, $P_{\text{lin}}(k)$, the red lines show one convergent Hamiltonian spectrum, $P_{\text{H}}(k)$, and the blue lines show the corrected power spectrum, $P_{\text{c}}(k)$. The left and right panels show the results for the LRR and the HRR, respectively. (A color version of this figure is available in the online journal.)

Figure 11. Probability distribution of $\delta_0(k)/\sqrt{P_{\text{lin}}(k)/2}$ at large (left), intermediate (middle), and small (right) scales for the LRR (upper panels) and the HRR (lower panels). The dashed and solid black lines show the results before and after correcting for the discrepancy, respectively. The dashed and solid lines are indistinguishable in all panels except the lower middle panel. The red lines are the best-fitting Gaussian curves of the solid black lines. We also present the best-fitting $\sigma$ in red text. (A color version of this figure is available in the online journal.)

the acceptance rate is about 35%. The $\chi^2$ value for a converged state is about 0.0029, indicating that the rms difference between $\rho_{\text{mod}}(x)$ and $\rho_{\text{c}}(x)$ is only 3.8%. We show the phase correlation between $\rho_{\text{c}}$ and $\rho_{\text{mod}}$ at the 1700th chain step in the left panel of Figure 9. The correlation is almost unity at large scales, and drops quickly around $k_c$, consistent with our test results presented above.

In the left panel of Figure 10, we compare a converged Hamiltonian spectrum, $P_{\text{H}}(k)$, with the analytic linear power spectrum, $P_{\text{lin}}(k)$, used in the prior. As one can see, $P_{\text{H}}(k)$ is very close to $P_{\text{lin}}(k)$ over the entire range of scale. In particular, the discrepancy around $k_c$ is also small. The distribution of the reconstructed initial density field is extremely close to Gaussian, as shown in the upper three panels of Figure 11. As described above, we can also renormalize the reconstructed linear power spectrum by visually identifying the discrepancy region ($0.28 < k < 0.47 \ h^{-1} \text{ Mpc}^{-1}$) and scaling the corresponding $\delta_j(k)$ with a factor $\sqrt{P_{\text{lin}}(k)/P_{\text{H}}(k)}$. The new power spectrum so obtained and the distributions of the renormalized $\delta_j(k)$ are also shown in the corresponding figures. Since the discrepancy is tiny, the curves before and after the renormalization are indistinguishable in the figure. As shown in the upper panels of Figure 11, these renormalized $\delta_j(k)$ are well described by a Gaussian function with unity variance. These results demonstrate clearly that our HMC method works well on large scales.

To examine the performance of our HMC method on small scales, we perform a high-resolution run (HRR) with a small smoothing scale. This is a cubic box of side $100 \ h^{-1} \text{ Mpc}$ located in the inner region of the survey volume, put inside a larger periodic box with $L = 181.5 \ h^{-1} \text{ Mpc}$. We divide the larger box into $N_c = 256$ grids in each dimension and adopt a smoothing scale of $R_s = 2.84 \ h^{-1} \text{ Mpc}$, for which our reconstructed density field is in good agreement with the original simulation. Only grid cells that are located within both the small box and the survey volume are assigned a weight of unity. All other grid cells are assigned a weight of zero. Note that some grids in the small box
may not be in the survey volume, because of the existence of small holes in the survey mask. The other parameters are chosen to be the same as in the LRR. On average, the HRR takes 222 s for each HMC step, and the acceptance rate is about 58%. The chain finally converges to $\chi^2_w \simeq 0.0038$, corresponding to an rms of 4.4% in the difference between $\rho_{\text{mod}}(x)$ and $\rho_c(x)$. The corresponding phase correlation is shown in the right panel of Figure 9. Here, we see a significant correlation all the way to $k \sim 1 \text{ h Mpc}^{-1}$, a scale much smaller than the translinear scale, which corresponds to $k \sim 0.15 \text{ h Mpc}^{-1}$.

The converged $P_h(k)$ and the distributions of $\delta_j(k)/\sqrt{P_{\text{lin}}(k)/2}$ for the HRR are shown in Figures 10 and 11. Here, we see a significant bump at $0.3 < k < 1 \text{ h Mpc}^{-1}$ $P_h(k)$ compared with $P_{\text{lin}}(k)$. The reason for this bump is twofold. First, the bump is around $k_c$, suggesting that it is a compromise between the prior constraint and the likelihood (see Section 3). Second, the bump is partly ascribed to the inaccuracy in the adopted approximation of the structure formation model on small scales. According to TZ12, the mode-coupling term, $\rho_{\text{MC}}(k)$, cannot be neglected at $k > 0.4 \text{ h Mpc}^{-1}$ (see their Figure 1). On such scales, the amplitude of $\rho_{\text{mod}}(k)$ predicted by the MZA is somewhat lower than that of the fully evolved density field. To achieve a small $\chi^2_w$ in the HMC, the Hamiltonian spectra have to be enhanced to compensate for the deficit. On even smaller scales, $k > 1 \text{ h Mpc}^{-1}$, however, the Hamiltonian force is dominated by the prior term so that $P_{\text{HT}}(k)$ is forced back to $P_{\text{lin}}(k)$. Despite this inaccuracy, our HMC method can still recover more than half of the phase correlation all the way to $k \sim 1 \text{ h Mpc}^{-1}$, as demonstrated in the next section. As before, we renormalize the amplitudes of the Fourier modes to correct for the discrepancy in the range of $0.35 < k < 1 \text{ h Mpc}^{-1}$. The corrected power spectrum and distribution of the renormalized $\delta_j(k)$ are shown in the right panel of Figure 10 and the lower panels of Figure 11, respectively.

We only show the results at the 1700th chain steps for both the simulated and reconstructed density fields in all figures (except in Figures 2 and 3, where the results are shown for different steps). Because we just want to reconstruct the linear density field rather than draw a sample for a statistical study (see Section 2.1 for our objective in detail), it is not necessary to show the results for all chain steps. In fact, the accepted samples after burn-in have very similar Hamiltonian power spectra and $\chi^2_w$ (see, e.g., Figures 2 and 3); the results at all other steps are very similar to those that are shown. The choice of the 1700th step is arbitrary; the only requirement is that the chain at this step has already converged. Moreover, in order to investigate whether the results are sensitive to the choice of the initial set of $\delta_j(k)$, we have performed tests with different initial sets of $\delta_j(k)$ and found the results change very little. For example, the changes in $\chi^2_w$ and the phase correlation functions are small.

5. RESIMULATIONS OF THE RECONSTRUCTED LINEAR DENSITY FIELD

Up until now, all of our results have been based on the structure formation model of TZ12. The advantage of using the TZ12 model is that it is very fast and can thus be implemented into our HMC to infer the initial linear density field. However, the TZ12 model is not expected to work accurately in the highly nonlinear regime. Although the modeled density field shown above is closely correlated with the input present-day density, it is unclear as to what extent the density field fully evolved from our reconstructed linear density field matches the original simulated density field, especially on small scales where nonlinear evolution becomes important. In order to test the model in the highly nonlinear regime, we need to use full $N$-body simulations to evolve our reconstructed initial linear density field to the present day and to compare the resimulation with the original simulation.

To do this, we set up the initial condition for our constrained $N$-body simulation using the renormalized $\delta(k)$. We generate the initial displacement field at a given high redshift, $z_i$, using the Zel’dovich approximation. The displacement field is used to perturb the positions of the $N$-body particles that initially have a uniform distribution. Each particle is assigned a velocity according to the growing mode solution of the linear perturbations. We then use the $N$-body code Gadget-2 (Springel 2005) to evolve the initial conditions to the present day. The fully evolved density field is referred to as the resimulated density field, and is denoted by $\rho_{\text{rs}}$.

5.1. Initial Conditions from the Simulated Density Field

Let us first consider $\delta(k)$ reconstructed from the original simulated density field, i.e., $\rho_p \equiv \rho_i$ (Section 3). For our primary test, we use $N_p = 128^3$ particles in a box of $L = 500 \text{ h}^{-1} \text{ Mpc}$ to trace the evolution of the density field. As shown in Table 1, we adopt an initial redshift $z_i = 20$, a particle mass $m_p \simeq 4.14 \times 10^{12} \text{ h}^{-1} M_\odot$, and a force softening length $\epsilon = 80 \text{ h}^{-1} \text{ kpc}$. The dashed black line in Figure 4 shows the phase correlation between $\rho_p$ and $\rho_i$. As can be seen, this phase correlation is very similar to that between $\rho_{\text{mod}}$ and $\rho_i$. We also show the results of the resimulation from the reconstructed linear density field using $R_s = 5.86 \text{ h}^{-1} \text{ Mpc}$ and $3.91 \text{ h}^{-1} \text{ Mpc}$, respectively. For the test with $R_s = 5.86 \text{ h}^{-1} \text{ Mpc}$, the phase correlation is again very similar to that between $\rho_{\text{mod}}$ and $\rho_i$, suggesting that the MZA works well up to $k \gtrsim 0.3 \text{ h Mpc}^{-1}$. In the test with $R_s = 3.91 \text{ h}^{-1} \text{ Mpc}$, however, the $\rho_{\text{rs}}$–$\rho_i$ correlation is much stronger than the $\rho_{\text{mod}}$–$\rho_i$ correlation at $k > k_c$.

Given that the HMC method tends to minimize the difference between $\rho_{\text{mod}}$ and $\rho_i$, it is unexpected that the $\rho_{\text{mod}}$–$\rho_i$ correlation is much weaker than the $\rho_{\text{rs}}$–$\rho_i$ correlation at $k > k_c$. The most important difference between $\rho_{\text{mod}}$ and $\rho_{\text{rs}}$ is that the latter is the result of fully nonlinear processes in which the mode of the nonlinear density field on small scales may be coupled to that on large scales (see, e.g., Tassev & Zaldarriaga 2012a). Consequently, part of the phases at $k > k_c$, where the initial phases are not well constrained, are reproduced in the resimulation. Such mode coupling is not included in the TZ12 model based on quasi-linear theory; so the phase information in $\rho_i$ at $k \gg k_c$ is almost completely lost in $\rho_{\text{mod}}$.

Our above results clearly show that the match between the resimulation and the original simulation is better at smaller $R_s$. To quantify this trend, we introduce a quantity $k_0$ to measure the scale at which $\rho_{\text{rs}}$ can well match $\rho_i$. $k_0$ is defined in such a way that the phase correlation between the two density fields at $k_0$ is half. In Figure 12, we show $k_0$ as a function of $R_s$. On large scales, $k_0$ increases with decreasing $R_s$, consistent with expectations because information of the density field on scales below $R_s$ is lost due to the smoothing. As it reaches about unity, however, the value of $k_0$ becomes insensitive to $R_s$. This is also expected, because the TZ12 model is not expected to work accurately on very small scales. This demonstrates that in order to reconstruct the density field on scales below $k \sim 1 \text{ h Mpc}^{-1}$, one has to use a model that is more accurate than the TZ12 model adopted here.
5.2. Initial Conditions from the Reconstructed Density Field

In this subsection, we use N-body simulations to evolve the initial conditions obtained from the present-day density field reconstructed from the mock catalogs ($\rho_p \equiv \rho_{rc}$; Section 4). For reference, we list the parameters for both LRR and HRR in Table 1. To inspect our results visually, we present density maps of the same thin slices in the original simulation used to construct the mock catalog, the density field reconstructed from the mock catalog, and the density field in the resimulations. Figure 13 shows the results for the LRR. Here, all density fields are smoothed with a Gaussian kernel with $R_s = 5.67 h^{-1}$ Mpc. Within the survey volume, the three maps look quite similar; almost all structures in the original simulation, such as massive clusters, filaments, and underdense voids, are reproduced in the resimulation. The density maps for the HRR, smoothed with $R_s = 2.84 h^{-1}$ Mpc, are presented in Figure 14. There are about 20 bright spots in the original simulation, which correspond to a single halo or a cluster of a few halos with masses down to about a few times $10^{12} h^{-1} M_\odot$. Most of these structures are clearly reproduced in our resimulation. In addition, some small filaments in the original simulation are also correctly reproduced in the resimulation. This is quite remarkable, given that our reconstruction from the mock catalog uses only groups with assigned masses above $M_{th} = 10^{12} h^{-1} M_\odot$ and that nonlinear effects are important on such small scales.

In the left panel of Figure 15, we show the comparison of $\rho_{rs}$ with $\rho_{rc}$ and $\rho_f$ for the LRR. There is a weak bias at the high-density end in both relations; while $\rho_{rs}$ is higher than $\rho_{rc}$, it is slightly lower than $\rho_f$. Since the initial conditions for the resimulation are constrained by the reconstructed density field, the $\rho_{rs} - \rho_{rc}$ relation is much tighter than the $\rho_{rs} - \rho_f$ relation. The typical dispersion in the former relation is about 0.05 dex, while it is about 2–3 times larger in the latter relation. The phase correlations among the three density fields are shown in the left panel of Figure 9. Similar to the $\rho_{mod} - \rho_{rc}$ correlation, there is a sharp transition in the correlation coefficient from unity to

**Figure 12.** $k_h$, at which the phase correlation between the resimulated density field and original simulated density field is half, as a function of $R_s$. The solid line shows the results for the resimulations constrained directly from the original simulation, while the dashed line shows the results for resimulations constrained from the reconstructed density field.
Figure 14. High-resolution density maps in a slice of $100 \times 100 \times 6.4 h^{-1}$ Mpc. The left panel shows the resimulated density field from the HRR. The middle and right panels show the original simulated and the reconstructed density fields, respectively. All these density fields are smoothed with a Gaussian kernel with $R_s = 2.84 h^{-1}$ Mpc and scaled with the mean density of the universe. (A color version of this figure is available in the online journal.)

Figure 15. Black lines show the comparison between $\rho_{rs}$ and $\rho_{rc}$. Red lines show the comparison between $\rho_{rs}$ and $\rho_f$. All these densities are scaled with $\bar{\rho}$, the mean density of the universe. The left panel shows the results for the LRR and the densities are smoothed with a Gaussian kernel with $R_s = 5.67 h^{-1}$ Mpc. The right panel shows the results for the HRR and the densities are smoothed with a Gaussian kernel with $R_s = 2.84 h^{-1}$ Mpc. The dashed lines indicate the one-to-one relation. (A color version of this figure is available in the online journal.)

about zero around $k_c$. Upon closer examination, we find that the $\rho_{rs}-\rho_f$ phase correlation is always lower than the minimum of the $\rho_{rs}-\rho_{rc}$ and $\rho_{rc}-\rho_f$ phase correlations. This is expected, as the accuracy of the resimulation depends both on the accuracy of the HMC method, which determines the strength of the $\rho_{rs}-\rho_{rc}$ correlation, and the accuracy in the reconstruction of the present-day density field, which determines the strength of the $\rho_{rc}-\rho_f$ correlation.

The comparisons of $\rho_{rs}$ with $\rho_{rc}$ and $\rho_f$ for the HRR are shown in the right panel of Figure 15. As one can see, $\rho_{rs}$ is also strongly correlated with both $\rho_{rc}$ and $\rho_f$. The scatter in the $\rho_{rs}-\rho_f$ correlation is less than 0.2 dex in most density bins. At the high-density end, a weak bias is present in the $\rho_{rc}-\rho_f$ relation, but such a bias is absent in the $\rho_{rs}-\rho_f$ relation. At the low-density end ($\rho < 0.3 \bar{\rho}$), $\rho_{rc}$ is not correlated with either $\rho_{rc}$ nor $\rho_f$. The reason is that in our reconstruction of the present-day density field using mass distributions around halos, the minimum of the density profiles in the domain is about $0.25 \bar{\rho}$ (Figure 7). Therefore, the information in the most underdense regions is totally lost when reconstructing the present-day density field. This bias can be mitigated by adopting a smaller mass threshold $M_{th}$ for the group catalog. The usage of a smaller $M_{th}$ can lower the minimum density that our reconstruction can reach (see Wang et al. 2009b).

The phase correlations for the HRR are presented in the right panel of Figure 9. The phase correlation between $\rho_{rs}$ and $\rho_{rc}$ declines gradually around $k_c$. Similar to the results shown in the previous subsection, this correlation is much stronger than the $\rho_{mod}-\rho_{rc}$ correlation at $k > k_c$. As discussed above, this is due to the mode coupling that is not fully included in the TZ12 model. Moreover, the $\rho_{rc}-\rho_f$ phase correlation lies below the $\rho_{rs}-\rho_{rc}$ phase correlation at almost all scales. It indicates
that, on the smoothing scale $R_s = 2.84 h^{-1}$ Mpc, the accuracy of the resimulation in matching the original density field is mainly limited by the reconstruction of the present-day density rather than by the HMC method. Despite all of these, the match between the resimulation and the original simulation is remarkable. At $k = k_c$, the phase correlation between $\rho_s$ and $\rho_f$ is still as high as 0.6; even at $k = 1.0 h$ Mpc$^{-1}$, about half (47%) of the phase information is reproduced. We recall again that the translinear scale corresponds to $k = 0.15 h$ Mpc$^{-1}$.

We also perform tests with other values of $R_s$ and measure $k_s$, at which the phase correlation between the resimulation and original simulation is half. We show $k_s$ as a function of $R_s$ as the dashed line in Figure 12. One sees that the value of $k_s$ first increases with decreasing $R_s$, then remains almost constant, and has a maximum of 0.94 $h$ Mpc$^{-1}$ at $R_s = 2.84 h^{-1}$ Mpc. The curve generally lies below that based on the original simulated density field (solid line), because the reconstruction of the present-day density field is not perfect. Note that at $R_s = 2.84 h^{-1}$ Mpc, the value of $k_s$ obtained from the reconstructed present-day density field is similar to that obtained from the simulated present-day density field, because on such small scales the inaccuracy of the TZ12 model becomes the dominating source of error in the reconstructed initial condition.

6. SUMMARY AND DISCUSSION

In this paper, we have developed an effective method to reconstruct the linear density field that underlies the formation of the cosmic density field in the local universe. To this end, we have developed an HMC Monte Carlo method that allows us to generate the linear density field based on a posterior probability function. This distribution consists of two components, a prior term that takes into account the Gaussianity and power spectrum assumed for the linear density field and a likelihood term designed to ensure that the predicted density field from the initial condition matches a given final density field. We adopt the MZA developed by TZ12 to model the final, evolved density field of the initial, linear density field.

The HMC method is based on an analogy to a physical system. The potential is taken to be the negative of the logarithm of the posterior function. The momenta are drawn from given distributions before each chain step so that the fictitious system can continue to equilibrate and “orbit” within the extended potential well with the passage of “time.” The system eventually converges to a state in which a balance between kinetic and potential “energy” is achieved. Using a simulated density field, we demonstrate that our HMC method converges very quickly and that the converged linear density fields closely follow a Gaussian distribution with a spectrum that accurately matches the input linear power spectrum. A small discrepancy is found at scales where the likelihood and prior terms in the Hamiltonian force are comparable. This discrepancy, however, can straightforwardly be corrected for by renormalizing the amplitudes of the corresponding Fourier modes (while keeping their phases fixed) with the input linear spectrum. We find that the modeled density field matches the input density field with high precision, with an rms difference typically smaller than 5%.

Since our HMC method needs the present-day density field as a constraint in reconstructing the initial linear density field, we also present a method to reconstruct the present-day density field from mock galaxy and group catalogs. The mock catalogs are constructed from the MS for the SDSS DR7, taking detailed account of the angular variation of the magnitude limit and the survey completeness (Wang et al. 2012a, and references therein) so that we can verify the reliability of our method in real applications. We use the method developed by Wang et al. (2009b) to reconstruct the density field based on the mock group catalog, taking into account inaccuracies in the group finder, as well as uncertainties arising from the assignment of a halo mass to each individual group and the redshift-space distortions. We find that the phase correlation between the reconstructed and simulated density fields is almost perfect at large scales, with a correlation coefficient close to one. The scale at which the correlation coefficient drops to 0.5 is $k \sim 1 h$ Mpc$^{-1}$, indicating that our method works surprisingly well down to scales that are well into the nonlinear regime.

We apply the HMC method to the reconstructed density field in two different volumes. The first one (LRR) is the entire survey volume of the SDSS embedded in a periodic box of size 726 $h^{-1}$ Mpc and the second one (HRR) is a cubic box of size 100 $h^{-1}$ Mpc covering the inner region of the survey volume. These two applications are used to test and verify the performance of the HMC method over a wide dynamic range. As an additional test of the performance of our methods, we use the reconstructed linear density fields of LRR and HRR to generate initial conditions, which we subsequently evolve to the present day using an N-body simulation code. Both visual inspection and quantitative analysis show that the density field obtained from these resimulations accurately matches the density field of the original simulation used to construct the mock catalog. In particular, the phase correlation between the resimulation and the original simulation has a coefficient close to unity on large scales and only starts to drop to 0.5 at $k \sim 1 h$ Mpc$^{-1}$. This clearly demonstrates that our HMC method together with the reconstruction method of Wang et al. (2009b) provides a robust way to reconstruct the initial conditions for the local cosmological density field from observational data.

Numerous studies in the past have tried to infer the initial conditions of structure formation in the local universe using observational data, such as galaxy distributions and/or peculiar velocity surveys (e.g., Nusser & Dekel 1992; Weinberg 1992; Kolatt et al. 1996; Klypin et al. 2003; Dolag et al. 2005; Lavaux 2010). Most of these studies integrate the observed density field backward in time to some initial time. However, these approaches suffer from complications in the observational data such as spatial variations in the magnitude limit and complex survey boundaries, as well as the amplification of noise and numerical errors by the decaying mode during backward integration (Nusser & Dekel 1992). As pointed out by JW13, these problems can be overcome by the HMC method. The amplification of noise and numerical errors is not an issue, since the HMC method uses forward evolution of the cosmic density field (see also Kitaura 2013) and the survey geometry is taken into account by the weight field in the likelihood. Finally, it is worth emphasizing that some of the previous methods had to Gaussianize the inferred initial density field using some order-preserving transformation. In the HMC method adopted here, however, the initial density field is Gaussian by the construction of the posterior.

Our own HMC method has some unique advantages. We design the likelihood using the present-day density field reconstructed from galaxy groups (i.e., dark matter halos), rather than the galaxy distribution itself. The latter requires a detailed understanding of how galaxies are biased relative to the underlying
dark matter distribution (see, e.g., Kitaura & Enßlin 2008). As mentioned earlier, this bias between galaxies and dark matter is far from trivial; it depends on galaxy properties, has stochastic and nonlinear contributions, and may even be non-local. Adopting a simple linear bias model would significantly underestimate the density in high-density regions. Currently, it is still unclear how to directly use the galaxy distribution to model the density field, especially in a high-density region, in an unbiased way. Another problem with using the galaxy distribution is that the constraint becomes very poor in underdense regions, where only few or no galaxies can be observed in a uniformly selected galaxy sample (JW13). In our approach, these problems are largely absent. As shown in Section 4.2, the reconstructed density fields based on the detailed mock catalogs match the input density field very well over a large dynamic range. Furthermore, since our reconstruction relies on groups (halos), we can accurately reproduce the high-density regions within individual halos. In underdense regions, using the density profiles in the domains of halos can recover the density field down to $\rho \lesssim 0.25\bar{\rho}$. And in principle, we can recover even lower densities by simply using groups (halos) above a lower mass threshold, although this requires either a deeper redshift survey or the use of a more limited volume. The use of groups to trace the large-scale density field can effectively mitigate the problem due to the finger-of-God effect, which may severely impact the reconstruction if not properly handled. The reliability of our reconstruction is further demonstrated by the fact that the resimulations from the initial conditions constrained by the reconstruction match the original simulation remarkably well in the same density range.

Moreover, our HMC method works in Fourier space. Different Fourier modes are mutually independent in the prior, and so are the real and imaginary parts of individual modes. This enables us to derive simple formulae for both the prior and likelihood terms in the Hamiltonian force and makes the computation much faster. As shown in Table 1, it takes, on average, only about 21, 220, and 2100 s for each step for $N = 128, 256$, and 512, respectively. Particularly, our method can successfully handle more than one hundred million free parameters! Such efficiency is crucial when aiming to achieve high resolution in a large volume.

In forthcoming papers, we will apply our reconstruction and HMC methods to the SDSS DR7 group catalog in order to generate the initial conditions for structure formation in the SDSS volume. We will then use these initial conditions to run constrained simulations to study the evolution of the local cosmic density field. This will provide a unique opportunity to further our understanding of the formation and evolution of the galaxies we directly observe. For example, one can investigate the correlation between the large-scale environments, measured from the constrained simulation, and the observational galaxy properties. Recent studies have found significant dependencies of halo properties on large-scale environments, in particular the large-scale tidal fields (see, e.g., Wang et al. 2011 and references therein), and it would be interesting to see whether this is also the case for galaxies that reside in halos. One can also make semianalytical models of galaxy formation using halo merger trees extracted directly from the constrained simulations. The comparison between model galaxies and real galaxies in the same large-scale structures, such as filaments, sheets, and clusters, will provide us with an avenue to constrain galaxy formation in a way that is free of cosmic variance.

Finally, the constrained simulation can also be used to study the physics and dynamics of the IGM. For instance, the hot gas and peculiar velocities predicted by the constrained simulations can be used to make predictions for the (both thermal and kinetic) SZ effects, which can be compared with forthcoming observations. Moreover, a comparison of the simulated density field with quasar absorption lines in a wide range of ionization potentials can provide constraints on the metallicity and temperature of the baryonic gas inside the cosmic web (Cen & Ostriker 1999). Such studies will provide a unique way for understanding the nature of the low-$z$ absorption systems and the state and structure of the IGM. In particular, it will allow a detailed exploration of the connection and interaction between the galaxy population and the IGM.

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