Generation of Gaussian Density Fields

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ABSTRACT

This document describes analytical and numerical techniques for the generation of Gaussian density fields, which represent cosmological density perturbations. The mathematical techniques involved in the generation of density harmonics in k-space, the filtering of the density fields, and the normalization of the power spectrum to the measured temperature fluctuations of the Cosmic Microwave Background, are presented in details. These techniques are well-known amongst experts, but the current literature lacks a formal description. I hope that this technical report will prove useful to new researchers moving into this field, sparing them the task of reinventing the wheel.

Subject headings: cosmology: theory — methods: numerical

1. INTRODUCTION

Gaussian density field play a major role in cosmology. There is now strong evidence that the large-scale structure of the universe originated from the growth, by gravitational instability, of primordial density fluctuations. Observations of the temperature fluctuations of the Cosmic Microwave Background (CMB) indicate that these primordial fluctuation were Gaussian.

The formation of evolution of large-scale structure in the universe is a complex problem that requires a numerical approach. Typically, one creates a realization of the density fluctuations at early time, and uses a numerical algorithm to evolve this fluctuation all the way to the present (or to some redshift of interest). Since it is impossible to simulate the entire universe (which might very well be infinite), we normally assume that the universe is periodic at large scales. We can then divide the universe into identical cubes of volume $V_{\rm box} = L_{\rm box}^3$, and we only need to simulate one cube. This approximation is valid as long as the box size $L_{\rm box}$ is much larger than any existing large-scale structure in the universe. We can rephrase this by saying that the box must contain a "fair" sample of the universe.

The density field can be represented in two different ways. In the *Eulerian Representation*, the box is divided into $N \times N \times N$ cells, and the density contrast δ is calculated at the center of each cell. In the *Lagrangian Representation*, $N_p \times N_p \times N_p$ equal-mass particles are laid down on a cubic grid inside the box, and are then displaced in order to represent the density fluctuation. The choice of representation depends on the particular algorithm that will be used to evolve the system from these initial conditions.

1.1. The Power Spectrum

A Gaussian density field can be represented as a superposition of plane waves of wavevectors $\mathbf{k}$ and complex amplitudes $\delta_{\mathbf{k}}^{\rm cont}$, where the superscript "cont" stands for *continuous*, indicating that all values of

$\mathbf{k}$ are allowed. The amplitudes are related to the power spectrum $P(k)$ by

$$|\delta_{\mathbf{k}}^{\mathrm{cont}}|^2 \propto P(k) \,, \tag{1}$$

where $k = |\mathbf{k}|$. However, there is a lot of confusion in the literature about the constant of proportionality between $|\delta_{\mathbf{k}}^{\mathrm{cont}}|^2$ and $P(k)$, and even the *units* of $\delta_{\mathbf{k}}^{\mathrm{cont}}$ can vary from one author to another. We will clarify this issue in §2.

Note: Equation (1) is a convenient simplification. As we will discuss later, in a truly Gaussian random field, the amplitudes $\delta_{\mathbf{k}}$ are determined only in a statistical sense. Their real and imaginary parts are separately given by a Gaussian distribution whose variance is proportional to $P(k)$. However, using equation (1) greatly simplifies the derivation presented in §2, without affecting the results.

2. THE AMPLITUDES OF THE DENSITY MODES

We assume that the universe is periodic over a comoving cubic volume $V_{\mathrm{box}} = L_{\mathrm{box}}^3$. The density contrast δ can be decomposed into a sum of plane waves.

$$\delta(\mathbf{r}) = \frac{1}{N^3} \sum_{\mathbf{k}} \delta_{\mathbf{k}}^{\mathrm{disc}} e^{-i\mathbf{k}\cdot\mathbf{r}} \,, \tag{2}$$

where $\mathbf{r}$ is the comoving position. The wavevectors $\mathbf{k}$ are given by

$$\mathbf{k} = (l, m, n)k_0 \,, \qquad l, m, n = -\infty, \ldots, -1, 0, 1, \ldots, \infty \,. \tag{3}$$

where the fundamental wavenumber is

$$k_0 = \frac{2\pi}{L_{\mathrm{box}}} \,. \tag{4}$$

The superscript "disc" indicates that the amplitudes $\delta_{\mathbf{k}}^{\mathrm{disc}}$ form a discrete spectrum, that is, they are defined for particular, discrete values of $\mathbf{k}$.[1] The factor $1/N^3$ is not necessary at this point, and could be absorbed into the definition of $\delta_{\mathbf{k}}^{\mathrm{disc}}$. We introduce it to make the notation consistent with §3. To make $\delta(\mathbf{r})$ real, the coefficients $\delta_{\mathbf{k}}^{\mathrm{disc}}$ must satisfy the *reality condition*:

$$\delta_{-\mathbf{k}}^{\mathrm{disc}} = (\delta_{\mathbf{k}}^{\mathrm{disc}})^* \,. \tag{5}$$

Our first challenge is to relate the discrete sum in equation (2) to the continuous sum of modes present in the real universe, and to express the amplitudes $\delta_{\mathbf{k}}^{\mathrm{disc}}$ in terms of the power spectrum $P(k)$. To do so, we will consider the rms fluctuation of the density at a certain scale R, and match the expressions obtained in the discrete and continuous limits.

2.1. The Discrete Limit

Consider a sphere of radius R centered at $\mathbf{r}_0$. The mass inside that sphere is given by

$$M(\mathbf{r}_0) = \int_{\mathrm{sph}(\mathbf{r}_0)} \bar{\rho}\,[1 + \delta(\mathbf{r})]\,d^3r = \bar{\rho}V_{\mathrm{sph}} + \frac{\bar{\rho}}{N^3} \int_{\mathrm{sph}(\mathbf{r}_0)} d^3r \sum_{\mathbf{k}} \delta_{\mathbf{k}}^{\mathrm{disc}} e^{-i\mathbf{k}\cdot\mathbf{r}} \,, \tag{6}$$

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[1]Other values of $\mathbf{k}$ would not satisfy the periodic boundary conditions

where $\bar{\rho}$ is the average density, $V_{\mathrm{sph}} = 4\pi R^3/3$ is the volume of the sphere, and the integral is computed over that volume. The relative mass excess in the sphere is given by

$$\frac{\Delta M}{M}(\mathbf{r}_0) = \frac{M(\mathbf{r}_0) - \bar{\rho}V_{\mathrm{sph}}}{\bar{\rho}V_{\mathrm{sph}}} = \frac{1}{N^3 V_{\mathrm{sph}}} \int_{\mathrm{sph}(\mathbf{r}_0)} d^3r \sum_{\mathbf{k}} \delta_{\mathbf{k}}^{\mathrm{disc}} e^{-i\mathbf{k}\cdot\mathbf{r}} \,. \tag{7}$$

We introduce the following change of variables,

$$\mathbf{r} = \mathbf{r}_0 + \mathbf{y} \,. \tag{8}$$

In $\mathbf{y}$-space, the sphere is now located at the origin, and equation (7) becomes

$$\frac{\Delta M}{M}(\mathbf{r}_0) = \frac{1}{N^3 V_{\mathrm{sph}}} \int_{\mathrm{sph}(0)} d^3y \sum_{\mathbf{k}} \delta_{\mathbf{k}}^{\mathrm{disc}} e^{-i\mathbf{k}\cdot\mathbf{r}_0} e^{-i\mathbf{k}\cdot\mathbf{y}} \,. \tag{9}$$

We now square this expression, and get

$$\left(\frac{\Delta M}{M}\right)^2(\mathbf{r}_0) = \frac{9}{16\pi^2 R^6 N^6}\left[\int_{\mathrm{sph}(0)} d^3y \sum_{\mathbf{k}} \delta_{\mathbf{k}}^{\mathrm{disc}} e^{-i\mathbf{k}\cdot\mathbf{r}_0} e^{-i\mathbf{k}\cdot\mathbf{y}}\right]\left[\int_{\mathrm{sph}(0)} d^3z \sum_{\mathbf{k}'} \delta_{\mathbf{k}'}^{\mathrm{disc}} e^{-i\mathbf{k}'\cdot\mathbf{r}_0} e^{-i\mathbf{k}'\cdot\mathbf{z}}\right] \,. \tag{10}$$

The variance of the density contrast at scale R is obtained by averaging the above expression over all possible locations $\mathbf{r}_0$ of the sphere inside the computational box,

$$\begin{aligned}\sigma_R^2 &\equiv \left\langle\left(\frac{\Delta M}{M}\right)^2\right\rangle_{V_{\mathrm{box}}} = \frac{1}{V_{\mathrm{box}}} \int_{V_{\mathrm{box}}} d^3r_0 \left(\frac{\Delta M}{M}\right)^2(\mathbf{r}_0)\\ &= \frac{1}{V_{\mathrm{box}}} \frac{9}{16\pi^2 R^6 N^6} \int_{V_{\mathrm{box}}} d^3r_0 \int_{\mathrm{sph}(0)} d^3y \int_{\mathrm{sph}(0)} d^3z \sum_{\mathbf{k}}\sum_{\mathbf{k}'} \delta_{\mathbf{k}}^{\mathrm{disc}}\delta_{\mathbf{k}'}^{\mathrm{disc}} e^{-i\mathbf{k}\cdot\mathbf{y}} e^{-i\mathbf{k}'\cdot\mathbf{z}} e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}_0} \,.\end{aligned} \tag{11}$$

The integral over V_{box} reduces to

$$\int_{V_{\mathrm{box}}} d^3r_0 e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}_0} = V_{\mathrm{box}}\delta_{\mathbf{k},-\mathbf{k}'} \,. \tag{12}$$

We substitute this expression in equation (11), and use the Kronecker δ to eliminate the summation over $\mathbf{k}'$. Equation (11) reduces to

$$\sigma_R^2 = \frac{9}{16\pi^2 R^6 N^6} \sum_{\mathbf{k}} |\delta_{\mathbf{k}}^{\mathrm{disc}}|^2\left[\int_{\mathrm{sph}(0)} d^3y\, e^{-i\mathbf{k}\cdot\mathbf{y}}\right]^2 \,, \tag{13}$$

where we used equation (5) to get $\delta_{-\mathbf{k}}^{\mathrm{disc}}\delta_{\mathbf{k}}^{\mathrm{disc}} = (\delta_{\mathbf{k}}^{\mathrm{disc}})^*\delta_{\mathbf{k}}^{\mathrm{disc}} = |\delta_{\mathbf{k}}^{\mathrm{disc}}|^2$. The remaining integral can be evaluated easily (see Appendix A). Equation (13) reduces to

$$\sigma_R^2 = \frac{1}{N^6} \sum_{\mathbf{k}} |\delta_{\mathbf{k}}^{\mathrm{disc}}|^2 W^2(kR) \,, \tag{14}$$

where

$$W(u) \equiv \frac{3}{u^3}(\sin u - u\cos u) \,. \tag{15}$$

2.2. The Continuous Limit

The real universe is of course not periodic, in which case all values of $\mathbf{k}$ are allowed. To convert the expressions derived in §2.1 from the discrete limit to the continuous one, consider any function $f_{\mathbf{k}}$ that is summed over all allowed values of $\mathbf{k}$. In the discrete limit, we have

$$\sum_{\mathbf{k}} f_{\mathbf{k}}^{\text{disc}} = \sum_{\text{all V.E.}} f_{\mathbf{k}}^{\text{disc}} = \frac{1}{k_0^3} \sum_{\text{all V.E.}} f_{\mathbf{k}}^{\text{disc}} k_0^3 = \frac{V_{\text{box}}}{(2\pi)^3} \sum_{\text{all V.E.}} f_{\mathbf{k}}^{\text{disc}} \int_{\text{V.E.}} d^3 k \,, \tag{16}$$

where "V.E." represent a *volume element* in $\mathbf{k}$-space, which is a cube of volume k_0^3 centered around an allowed value of $\mathbf{k}$ (with $k_0 = 2\pi/L_{\text{box}}$). Assuming that the function $f_{\mathbf{k}}^{\text{disc}}$ does not vary significantly over one volume element, we can pull it inside the integral,

$$\sum_{\mathbf{k}} f_{\mathbf{k}}^{\text{disc}} \approx \frac{V_{\text{box}}}{(2\pi)^3} \sum_{\text{all V.E.}} \int_{\text{V.E.}} f_{\mathbf{k}}^{\text{disc}} d^3 k \,. \tag{17}$$

Of course, the effect of integrating over the volume element, and then summing over all volume elements, is to effectively integrate over all k-space, so equation (17) reduces to

$$\sum_{\mathbf{k}} f_{\mathbf{k}}^{\text{disc}} \approx \frac{V_{\text{box}}}{(2\pi)^3} \int f_{\mathbf{k}}^{\text{disc}} d^3 k \,. \tag{18}$$

We can rewrite this expression as

$$\sum_{\mathbf{k}} f_{\mathbf{k}}^{\text{disc}} \approx \int f_{\mathbf{k}}^{\text{cont}} d^3 k \,, \tag{19}$$

where the continuous and discrete functions are related by

$$f_{\mathbf{k}}^{\text{cont}} = \frac{V_{\text{box}}}{(2\pi)^3} f_{\mathbf{k}}^{\text{disc}} \,. \tag{20}$$

Using these formulae, we can rewrite equation (2) as

$$\delta(\mathbf{r}) = \frac{1}{N^3} \int d^3 k \, \delta_{\mathbf{k}}^{\text{cont}} e^{-i\mathbf{k}\cdot\mathbf{r}} \,, \tag{21}$$

where

$$\delta_{\mathbf{k}}^{\text{cont}} = \frac{V_{\text{box}}}{(2\pi)^3} \delta_{\mathbf{k}}^{\text{disc}} \,. \tag{22}$$

Let us now convert equation (14) into an integral, as we did for equation (16). We get

$$\sigma_R^2 = \frac{V_{\text{box}}}{(2\pi)^3 N^6} \int d^3 k |\delta_{\mathbf{k}}^{\text{disc}}|^2 W^2(kR) \,. \tag{23}$$

We substitute equation (22) into equation (23), and get

$$\sigma_R^2 = \frac{(2\pi)^3}{V_{\text{box}} N^6} \int d^3 k |\delta_{\mathbf{k}}^{\text{cont}}|^2 W^2(kR) \,. \tag{24}$$

We then need to related σ_R^2 to the power spectrum $P(k)$. The relation is given by Bunn & White (1997) as

$$\sigma_R^2 = \frac{1}{2\pi^2} \int_0^\infty dk\, k^2 P(k) W^2(kR)\,.$$

(25)

This relation is obtained by performing an integration over angles, using the fact that $P(\mathbf{k})$ is a function of $k = |\mathbf{k}|$ only. We can "undo" this integration, simply by dividing equation (25) by 4π. We get

$$\sigma_R^2 = \frac{1}{(2\pi)^3} \int d^3k\, P(k) W^2(kR)\,.$$

(26)

Comparing equations (23), (24), and (26), we get

$$P(k) = \frac{V_{\text{box}}}{N^6} |\delta_{\mathbf{k}}^{\text{disc}}|^2 = \frac{(2\pi)^6}{V_{\text{box}} N^6} |\delta_{\mathbf{k}}^{\text{cont}}|^2\,.$$

(27)

This gives us the relation between $P(k)$, $\delta_{\mathbf{k}}^{\text{disc}}$, and $\delta_{\mathbf{k}}^{\text{cont}}$. Notice the $P(k)$ is neither the square of $\delta_{\mathbf{k}}^{\text{disc}}$ nor the square of $\delta_{\mathbf{k}}^{\text{cont}}$. Both $P(k)$ and $\delta_{\mathbf{k}}^{\text{cont}}$ have dimensions of a volume while $\delta_{\mathbf{k}}^{\text{disc}}$ is dimensionless.

Equations (25) and (26) define the normalization of the power spectrum. When using any power spectrum obtained from the literature, *it is essential to check that these relations are satisfied.* Variations by factors of 2π between different papers are quite common.

3. DIRECT CALCULATION OF THE DENSITY HARMONICS

Using the formalism described in §2, we now want to compute the density harmonics $\hat{\delta}_{\mathbf{k}}$. We first lay down inside the computational volume V_{box} a regular cubic grid of size $N \times N \times N$, with grid spacing $\Delta = L_{\text{box}}/N$. The coordinates $\mathbf{r}$ of the grid points are given by

$$\mathbf{r} = (\alpha, \beta, \gamma)\Delta\,, \qquad \alpha, \beta, \gamma = 0, 1, \ldots, N-1\,.$$

(28)

The presence of a grid results in a discretization of space, which in turns modifies the structure of the k-space. In equation (3), the values of $\mathbf{k}$ form an infinite cubic grid in k-space, since the indicies l, m, n can take any integer value from $-\infty$ to $+\infty$. However, the discretization of space limits the number of modes. Consider a mode with wavenumber

$$\mathbf{k}' = \mathbf{k} + (uN, vN, wN)k_0\,,$$

(29)

where u, v, and w are integers. The exponential in equation (2) becomes

$$
\begin{aligned}
e^{-i\mathbf{k}'\cdot\mathbf{r}} &= e^{-i\mathbf{k}\cdot\mathbf{r}} e^{-i[uN,vN,wN]\cdot[\alpha,\beta,\gamma]k_0\Delta} = e^{-i\mathbf{k}\cdot\mathbf{r}} e^{-i[uN,vN,wN]\cdot[\alpha,\beta,\gamma](2\pi/N)} \\
&= e^{-i\mathbf{k}\cdot\mathbf{r}} e^{-2\pi i[u,v,w]\cdot[\alpha,\beta,\gamma]} = e^{-i\mathbf{k}\cdot\mathbf{r}}\,.
\end{aligned}
$$

(30)

Hence, the modes $\mathbf{k}'$ and $\mathbf{k}$ are *inseparable.* They represent a plane wave with the same effective wavenumber. Consequently, we will consider a finite k-space, in which the values l, m, n do not run from $-\infty$ to $+\infty$, but instead are limited to the range 0 to $N-1$. Hence, in k-space, the density harmonics $\hat{\delta}(\mathbf{k})$ are also defined on a regular cubic grid of size $N \times N \times N$. The wavevectors are given by

$$\mathbf{k} = (l, m, n)k_0\,, \qquad l, m, n = 0, 1, \ldots, N-1\,.$$

(31)

In doing so, we are simply neglecting high-frequency modes. This is justified since the discreteness of the grid in r-space prevents us from resolving any structure that these modes represent. Hence, by using a grid in r-space, we are effectively performing a filtering of the density fluctuation at the scale of Δ, and such filtering eliminates high-frequency modes.

The Fourier transform and inverse Fourier transform are given respectively by

$$\hat{\delta}(\mathbf{k}) = \sum_{\mathbf{r}} \delta(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{32}$$

$$\delta(\mathbf{r}) = \frac{1}{N^3} \sum_{\mathbf{k}} \hat{\delta}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}}. \tag{33}$$

Notice that equation (33) is the same as equation (2), with a slight change of notation: $\delta_{\mathbf{k}}^{\text{disc}} \to \hat{\delta}(\mathbf{k})$. We introduce the notation

$$\hat{\delta}(\mathbf{k}) = \hat{\delta}_{lmn}, \tag{34}$$

$$\delta(\mathbf{r}) = \delta_{\alpha\beta\gamma}. \tag{35}$$

Equation (32) becomes

$$\hat{\delta}_{lmn} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} e^{i(2\pi/\Delta N)\Delta[l,m,n]\cdot[\alpha,\beta,\gamma]} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} e^{2\pi il\alpha/N} e^{2\pi im\beta/N} e^{2\pi in\gamma/N}$$

$$= \sum_{\alpha,\beta,\gamma=0}^{N-1} \left(\cos\frac{2\pi l\alpha}{N} + i\sin\frac{2\pi l\alpha}{N} \right) \left(\cos\frac{2\pi m\beta}{N} + i\sin\frac{2\pi m\beta}{N} \right) \left(\cos\frac{2\pi n\gamma}{N} + i\sin\frac{2\pi n\gamma}{N} \right). \tag{36}$$

After expansion, this expression becomes

$$\hat{\delta}_{lmn} = (\hat{\delta}_{eee} + \hat{\delta}_{eoo} + \hat{\delta}_{oeo} + \hat{\delta}_{ooe}) + i(\hat{\delta}_{eeo} + \hat{\delta}_{eoe} + \hat{\delta}_{oee} + \hat{\delta}_{ooo}), \tag{37}$$

where we define

$$\hat{\delta}_{eee} \equiv \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \cos\frac{2\pi l\alpha}{N} \cos\frac{2\pi m\beta}{N} \cos\frac{2\pi n\gamma}{N}, \tag{38}$$

$$\hat{\delta}_{eeo} \equiv \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \cos\frac{2\pi l\alpha}{N} \cos\frac{2\pi m\beta}{N} \sin\frac{2\pi n\gamma}{N}, \tag{39}$$

$$\hat{\delta}_{eoe} \equiv \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \cos\frac{2\pi l\alpha}{N} \sin\frac{2\pi m\beta}{N} \cos\frac{2\pi n\gamma}{N}, \tag{40}$$

$$\hat{\delta}_{eoo} \equiv -\sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \cos\frac{2\pi l\alpha}{N} \sin\frac{2\pi m\beta}{N} \sin\frac{2\pi n\gamma}{N}, \tag{41}$$

$$\hat{\delta}_{oee} \equiv \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \sin\frac{2\pi l\alpha}{N} \cos\frac{2\pi m\beta}{N} \cos\frac{2\pi n\gamma}{N}, \tag{42}$$

$$\hat{\delta}_{oeo} \equiv -\sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \sin\frac{2\pi l\alpha}{N} \cos\frac{2\pi m\beta}{N} \sin\frac{2\pi n\gamma}{N}, \tag{43}$$

$$\hat{\delta}_{ooe} \equiv - \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \sin \frac{2\pi l\alpha}{N} \sin \frac{2\pi m\beta}{N} \cos \frac{2\pi n\gamma}{N} , \qquad (44)$$

$$\hat{\delta}_{ooo} \equiv - \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \sin \frac{2\pi l\alpha}{N} \sin \frac{2\pi m\beta}{N} \sin \frac{2\pi n\gamma}{N} . \qquad (45)$$

Consider now the mode $\hat{\delta}_{N-l,m,n}$. We replace l by $N-l$ in equation (36), and get

$$\hat{\delta}_{N-l,mn} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} e^{2\pi i(N-l)\alpha/N} e^{2\pi im\beta/N} e^{2\pi in\gamma/N} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} e^{2\pi i\alpha} e^{-2\pi il\alpha/N} e^{2\pi im\beta/N} e^{2\pi in\gamma/N} . \qquad (46)$$

Since α is an integer, the first exponential is always unity, and equation (46) reduces to

$$\hat{\delta}_{N-l,mn} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \left(\cos \frac{2\pi l\alpha}{N} - i \sin \frac{2\pi l\alpha}{N} \right) \left(\cos \frac{2\pi m\beta}{N} + i \sin \frac{2\pi m\beta}{N} \right) \left(\cos \frac{2\pi n\gamma}{N} + i \sin \frac{2\pi n\gamma}{N} \right) . \qquad (47)$$

Comparing equations (36) and (47), we see that the effect of replacing l by $N-l$ amounts to a change of sign of the first sine function. In equations (38)–(45), that sine appears only in the $\hat{\delta}$'s for which the first subscript is "o." Hence, these $\hat{\delta}$'s will change sign, and equation (37) will become

$$\hat{\delta}_{N-l,mn} = (\hat{\delta}_{eee} + \hat{\delta}_{eoo} - \hat{\delta}_{oeo} - \hat{\delta}_{ooe}) + i(\hat{\delta}_{eeo} + \hat{\delta}_{eoe} - \hat{\delta}_{oee} - \hat{\delta}_{ooo}) , \qquad (48)$$

We can directly generalize to the other indicies, or combinations of them. Replacing m by $N-m$ changes the sign of the $\hat{\delta}$'s for which the second subscript is "o," and replacing n by $N-n$ changes the sign of the $\hat{\delta}$'s for which the third subscript is "o." Hence,

$$\hat{\delta}_{l,N-m,n} = (\hat{\delta}_{eee} - \hat{\delta}_{eoo} + \hat{\delta}_{oeo} - \hat{\delta}_{ooe}) + i(\hat{\delta}_{eeo} - \hat{\delta}_{eoe} + \hat{\delta}_{oee} - \hat{\delta}_{ooo}) , \qquad (49)$$

$$\hat{\delta}_{lm,N-n} = (\hat{\delta}_{eee} - \hat{\delta}_{eoo} - \hat{\delta}_{oeo} + \hat{\delta}_{ooe}) + i(-\hat{\delta}_{eeo} + \hat{\delta}_{eoe} + \hat{\delta}_{oee} - \hat{\delta}_{ooo}) , \qquad (50)$$

$$\hat{\delta}_{N-l,N-m,n} = (\hat{\delta}_{eee} - \hat{\delta}_{eoo} - \hat{\delta}_{oeo} + \hat{\delta}_{ooe}) + i(\hat{\delta}_{eeo} - \hat{\delta}_{eoe} - \hat{\delta}_{oee} + \hat{\delta}_{ooo}) , \qquad (51)$$

$$\hat{\delta}_{N-l,m,N-n} = (\hat{\delta}_{eee} - \hat{\delta}_{eoo} + \hat{\delta}_{oeo} - \hat{\delta}_{ooe}) + i(-\hat{\delta}_{eeo} + \hat{\delta}_{eoe} - \hat{\delta}_{oee} + \hat{\delta}_{ooo}) , \qquad (52)$$

$$\hat{\delta}_{l,N-m,N-n} = (\hat{\delta}_{eee} + \hat{\delta}_{eoo} - \hat{\delta}_{oeo} - \hat{\delta}_{ooe}) + i(-\hat{\delta}_{eeo} - \hat{\delta}_{eoe} + \hat{\delta}_{oee} + \hat{\delta}_{ooo}) , \qquad (53)$$

$$\hat{\delta}_{N-l,N-m,N-n} = (\hat{\delta}_{eee} + \hat{\delta}_{eoo} + \hat{\delta}_{oeo} + \hat{\delta}_{ooe}) + i(-\hat{\delta}_{eeo} - \hat{\delta}_{eoe} - \hat{\delta}_{oee} - \hat{\delta}_{ooo}) . \qquad (54)$$

Hence, 8 different, but related harmonics can be represented by various combinations of 8 numbers: $\hat{\delta}_{eee}$, $\hat{\delta}_{eeo}$, $\hat{\delta}_{eoe}$, $\hat{\delta}_{oee}$, $\hat{\delta}_{eoo}$, $\hat{\delta}_{oeo}$, $\hat{\delta}_{ooe}$, and $\hat{\delta}_{ooo}$. This implies that the Fourier transform of a real field defined on a grid $N \times N \times N$ can be represented by N^3 real numbers stored on a similar grid, even though the Fourier transform $\hat{\delta}(\mathbf{k})$ is complex. Notice also that the 8 "related" modes are located, in k-space, at the verticies of a rectangular box centered on the center of the k-space grid ($l, m, n = N/2$). This is illustrated in Figure 1.

From equations (37) and (48)–(54), we see that related modes form 4 pairs of complex conjugates:

$$\hat{\delta}_{lmn} = \hat{\delta}^*_{N-l,N-m,N-n} , \qquad (55)$$

$$\hat{\delta}_{lm,N-n} = \hat{\delta}^*_{N-l,N-m,n} , \qquad (56)$$

$$\hat{\delta}_{l,N-m,n} = \hat{\delta}^*_{N-l,m,N-n} , \qquad (57)$$

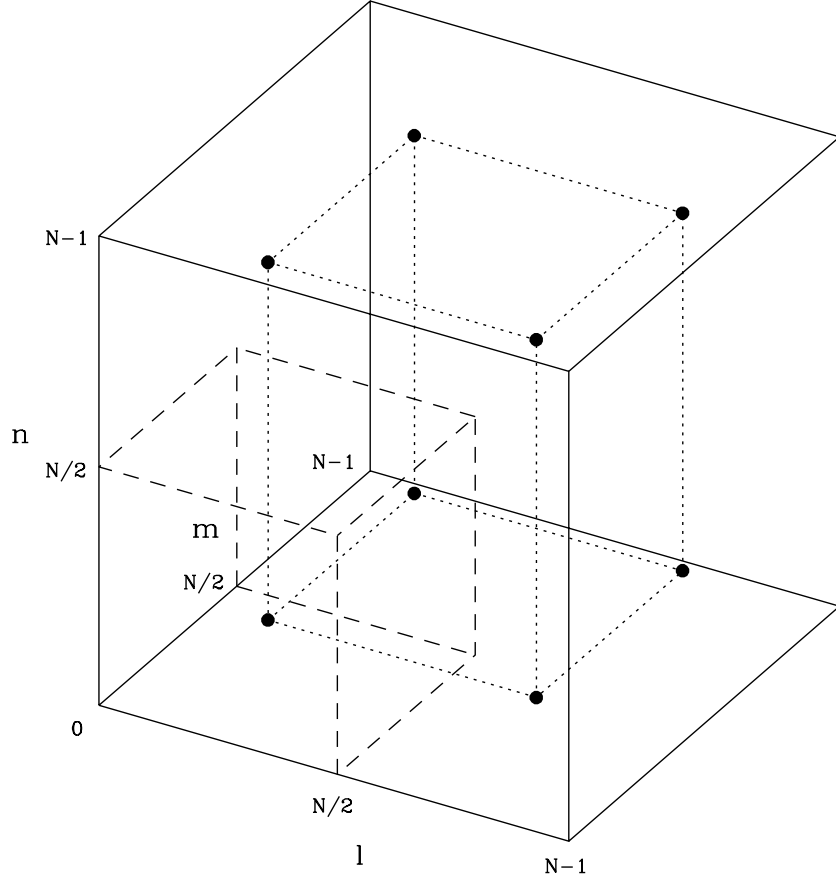$$\hat{\delta}_{l,N-m,N-n} = \hat{\delta}^*_{N-l,mn} . \qquad (58)$$

Fig. 1.— Representation of the system in k-space. The 3 axes correspond to the 3 indicies l, m, n, which run from 0 to $N-1$, with $N = 64$ in this case. The dots indicate the particular mode $(l, m, n) = (14, 15, 8)$ and the seven related modes. Notice that only one of these modes is located in the first octant, indicated by the dashed lines.

3.1. General Case

Consider first the modes for which the indicies l, m, and n are neither 0 nor $N/2$. In equations (55)–(58), the amplitudes $\hat{\delta}$ are provided by the power spectrum. From equation (27), we get

$$|\hat{\delta}_{\mathbf{k}}^{\text{disc}}| = N^3 \left[\frac{P(k)}{V_{\text{box}}} \right]^{1/2} . \tag{59}$$

Equation (59) provides the correct normalization of the power spectrum. However, there are two problems with this equation. First, it provides no mean of determining the phases of the complex numbers $\hat{\delta}_{\mathbf{k}}^{\text{disc}}$, and second, choosing random phases would result in a field that is not Gaussian. In a truly Gaussian field, equation (59) is only valid in a statistical sense. The correct approach is to compute the real and imaginary

parts of $\hat{\delta}_{\mathbf{k}}^{\mathrm{disc}}$ independently, by drawing them from a Gaussian distribution,

$$\mathrm{Re}\,\hat{\delta}_{\mathbf{k}}^{\mathrm{disc}} = G_1(0,1)N^3\left[\frac{P(k)}{2V_{\mathrm{box}}}\right]^{1/2}, \tag{60}$$

$$\mathrm{Im}\,\hat{\delta}_{\mathbf{k}}^{\mathrm{disc}} = G_2(0,1)N^3\left[\frac{P(k)}{2V_{\mathrm{box}}}\right]^{1/2}, \tag{61}$$

where $G_1(0,1)$ and $G_2(0,1)$ are random numbers drawn from a Gaussian distribution with mean 0 and standard deviation 1. This ensures that the resulting field is Gaussian.

Equations (60) and (61) provide us with the left-hand-sides of equations (55)–(58). By equating these expressions with equations (37), (49), (50), and (53), and considering the real and imaginary parts separately, we get 8 equations,

$$\hat{\delta}_{eee} + \hat{\delta}_{eoo} + \hat{\delta}_{oeo} + \hat{\delta}_{ooe} = R_1, \tag{62}$$
$$\hat{\delta}_{eeo} + \hat{\delta}_{eoe} + \hat{\delta}_{oee} + \hat{\delta}_{ooo} = I_1, \tag{63}$$
$$\hat{\delta}_{eee} - \hat{\delta}_{eoo} - \hat{\delta}_{oeo} + \hat{\delta}_{ooe} = R_2, \tag{64}$$
$$-\hat{\delta}_{eeo} + \hat{\delta}_{eoe} + \hat{\delta}_{oee} - \hat{\delta}_{ooo} = I_2, \tag{65}$$
$$\hat{\delta}_{eee} - \hat{\delta}_{eoo} + \hat{\delta}_{oeo} - \hat{\delta}_{ooe} = R_3, \tag{66}$$
$$\hat{\delta}_{eeo} - \hat{\delta}_{eoe} + \hat{\delta}_{oee} - \hat{\delta}_{ooo} = I_3, \tag{67}$$
$$\hat{\delta}_{eee} + \hat{\delta}_{eoo} - \hat{\delta}_{oeo} - \hat{\delta}_{ooe} = R_4, \tag{68}$$
$$-\hat{\delta}_{eeo} - \hat{\delta}_{eoe} + \hat{\delta}_{oee} + \hat{\delta}_{ooo} = I_4, \tag{69}$$

where

$$R_1 \equiv \mathrm{Re}\,\hat{\delta}_{lmn}, \tag{70}$$
$$I_1 \equiv \mathrm{Im}\,\hat{\delta}_{lmn}, \tag{71}$$
$$R_2 \equiv \mathrm{Re}\,\hat{\delta}_{lm,N-n}, \tag{72}$$
$$I_2 \equiv \mathrm{Im}\,\hat{\delta}_{lm,N-n}, \tag{73}$$
$$R_3 \equiv \mathrm{Re}\,\hat{\delta}_{l,N-m,n}, \tag{74}$$
$$I_3 \equiv \mathrm{Im}\,\hat{\delta}_{l,N-m,n}, \tag{75}$$
$$R_4 \equiv \mathrm{Re}\,\hat{\delta}_{l,N-m,N-n}, \tag{76}$$
$$I_4 \equiv \mathrm{Im}\,\hat{\delta}_{l,N-m,N-n}. \tag{77}$$

Altogether, we get two separate systems of 4 equations and 4 unknowns. Written in matrix form, these systems are:

$$\mathbf{M}\begin{bmatrix}\hat{\delta}_{eee}\\\hat{\delta}_{eoo}\\\hat{\delta}_{oeo}\\\hat{\delta}_{ooe}\end{bmatrix} = \begin{bmatrix}R_1\\R_2\\R_3\\R_4\end{bmatrix}, \qquad \mathbf{M}\begin{bmatrix}\hat{\delta}_{eeo}\\\hat{\delta}_{eoe}\\\hat{\delta}_{oee}\\\hat{\delta}_{ooo}\end{bmatrix} = \begin{bmatrix}I_1\\-I_2\\I_3\\-I_4\end{bmatrix}, \tag{78}$$

where the matrix $\mathbf{M}$ is given by

$$\mathbf{M} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \end{bmatrix} . \tag{79}$$

The inverse of the matrix $\mathbf{M}$ is simply $\mathbf{M}^{-1} = \mathbf{M}/4$. Hence, the $\hat{\delta}$'s are given by

$$\begin{bmatrix} \hat{\delta}_{eee} \\ \hat{\delta}_{eoo} \\ \hat{\delta}_{oeo} \\ \hat{\delta}_{ooe} \end{bmatrix} = \frac{\mathbf{M}}{4} \begin{bmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \end{bmatrix} , \qquad \begin{bmatrix} \hat{\delta}_{eeo} \\ \hat{\delta}_{eoe} \\ \hat{\delta}_{oee} \\ \hat{\delta}_{ooo} \end{bmatrix} = \frac{\mathbf{M}}{4} \begin{bmatrix} I_1 \\ -I_2 \\ I_3 \\ -I_4 \end{bmatrix} , \tag{80}$$

3.2. On a Face

Consider now the case where one of the indicies, say l, is equal to either 0 or $N/2$. These cases correspond to values of $\mathbf{k}$ located on a face of the first octant in k-space. The problem becomes simpler. With $l = 0$, equation (36) reduces to

$$\begin{aligned} \hat{\delta}_{0mn} &= \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} e^{2\pi i m\beta/N} e^{2\pi i n\gamma/N} \\ &= \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \left(\cos\frac{2\pi m\beta}{N} + i\sin\frac{2\pi m\beta}{N} \right) \left(\cos\frac{2\pi n\gamma}{N} + i\sin\frac{2\pi n\gamma}{N} \right) . \end{aligned} \tag{81}$$

After expansion, this expression becomes

$$\hat{\delta}_{0mn} = (\hat{\delta}_{ee} + \hat{\delta}_{oo}) + i(\hat{\delta}_{eo} + \hat{\delta}_{oe}) , \tag{82}$$

where

$$\hat{\delta}_{ee} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \cos\frac{2\pi m\beta}{N} \cos\frac{2\pi n\gamma}{N} , \tag{83}$$

$$\hat{\delta}_{eo} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \cos\frac{2\pi m\beta}{N} \sin\frac{2\pi n\gamma}{N} , \tag{84}$$

$$\hat{\delta}_{oe} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \sin\frac{2\pi m\beta}{N} \cos\frac{2\pi n\gamma}{N} , \tag{85}$$

$$\hat{\delta}_{oo} = -\sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \sin\frac{2\pi m\beta}{N} \sin\frac{2\pi n\gamma}{N} . \tag{86}$$

Consider now the mode $\hat{\delta}_{0,N-m,n}$. We replace m by $N-m$ in equation (81), and get

$$\hat{\delta}_{0,N-m,n} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} e^{2\pi i(N-m)\beta/N} e^{2\pi i n\gamma/N} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} e^{2\pi i\beta} e^{-2\pi i m\beta/N} e^{2\pi i n\gamma/N} . \tag{87}$$

Since β in an integer, the first exponential is always unity, and equation (87) reduces to

$$\hat{\delta}_{0,N-m,n} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \left(\cos\frac{2\pi m\beta}{N} - i\sin\frac{2\pi m\beta}{N} \right) \left(\cos\frac{2\pi n\gamma}{N} + i\sin\frac{2\pi n\gamma}{N} \right) . \tag{88}$$

Comparing equations (81) and (88), the only difference is a change of sign of the first sine function. In equations (83)–(86), that sine appears only in the $\hat{\delta}$'s for which the first subscript is "o." Hence, these $\hat{\delta}$'s will change sign, and equation (82) will becomes

$$\hat{\delta}_{0,N-m,n} = (\hat{\delta}_{ee} - \hat{\delta}_{oo}) + i(\hat{\delta}_{eo} - \hat{\delta}_{oe}) , \tag{89}$$

Similarly, we can easily show that replacing n by $N - n$ results in a change of sign of the $\hat{\delta}$'s for which the second subscript is "o." Hence, we get

$$\hat{\delta}_{0m,N-n} = (\hat{\delta}_{ee} - \hat{\delta}_{oo}) + i(-\hat{\delta}_{eo} + \hat{\delta}_{oe}) , \tag{90}$$

$$\hat{\delta}_{0,N-m,N-n} = (\hat{\delta}_{ee} + \hat{\delta}_{oo}) + i(-\hat{\delta}_{eo} - \hat{\delta}_{oe}) . \tag{91}$$

These 4 modes are located at the vertices of a rectangle in k-space, as shown in Figure 2. They form two pairs of complex conjugates,

$$\hat{\delta}_{0mn} = \hat{\delta}_{0,N-m,N-n}^* , \tag{92}$$

$$\hat{\delta}_{0m,N-n} = \hat{\delta}_{0,N-m,n}^* . \tag{93}$$

By equating these expressions with equations (82) and (90), and considering the real and imaginary parts separately, we get 4 equations,

$$\hat{\delta}_{ee} + \hat{\delta}_{oo} = R_1 , \tag{94}$$

$$\hat{\delta}_{eo} + \hat{\delta}_{oe} = I_1 , \tag{95}$$

$$\hat{\delta}_{ee} - \hat{\delta}_{oo} = R_2 , \tag{96}$$

$$-\hat{\delta}_{eo} + \hat{\delta}_{oe} = I_2 , \tag{97}$$

where

$$R_1 \equiv \operatorname{Re}\hat{\delta}_{0mn} , \tag{98}$$

$$I_1 \equiv \operatorname{Im}\hat{\delta}_{0mn} , \tag{99}$$

$$R_2 \equiv \operatorname{Re}\hat{\delta}_{0m,N-n} , \tag{100}$$

$$I_2 \equiv \operatorname{Im}\hat{\delta}_{0m,N-n} . \tag{101}$$

Again, the numbers R_1, I_1, R_2, and I_2 are determined from equations (60) and (61). The solutions are

$$\hat{\delta}_{ee} = \frac{R_1 + R_2}{2} , \tag{102}$$

$$\hat{\delta}_{oo} = \frac{R_1 - R_2}{2} , \tag{103}$$

$$\hat{\delta}_{eo} = \frac{I_1 - I_2}{2} , \tag{104}$$

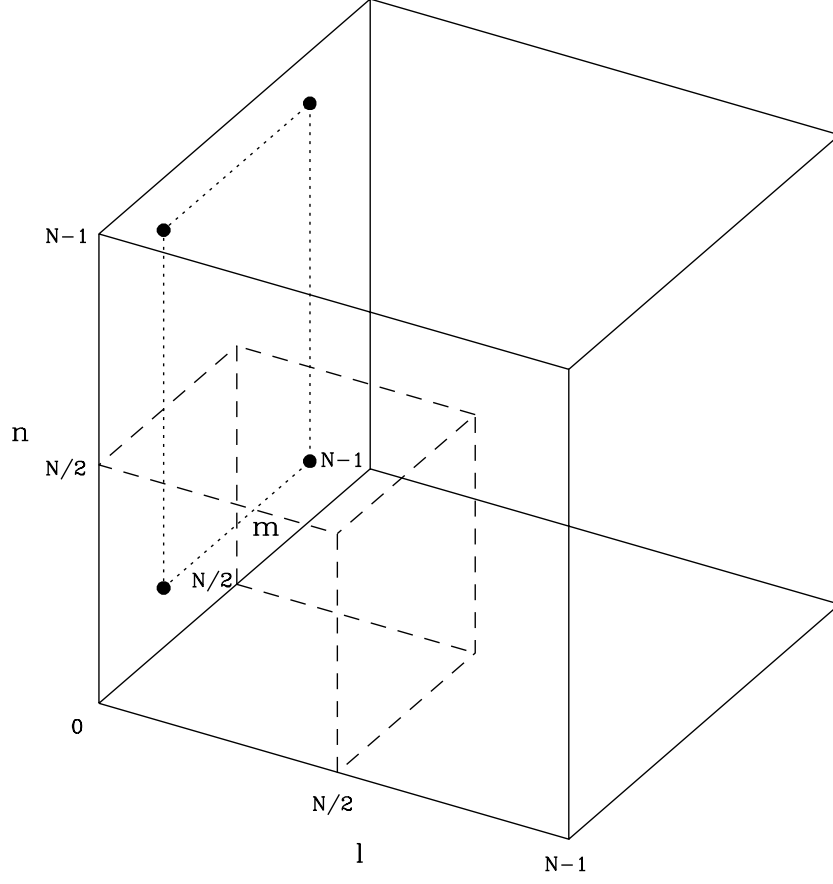$$\hat{\delta}_{oe} = \frac{I_1 + I_2}{2} . \tag{105}$$

Fig. 2.— Representation of the system in k-space. The dots indicate the particular mode $(l, m, n) = (0, 15, 8)$ and the three related modes.

Consider now the case $l = N/2$. Equation (36) reduces to

$$\hat{\delta}_{N/2,mn} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} e^{\pi i l \alpha} e^{2\pi i m \beta/N} e^{2\pi i n \gamma/N}$$

$$= \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma}(-1)^{\alpha} \left(\cos \frac{2\pi m \beta}{N} + i \sin \frac{2\pi m \beta}{N} \right) \left(\cos \frac{2\pi n \gamma}{N} + i \sin \frac{2\pi n \gamma}{N} \right). \quad (106)$$

After expansion, this expression becomes

$$\hat{\delta}_{0mn} = (\hat{\delta}_{ee} + \hat{\delta}_{oo}) + i(\hat{\delta}_{eo} + \hat{\delta}_{oe}), \quad (107)$$

where

$$\hat{\delta}_{ee} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma}(-1)^{\alpha} \cos \frac{2\pi m \beta}{N} \cos \frac{2\pi n \gamma}{N}, \quad (108)$$
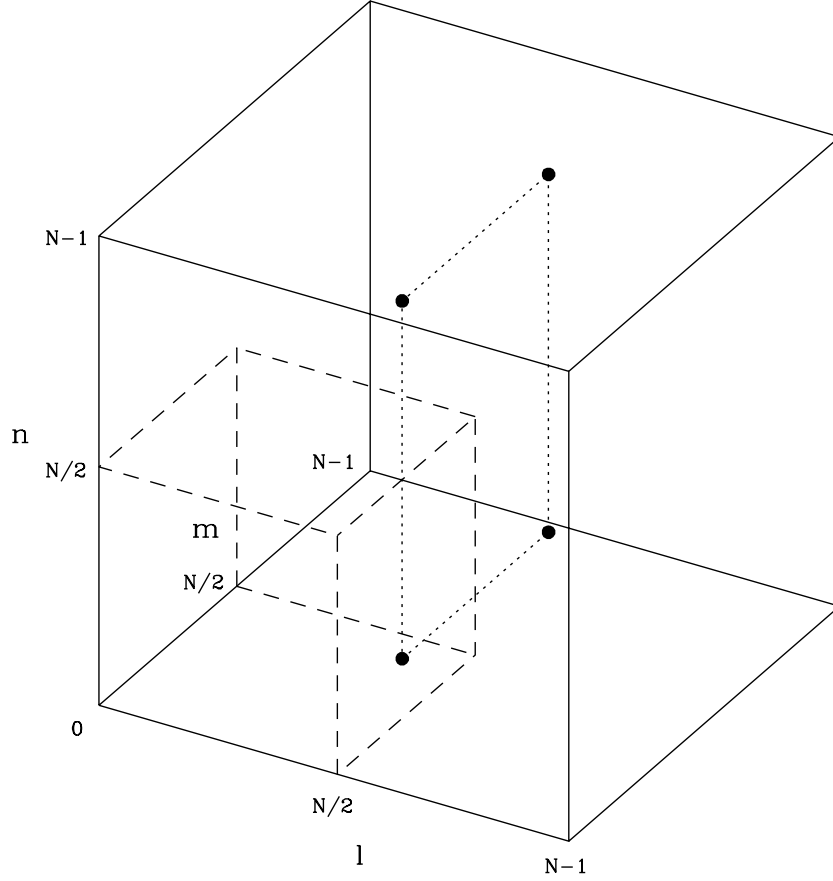
Fig. 3.— Representation of the system in k-space. The dots indicate the particular mode $(l,m,n) = (32, 15, 8)$, where $32 = N/2$, and the three related modes.

$$\hat{\delta}_{eo} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma}(-1)^\alpha \cos\frac{2\pi m\beta}{N}\sin\frac{2\pi n\gamma}{N}, \tag{109}$$

$$\hat{\delta}_{oe} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma}(-1)^\alpha \sin\frac{2\pi m\beta}{N}\cos\frac{2\pi n\gamma}{N}, \tag{110}$$

$$\hat{\delta}_{oo} = -\sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma}(-1)^\alpha \sin\frac{2\pi m\beta}{N}\sin\frac{2\pi n\gamma}{N}. \tag{111}$$

We find the same expressions as for the case $l = 0$, the only differences being the extra factor of $(-1)^\alpha$ in the definitions of the $\hat{\delta}$'s. Hence, the solutions (102)–(105) are still valid in this case. These modes are shown in Figure 3.

We have only considered the cases when the first index, l, is either 0 or $N/2$, but these results can be generalized to the other indicies m and n as well, since the entire problem has cubic symmetry.

3.3. On an Edge

Consider now the case when two of the indicies, say l and m, are equal to either 0 or $N/2$. These cases corresponds to values of $\mathbf{k}$ located on an edge of the first octant in k-space. With $l = m = 0$, equation (36) reduces to

$$\hat{\delta}_{00n} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} e^{2\pi in\gamma/N} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \left(\cos \frac{2\pi in\gamma}{N} + i \sin \frac{2\pi in\gamma}{N} \right). \tag{112}$$

This expression becomes

$$\hat{\delta}_{00n} = \hat{\delta}_e + i\hat{\delta}_o, \tag{113}$$

where

$$\hat{\delta}_e = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \cos \frac{2\pi n\gamma}{N}, \tag{114}$$

$$\hat{\delta}_o = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \sin \frac{2\pi n\gamma}{N}. \tag{115}$$

Consider now the mode $\hat{\delta}_{00,N-n}$. We replace n by $N-n$ in equation (112), and get

$$\hat{\delta}_{00,N-n} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} e^{2\pi i(N-n)\gamma/N} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} e^{2\pi i\gamma} e^{-2\pi in\gamma/N}. \tag{116}$$

Since γ in an integer, the first exponential is always unity, and equation (116) reduces to

$$\hat{\delta}_{0,0,N-n} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \left(\cos \frac{2\pi n\gamma}{N} - i \sin \frac{2\pi n\gamma}{N} \right). \tag{117}$$

Comparing equations (112) and (117), the only difference is a change of sign of the sine function. In equations (114) and (115), that sine appears only in the expression for $\hat{\delta}_o$. Hence, equation (113) becomes

$$\hat{\delta}_{00,N-n} = \hat{\delta}_e - i\hat{\delta}_o, \tag{118}$$

These two modes are complex conjugates,

$$\hat{\delta}_{00n} = \hat{\delta}^*_{00,N-n}. \tag{119}$$

They are shown in Figure 4. By equating equation (113) and (119), and considering the real and imaginary parts separately, we get

$$\hat{\delta}_e = R_1, \tag{120}$$

$$\hat{\delta}_o = I_1, \tag{121}$$

where

$$R_1 \equiv \operatorname{Re} \hat{\delta}_{00n}, \tag{122}$$

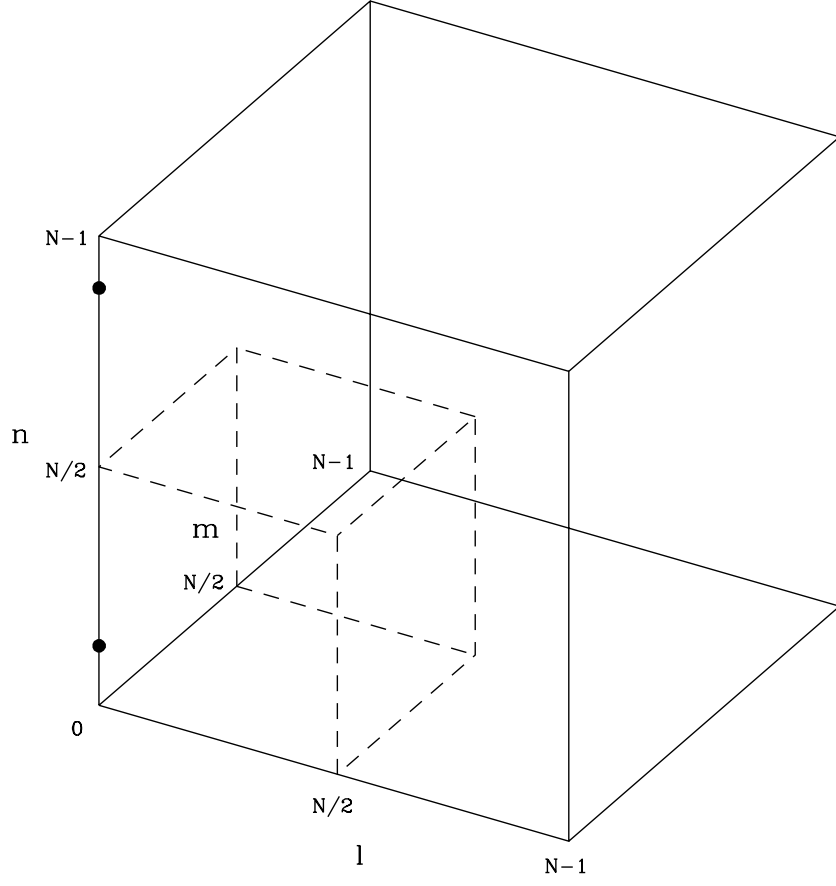$$I_1 \equiv \operatorname{Im} \hat{\delta}_{00n}. \tag{123}$$

Fig. 4.— Representation of the system in k-space. The dots indicate the particular mode $(l, m, n) = (0, 0, 8)$ and its related mode.

The numbers R_1 and I_1 are determined from equations (60) and (61).

Consider now the case $l = N/2$, $m = 0$, the case $l = 0$, $m = N/2$, and the case $l = m = N/2$. We can easily show that the solutions (120) and (121) are still valid, using the same approach as in §3.2. Again, the only difference will be extra factors of $(-1)^\alpha$ in the definitions of $\hat{\delta}_e$ and $\hat{\delta}_o$. These modes are shown in Figure 5. Using the cubic symmetry, we can then show that the solutions (120) and (121) applies to all cases for which two of the three indicies l, m, n are equal to 0 or $N/2$ (12 combinations).
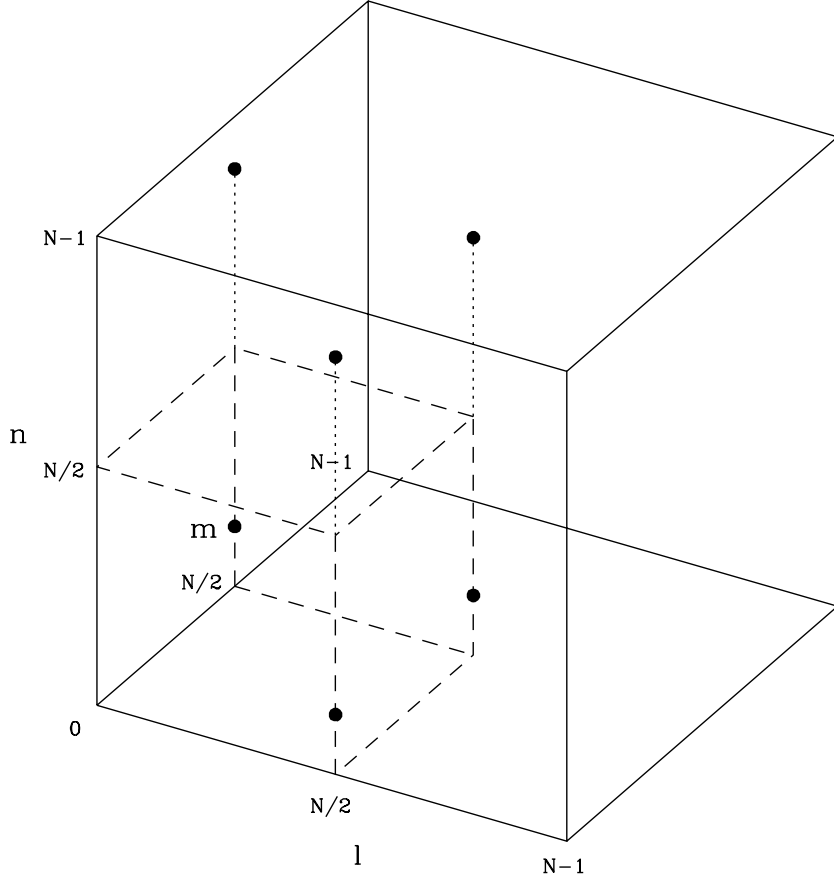
Fig. 5.— Representation of the system in k-space. The dots indicate the particular modes $(l, m, n) = (0, 32, 8)$, $(32, 0, 8)$, and $(32, 32, 8)$, where $32 = N/2$, and their related modes.

3.4. In a Corner

Finally, we consider the cases when all indicies are equal to 0 or $N/2$. These cases corresponds to values of $\mathbf{k}$ located in a corner of the first octant in k-space. With $l = m = n = 0$, equation (36) reduces to

$$\hat{\delta}_{000} = \sum_{\alpha,\beta,\gamma=0}^{N-1} \delta_{\alpha\beta\gamma} \equiv \delta_u \,, \tag{124}$$

where the subscript u stands for "uniform," since the mode 000 corresponds to a null wavenumber, or an infinite wavelength. Notice that since $\delta_{\alpha\beta\gamma}$ is real, δ_u is real as well. Hence, for this mode, there is no imaginary part, and δ_u is determined form equation (60). This mode is shown in Figure 6.

Consider now the case $l = N/2$, $m = 0$, $n = 0$. Again, we can easily show that the solution (124) is still valid, using the same approach as in §§3.2 and 3.3. The only difference will be an extra factor of $(-1)^\alpha$ in the expression for δ_u. Using the cubic symmetry, we can then show that the solution (124) applies to all
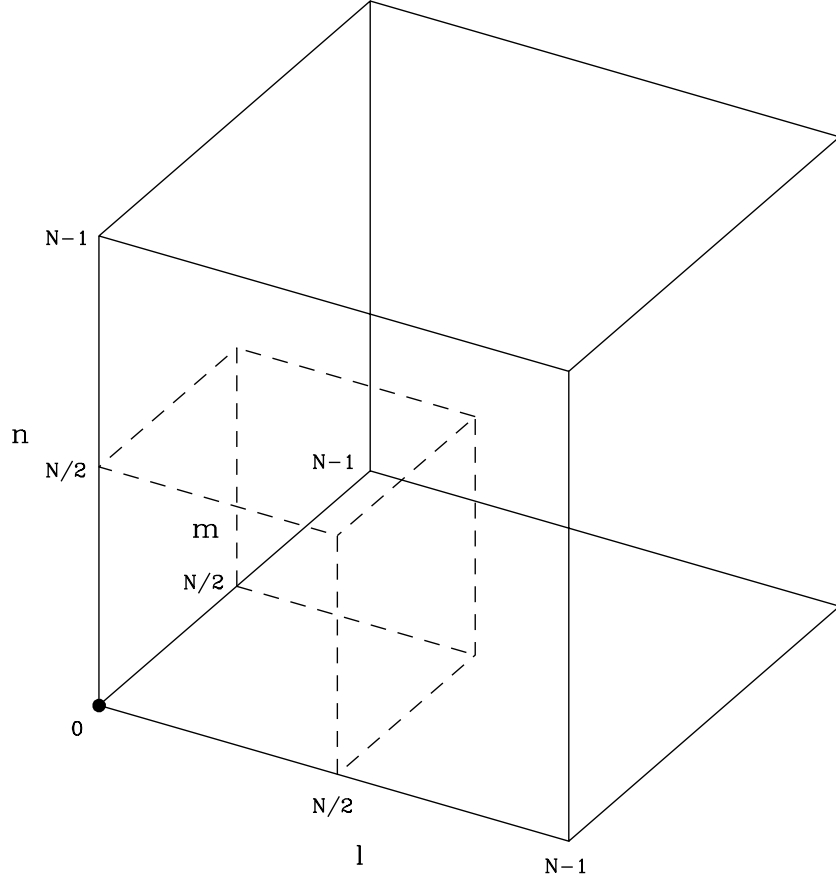
Fig. 6.— Representation of the system in k-space. The dot indicates the particular mode $(l, m, n) = (0, 0, 0)$. For that particular mode, we ignore equation (124) and set $\delta_u = 0$ instead.

cases for which the three indicies l, m, n are equal to 0 or $N/2$ (8 combinations).

Notice that there is a fundamental difference between the mode $\hat{\delta}_{000}$ and the other 7 modes, $\hat{\delta}_{00,N/2}$, $\hat{\delta}_{0,N/2,0}$, ..., $\hat{\delta}_{N/2,N/2,N/2}$, shown in Figures 6 and 7, respectively. The mode $\hat{\delta}_{000}$ represents a perturbation of infinite wavelength, that is, a constant. Clearly that constant must be zero, otherwise the mean value of $\delta(\mathbf{r})$ integrated over the entire volume would be nonzero, and this would violate the assumption that the volume contains a fair sample of the universe. Therefore, for the mode $\hat{\delta}_{000}$, *and that mode only*, we do not compute the amplitude $|\hat{\delta}_{000}|$ from the power spectrum, but instead set that amplitude equal to zero.

3.5. Putting it All Together

We can now count the number of independent quantities necessary to represent all the density harmonics. Consider first the modes $\hat{\delta}_{lmn}$ for which the indicies are neither 0 nor $N/2$. Excluding these values, each index can take $N-2$ different values, which gives us $(N-2)^3$ modes. As we showed in §3.1, these modes come
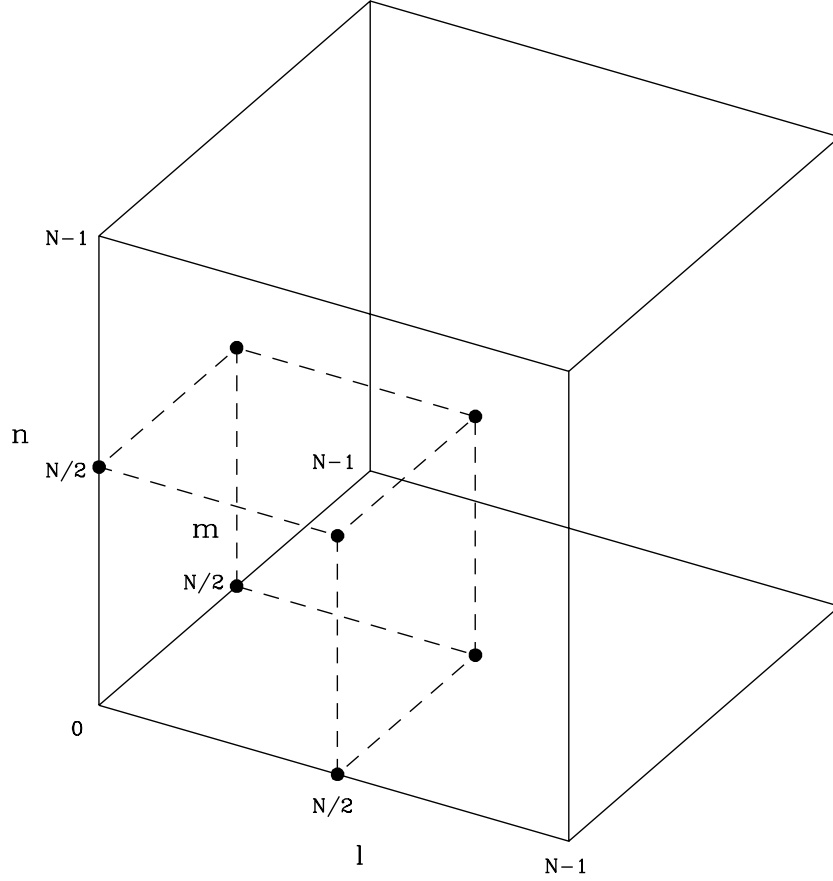
Fig. 7.— Representation of the system in k-space. The dots indicate the particular modes (l, m, n) located at corners of the first octant, excluding the mode $(0, 0, 0)$. For these modes, equation (124) applies.

in groups of 8, and within each group the complex values of the harmonics can be expressed as combinations of 8 real numbers $\hat{\delta}_{eee}$, $\hat{\delta}_{eeo}$, ..., $\hat{\delta}_{ooo}$. Hence, it takes a total of $(N-2)^3$ real numbers to represent these modes.

Consider now the modes for which one of the indicies is equal to 0 or $N/2$. There are 6 possibilities, and for each one, the remaining two indicies can take $N-2$ values each (all values except 0 and $N/2$). This gives us $6(N-2)^2$ modes. As we showed in §3.2, these modes come in groups of four, and within each group the complex values of the harmonics can be expressed as combinations of four real numbers $\hat{\delta}_{ee}$, $\hat{\delta}_{eo}$, $\hat{\delta}_{oe}$, and $\hat{\delta}_{oo}$. Hence, it takes a total of $6(N-2)^2$ real numbers to represent these modes.

Next, consider the modes for which two of the indicies are equal to 0 or $N/2$. There are 12 possibilities, and for each one, the remaining index can take $N-2$ values (all values except 0 and $N/2$). This gives us $12(N-2)$ modes. As we showed in §3.3, the amplitude these modes form complex conjugates pairs, and each pair can be represented by two real numbers $\hat{\delta}_e$, and $\hat{\delta}_o$. Hence, it takes a total of $12(N-2)$ real numbers to represent these modes.

Finally, consider the modes for which all three indicies are equal to 0 or $N/2$. There are 8 such modes. As we showed in §3.4, these modes are real, hence it takes 8 real numbers to represent them. The total number of variables necessary to represent all the density harmonics is therefore

$$(N - 2)^3 + 6(N - 2)^2 + 12(n - 2) + 8 = N^3 \,. \tag{125}$$

It takes N^3 numbers to represent the Fourier transform of a cube $N \times N \times N$ of real numbers, in spite of the fact that the Fourier transform is complex. Indeed, it is common for Fast Fourier Transform (FFT) subroutines to take a tridimensional array of number and to overwrite that array with the Fourier transform. This is the case for the FFT subroutines of *Numerical Recipes* (Press et al 1992). When these subroutines compute the Fourier transform of a cube $N \times N \times N$, the results are written in the same cube, and *the actual numbers stored in the cube are precisely the $\hat{\delta}_{xxx}$'s, $\hat{\delta}_{xx}$'s, $\hat{\delta}_x$'s, and δ_u's derived in this section.* Hence it is possible to generate the density harmonics directly in k-space, using the above formulae, store these numbers at the appropriate locations inside an $N \times N \times N$ cubic array, and then invoke the *Numerical Recipes* inverse FFT subroutines to generate the density field.

The *Numerical Recipes* convention for storing the density harmonics is the following: Consider a 3D array A, with indicies running from 0 to $N-1$. We loop over all modes located in the first octant in k-space: $0 \leq l, m, n \leq N/2$.

1. For modes with $0 < l, m, n < N/2$ (the general case), the numbers δ_{eee}, δ_{eeo}, ..., δ_{ooo} are stored in a $2 \times 2 \times 2$ cube located at `A(2l,2m,2n)`, `A(2l,2m,2n+1)`, ..., `A(2l+1,2m+1,2n+1)`.

2. For modes with $l = 0$, the numbers δ_{ee}, δ_{eo}, δ_{oe}, δ_{oo} are stored at `A(0,2m,2n)`, `A(0,2m,2n+1)`, `A(0,2m+1,2n)`, and `A(0,2m+1,2n+1)`, respectively. For modes with $l = N/2$, they are stored at `A(1,2m,2n)`, `A(1,2m,2n+1)`, `A(1,2m+1,2n)`, and `A(1,2m+1,2n+1)`, respectively. This is easily generalized to the other faces ($m = 0$, $m = N/2$, $n = 0$, $n = N/2$).

3. For modes with $l = m = 0$, the numbers δ_e and δ_o are stored at `A(0,0,2n)` and `A(0,0,2n+1)`, respectively. For modes with $l = 0$, $m = N/2$, they are stored are stored at `A(0,1,2n)` and `A(0,1,2n+1)`, respectively. This is easily generalized to the other edges.

4. The number δ_u is stored in a $2 \times 2 \times 2$ cube located in the corner of the array, at `A(0,0,0)`, `A(0,0,1)`, ..., `A(1,1,1)`. Then, the value of `A(0,0,0)` is set to 0, since this represents the mode $(0, 0, 0)$.

4. CALCULATION OF THE DENSITY FIELD

4.1. Eulerian Representation

With the expressions derived in §2, we have all the ingredients necessary to compute the density field on a grid. The steps are the following:

1. Choose a particular power spectrum $P(k)$, a box size L_{box}, and a grid size N. This determines the fundamental wavenumber $k_0 = 2\pi/L_{\mathrm{box}}$. The allowed modes are given by equation (31).

2. For all modes with $l, m, n \neq 0, N/2$, group these modes in groups of 8, and for each group, calculate the quantities δ_{eee}, δ_{eeo}, ..., δ_{ooo} using equations (70)–(77) and (80). The quantities R_1, I_1, ..., I_4 are determined from equations (60) and (61).

3. For all modes located on a face (one of the indicies l, m, n equal to 0 or $N/2$), group these modes in groups of four, and for each group, calculate the quantities δ_{ee}, δ_{eo}, δ_{oe}, δ_{oo} using equations (98)–(101) and (102)–(105).

4. For all modes located on an edge (two of the indicies l, m, n equal to either 0 or $N/2$), group these modes in groups of two, and for each group, calculate the quantities δ_e and δ_o, using equations (120)–(101).

5. For the modes located in a corner (all indicies l, m, n equal to either 0 or $N/2$), calculate the quantity δ_u using equation (124). For the mode $(l, m, n) = (0, 0, 0)$, replace the value of δ_u by 0.

6. Store the quantities δ_{eee}, ..., δ_{ooo}, δ_{ee}, δ_{eo}, δ_{oe}, δ_{oo}, δ_e, δ_o, δ_u in a 3D, $N \times N \times N$ array, at the proper locations. These depends on the convention used by the FFT subroutines.

7. Compute the inverse FFT of the 3D array. The result will be the density field $\delta(\mathbf{r})$.

4.2. Lagrangian Representation

In the Lagrangian representation, the density field is represented by a distribution of equal-mass particles. We start by laying down $N_p \times N_p \times N_p$ particles on a cubic grid with grid spacing $d = L_{\text{box}}/N_p$ inside the computational volume V_{box}. The mass of the particles are given by $M = \bar{\rho} V_{\text{box}}/N_p^3$, such that the mean density inside the box is equal to the mean background density $\bar{\rho}$. The particles are then displaced in order to represent the initial density field. This approach is valid only in the *linear regime*, defined by $|\delta(\mathbf{r})| \ll 1$. In this regime, the particle displacements $\Delta \mathbf{r}$ are significantly smallar than the initial separation d between the particles, and can be computed using the Zel'dovich approximation (Zel'dovich 1970). The displacements are given by

$$\Delta \mathbf{r}_j = -\frac{i}{N^3} \sum_{\mathbf{k}} \frac{\hat{\delta}_{\mathbf{k}} \mathbf{k}}{k^2} e^{-i\mathbf{k} \cdot \mathbf{r}_j} , \tag{126}$$

where $\mathbf{r}_j$ is the position of particle j before it is displaced, and $\mathbf{r}_j + \Delta \mathbf{r}_j$ is the position after. Notice that the reality condition (5) ensures that $\Delta \mathbf{r}_j$ is real.

This method is straightforward, but can rapidly become unpractical. Equation (126) involves a sum over N^3 modes, and that sum must be performed for each of the N_p^3 particles. Since in typical cosmological simulations N_p is chosen to be $N/2$, the number of operations scales like N^6. If it takes 5 minutes to set up initial conditions with 64^3 particles, it will take 5.3 hours for 128^3 particles, 2 weeks for 256^3 particles, and 2.5 years for 512^3 particles! An alternative method, which scales like N^3, was proposed by Efstathiou et al. (1985). Essentially, this approach uses the fact that the displacement of each particle is proportional to its peculiar acceleration, that can be calculated with a N-body simulation algorithm such as PM (Particle-Mesh) or P^{3}M (Particle-Particle/Particle-Mesh). With this method, the number of operations scales roughly as N^3. I refer the reader to Hockney & Eastwood (1981) and Efstathiou et al. (1985) for details. It is worth noting that, unlike equation (126), the approach of Efstathiou et al. (1985) is approximative, and the high-frequency modes, near the Nyquist frequency $k = (N_p/2)k_0$, are often poorly represented by the particle distribution.

5. FILTERING

Our next task in to filter the density field at some scale s. The choice of scale must obey two conditions: $s \gg \Delta$ and $s \ll L_{\text{box}}$. The first condition is required by the discreteness of the grid and the second by the

assumption of periodic boundary conditions. The filtered density field $\delta_s(\mathbf{r})$ at scale s is given by

$$\delta_s(\mathbf{r}) = \int_{V_{\text{box}}} \delta(\mathbf{r}')K_s(\mathbf{r} - \mathbf{r}')d^3r' \, , \tag{127}$$

where K_s is the filter function. We will use a Gaussian filter given by

$$K_s(\mathbf{x}) = \frac{e^{-x^2/2s^2}}{(2\pi)^{3/2}s^3} \, . \tag{128}$$

This filter function satisfied the normalization condition,

$$\int_{V_{\text{box}}} K_s(\mathbf{r})d^3r = 1 \, , \tag{129}$$

as long as $s \ll L_{\text{box}}$.

It is well known that filtering in real space is equivalent to a multiplication in k-space. However, it is useful to redo the derivation, to ensure that we have all the correct factors of 2π, N^3, and so on. First, we express the filter as an inverse Fourier transform,

$$K_s(\mathbf{r} - \mathbf{r}') = \frac{1}{N^3}\sum_{\mathbf{k}'}\hat{K}_s(\mathbf{k}')e^{-i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')} \, . \tag{130}$$

We substitute equations (33) and (130) in equation (127), and get

$$\begin{aligned}
\delta_s(\mathbf{r}) &= \frac{1}{N^6}\int_{V_{\text{box}}}\sum_{\mathbf{k}}\hat{\delta}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{r}}\sum_{\mathbf{k}'}\hat{K}_s(\mathbf{k}')e^{-i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')}d^3r' \\
&= \frac{1}{N^6}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\hat{\delta}(\mathbf{k})\hat{K}_s(\mathbf{k}')e^{-i\mathbf{k}\cdot\mathbf{r}}\int_{V_{\text{box}}}e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}'}d^3r' \, .
\end{aligned} \tag{131}$$

$$\tag{132}$$

The integral is equal to $V_{\text{box}}\delta_{\mathbf{k},\mathbf{k}'}$ (see eq. [12]), and we use the Kronecker δ to eliminate the sum over $\mathbf{k}'$. We get

$$\delta_s(\mathbf{r}) = \frac{V_{\text{box}}}{N^6}\sum_{\mathbf{k}}\hat{\delta}(\mathbf{k})\hat{K}_s(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{r}} \, . \tag{133}$$

We now need an expression for $\hat{K}_s(\mathbf{k})$. This function is the Fourier transform of the filter,

$$\hat{K}_s(\mathbf{k}) = \sum_{\mathbf{x}}K_s(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}} = \frac{1}{(2\pi)^{3/2}s^3}\sum_{\mathbf{x}}e^{-x^2/2s^2}e^{i\mathbf{k}\cdot\mathbf{x}} \, . \tag{134}$$

We rewrite this expression as

$$\hat{K}_s(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}s^3}\left(\frac{N^3}{V_{\text{box}}}\right)\sum_{\mathbf{x}}e^{-x^2/2s^2}e^{i\mathbf{k}\cdot\mathbf{x}}\left(\frac{V_{\text{box}}}{N^3}\right) \, . \tag{135}$$

The factor $V_{\text{box}}/N^3 = \Delta^3$ represents the volume element around each point $\mathbf{x}$ in the $N \times N \times N$ grid. Since we assume $s \gg \Delta$, we can approximate the sum as an integral over the volume of the box (or, equivalently, regard the sum as a numerical approximation for the integral). Hence,

$$\hat{K}_s(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}s^3} \left(\frac{N^3}{V_{\text{box}}} \right) \int_{V_{\text{box}}} e^{-x^2/2s^2} e^{i\mathbf{k}\cdot\mathbf{x}} d^3x \,. \tag{136}$$

Since we assume periodic boundary conditions, we are free to locate the origin anywhere inside the box. For instance, we can locate it in the center of the box. Since $s \ll L_{\text{box}}$, the integrant becomes negligible at the edge of the box. We can then extend the integration domain to all space,

$$\hat{K}_s(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}s^3} \left(\frac{N^3}{V_{\text{box}}} \right) \int_{\text{all space}} e^{-x^2/2s^2} e^{i\mathbf{k}\cdot\mathbf{x}} d^3x \,, \tag{137}$$

where this expression *no longer assumes boundary conditions*. The integral in equation (137) can be found in any textbook of Fourier transforms,

$$\int_{\text{all space}} e^{-x^2/2s^2} e^{i\mathbf{k}\cdot\mathbf{x}} d^3x = (2\pi)^{3/2} s^3 e^{-(ks)^2/2} \,. \tag{138}$$

Hence,

$$\hat{K}_s(\mathbf{k}) = \frac{N^3}{V_{\text{box}}} e^{-(ks)^2/2} \,. \tag{139}$$

We substitute this expression in equation (133), and get

$$\delta_s(\mathbf{r}) = \frac{1}{N^3} \sum_{\mathbf{k}} \hat{\delta}(\mathbf{k}) e^{-(ks)^2/2} e^{-i\mathbf{k}\cdot\mathbf{r}} \,. \tag{140}$$

Hence, to obtain a filtered density field, we generate the density harmonics using the method described in §3, and then multiply them by the factor $e^{-k^2 s^2/2}$ *before* taking the inverse Fourier transform.

6. SUMMARY

This paper presents in great detail the techniques used for generating Gaussian density fields. These techniques are well-known among experts in cosmological numerical simulations, but the specific details of the implementation are often difficult to find in the literature. Also, the notation tends to vary significantly from one author to another. The consequences is that any new researcher moving into this field has to either spend a great deal of effort rederiving all the technical details, or else rely on existing codes and use them as black boxes. The goal of this document is to improve the situation by presenting in a comprehensive form the basic theory behind the generation of Gaussian random fields.

A.   FOURIER TRANSFORM OF THE TOP HAT

Consider the following integral,

$$I = \int_{\text{sph}(0)} d^3 y \, e^{-i\mathbf{k} \cdot \mathbf{y}} \,, \tag{A1}$$

where the domain of integration is a sphere of radius R centered at the origin. We consider a spherical coordinate system centered at the origin, with the z-axis pointing in the direction of $\mathbf{k}$. Equation (A1) becomes

$$I = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \int_0^R dy \, (y^2 \sin \theta) e^{-iky \cos \theta} \,, \tag{A2}$$

where $k \equiv |\mathbf{k}|$, $y \equiv |\mathbf{y}|$, and θ is the angle between $\mathbf{k}$ and $\mathbf{y}$. The integrations over ϕ and θ are trivial. We get

$$I = 2\pi \int_0^R dy \, y^2 \left[\frac{e^{-iky \cos \theta}}{iky} \right]_0^{\pi} = 2\pi \int_0^R dy \, y^2 \left[\frac{e^{iky} - e^{-iky}}{iky} \right] = 4\pi \int_0^R dy \, \frac{y \sin ky}{k} \,. \tag{A3}$$

The integral over y is now trivial. We get

$$I = \frac{4\pi}{k^3} (\sin kR - kR \cos kR) = \frac{4\pi R^3}{u^3} (\sin u - u \cos u) \,, \tag{A4}$$

where $u = kR$.

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