Best unbiased estimates for the microwave background anisotropies

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It is likely that the observed distribution of the microwave background temperature over the sky is only one realization of the underlying random process associated with cosmological perturbations of quantum-mechanical origin. If so, one needs to derive the parameters of the random process, as accurately as possible, from the data of a single map. These parameters are of the utmost importance, since our knowledge of them would help us to reconstruct the dynamical evolution of the very early Universe. It appears that the lack of ergodicity of a random process on a two-sphere does not allow us to do this with arbitrarily high accuracy. We are left with the problem of finding the best unbiased estimators of the participating parameters. A detailed solution to this problem is presented in this article. The theoretical error bars for the best unbiased estimates are derived and discussed. [S0556-2821(97)04616-X]

I. INTRODUCTION

The existing and planned measurements of the cosmic microwave background (CMB) anisotropies belong to the category of astronomical observations which promise a direct link to fundamental physics and, therefore, they attract additional attention.

The mere detection of the quadrupole anisotropy at the level $\delta T/T = 5 \times 10^{-6}$ [1] allows us to conclude that the Universe remains to be homogeneous and isotropic (all dimensionless deviations are smaller than 1) at scales much larger than the present-day Hubble radius l_H and up to distances about 500 times longer than l_H [2]. The significance of this result lies in the fact that such large scales are not directly observable now and will be accessible only to astronomers of a very remote future. At still longer scales, the homogeneity and isotropy of the Universe cannot be guaranteed, in the sense that some deviations can be larger than 1 without conflicting the CMB observations [2]. The transition from spatially flat cosmological models to open models does not affect these conclusions considerably [3].

The mere existence of the long-wavelength cosmological perturbations, responsible for the observed large-angular-scale anisotropy, requires them to have special phases and to exist at the previous radiation-dominated stage in the form of standing, rather than traveling, waves [4]. This conclusion follows from the Einstein equations, if we trust them to propagate the observed perturbations back in time up to, at least, the era of primordial nucleosynthesis without destroying the homogeneity and isotropy of that era. The distribution of phases can be only very narrow (highly squeezed) with two peaks separated by π (see [4] and references

therein), a sort of the ''phase bifurcation'' [5].

The already identified properties of the presently existing long-wavelength cosmological perturbations raise sharply the issue of their origin. Although several schemes are logically possible, it was argued [4] that the quantum-mechanical generation of cosmological perturbations was likely to be the one to do the job. If so, not only the existing requirements are satisfied but also some new specific consequences follow.

In a broad sense, the quantum-mechanical generation of cosmological perturbations means the Schrödinger evolution of the initial vacuum state (no ''particles'' perturbations) into the present-day multi-particle state (many ''particles'' perturbations). Even the simplest, linear and quadratic, interaction Hamiltonians are capable of producing a variety of multi-particle states: coherent states (result of the action of a force, linear Hamiltonians), squeezed vacuum states (result of the parametric influence, quadratic Hamiltonians), squeezed coherent states (combination of the two above). All these states have Gaussian wave functions and are in this sense Gaussian. A single word ''Gaussian'' is too general to distinguish between these states. The difference between them lies in the statements regarding the mean values (zero for squeezed vacuum states, nonzero for the rest of the states) and the variances (equal for coherent states, nonequal for other states) of the conjugate variables characterizing the state, such as generalized coordinates and momenta, or quadrature components of the field, or, loosely, amplitude and phase, etc. In case of cosmological perturbations, there is no natural and unavoidable mechanism for generation of coherent states, but there is one such for generation of squeezed vacuum states: parametric (superadiabatic) interaction of the quantized perturbations with strong variable gravitational field of the very early Universe (see [4] and references therein). The fact that the cosmological perturbations are being generated specifically in the squeezed vacuum quantum states (and not, say, in the ''most classical'' coherent states)

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dictates a number of properties of the perturbations themselves and the CMB anisotropies caused by them [6]. Squeezing is a physical phenomenon, not a formalism or a language.

Let us imagine that the accurately measured distribution of the CMB temperature over the sky is decomposed over spherical harmonics (for precise definitions see Sec. II):

$$\frac{\delta T}{T}(\theta,\varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_{lm} Y_{lm}(\theta,\varphi).$$

A priori, there may be nothing inherently random or quantum mechanical behind this observed distribution of the cosmic temperature, in the same sense in which there is nothing inherently random or quantum mechanical behind, say, the observed distribution of the stars of our galaxy over the sky. If the measured CMB temperature map is a reflection of a given classical distribution of matter and gravitational fields, the derived fixed numbers c_{lm} is about all what we can extract from the map. The notion of the random temperature arises if the cosmological perturbations responsible for the anisotropies were randomly generated. We should then interpret a particular perturbation field and the observed numbers c_{lm} caused by this field as one specific realization of the random process. The objective then is to find out and characterize the underlying random process, as accurately as possible, using the data of a single observed map.

We maintain the view that the cosmological perturbations responsible for the observed anisotropies were generated quantum mechanically. If they could be generated in coherent states, the mean quantum-mechanical values of the perturbation field would be nonzero, and they would be surrounded by small (at the level of the zero-point quantum oscillations) Gaussian fluctuations. Correspondingly, the theoretical distributions for the c_{lm} coefficients would have had nonzero means with small Gaussian fluctuations around them. Roughly speaking, in this case, the mean numerical values of $\delta T/T$ would be determined by the mean values of the perturbation field. In contrast, in case of the squeezed vacuum states, the mean values of the perturbation field and the mean values of the c_{lm} coefficients are zero, but the Gaussian fluctuations around them are large. Roughly speaking, in this case, the numerical values of $\delta T/T$ are determined by the dispersion (square root of variance) of the perturbation field. In both cases, the words about Gaussian distributions should be taken with a great care. Whatever we are able to calculate presently, relies on the assumption that cosmological perturbations are weak and that the absolute value of $\delta T/T$ is a small, less than 1, number. On the other hand, if the variable $\delta T/T$ obeys a Gaussian (normal) distribution law, this quantity may take, even though with a small probability density, arbitrarily large values, which is in conflict with our initial assumption. In addition, the short-wavelength perturbations became nonlinear in the course of evolution, and many extra physical processes were involved in the producing of the small-angular-scale anisotropies. However, in this paper, we will ignore these difficulties and will work with exact normal zero-mean distributions (Secs. II and III).

In case of squeezed vacuum quantum states, and the corresponding normal zero-mean distributions for the c_{lm} coefficients, the underlying random process is completely characterized by the set of variances σ_l^2 ($l = 0, 1, 2, 3, \dots$) of the c_{lm} distributions. These quantities are calculable if the cosmological model is postulated and, vice versa, the cosmological model can be determined if these quantities are known from observations. Specifically, the quantities σ_l^2 are calculable if the time dependence of the cosmological scale factor describing the very early Universe is chosen, and assuming that the rest of the evolution is known. Moreover, for simple cosmological models, the quantities σ_l^2 are related to each other and are all expressible through a small number of parameters. This happens, for example, if one assumes that the scale factor of the very early Universe had obeyed one of the power-law time dependences. In these cases, the problem of extracting cosmological information from a given map simplifies and reduces to the problem of determining those few parameters and testing those models. However, the real situation with the data can be more complicated [7]. The observer may not be willing to believe any of theoretical cosmological models, even if he/she accepts the view that the underlying distributions should be normal zero-mean distributions. A more ambitious task than testing each of many possible models is the derivation of the true behavior of the very early Universe from the observations, that is, from the observed set of numbers σ_l^2. This is the position that we adopt in this paper. We begin from observations rather than from theory. Concretely, we want to answer the following question: What can be stated about the set of independent σ_l^2 on the grounds of a single observed map?

We assume that the sky coverage is complete, the foreground sources and contaminating signals are under full control, the instrumental errors are negligibly small, the angular resolution is arbitrarily high, and the map is constructed from the raw data in the most intelligent and effective way [8,9]. At the first sight, under these conditions, an arbitrarily accurate determination of all the σ_l^2 should not present a big problem. Indeed, the angular correlation function $K(\delta)$, constructed as a result of averaging over many maps (''many universes''), has the form

$$\left\langle \frac{\delta T}{T}(\vec{e}_1) \frac{\delta T}{T}(\vec{e}_2) \right\rangle = K(\delta)$$

$$= \frac{1}{4\pi} \sum_{l=0}^{\infty} \sigma_l^2 (2l+1) P_l(\cos\delta).$$

If the function $K(\delta)$ is known, each of the σ_l^2 can be easily obtained from it. One simply needs to integrate over δ the product of $K(\delta)$ with the respective Legendre polynomial $P_l(\cos\delta)$. It is true that we have access to only one realization of the random process, not to infinitely many implied in the construction of the $K(\delta)$, but this is not an obstacle by itself. If the process is ergodic [10,11] (see Sec. IV), the correlation functions can be built from a single realization, and the parameters of the random process, such as σ_l^2, can be determined with arbitrarily high accuracy. What is required for the ergodicity of a random process in time or in three-space is the decay of correlations in the limit of very large temporal or spatial separations. Then, the ensemble averages can be replaced by integrals over time or three-space,

and the parameters derived from one realization are true parameters with probability 1. In theoretical cosmology, the long-distance behavior of the perturbation field is partially in our hands. It can be assumed to be appropriate, so that the field in three-space can be made ergodic: the access to one realization would be sufficient for the determination of all parameters of the perturbation field. The difficulty apparently comes about when the three-dimensional ergodic process is being reduced to a two-dimensional random process on a sphere, what effectively takes place when cosmological perturbations produce anisotropies in the temperature distribution over the sky. It appears that a random process on a two-sphere can never be ergodic (in the sense of replacement of the ensemble averages by the integrations over the sphere) and the σ_l^2 can never be determined with arbitrarily high accuracy from a single map (Sec. IV). Possibly, this is a statement well known to mathematicians but we could not find an adequate reference.

Without being able to find the true values of σ_l^2 we are left with the problem of estimating these parameters as accurately as possible. One can imagine that one is given a very precise map of the CMB sky, but the question is what to do with this map. This is a problem from the quite well-developed theory of estimation and statistical inference (see, for example [12,13]). To evaluate a parameter we need to build an estimator, a random variable constructed from the original random process. The estimator is ''unbiased'' if its expectation value is equal to the true value of the parameter. And the estimator is the ''best'' if its variance is minimal among all possible estimators. In Sec. V, we find the best unbiased estimator for σ_l^2, and in Sec. VI we find the best unbiased estimator for $K(\delta)$.

A concrete numerical value of the best unbiased estimator acquired at the observed map is the best unbiased estimate of the corresponding parameter. Usually, one is not satisfied with the best estimate alone, but wants to surround the estimate by appropriate error bars. This requires new definitions and criteria (see Sec. VII). Approximately, but not exactly, the size of the error box is characterized by the variance of the best unbiased estimator. Not surprisingly, since we have limited our discussion to normal zero-mean distributions, the most ''natural'' estimators turn out to be also the best unbiased estimators, and the maximum likelihood estimators, etc. In this way, this paper makes contact with previous work on the subject [14].

Before concluding the Introduction we need to make two comments.

First, our analysis is built on the assumptions that the observed map is only one realization of a random process, and that the underlying distributions are normal zero-mean distributions. These assumptions are in fact consequences of the parametric quantum-mechanical generating mechanism of the perturbations, but they are also testable hypotheses on their own. Logically, one needs first to show that one is dealing with a random process before trying to find out its characteristics. If we were experimenting with a noisy voltage generator, we could compare several sufficiently long records in order to argue that we were dealing with the different realizations of one and the same random process. In

cosmology, we have control over only one record, only one CMB map. The assumptions made above can hardly be proven rigorously, but one can possibly find evidence in their support. Alternatively, they can be disproved at some level of confidence. One possibility to test these assumptions was indicated in Ref. [6]. The product of two random variables $\delta T/T(\vec{e}_1)$ and $\delta T/T(\vec{e}_2)$ is a new random variable v. The probability density function (PDF) for v was derived, and its functional form was shown to be quite special [6]. The mean value of v is $K(\delta)$ but the variable v is not supposed to be a good estimator of $K(\delta)$ since the variance of v is very big. However, this big variance should be present in the original observational data (before any angular integrations over the map are performed) if our statistical assumptions are correct. It looks unlikely that the quite special functional form of the PDF for v can be mimicked by the anisotropies caused by perturbations of any other origin. In view of the forthcoming massive ''pixelization'' of the CMB sky, it will probably be possible to test directly whether the map values of the v satisfy, at least approximately, the theoretically derived PDF for v. In this paper, we effectively assume that this is the case.

Second, in our analysis we do not need to specify the nature of the cosmological perturbations responsible for the observed large-angular-scale anisotropy. They can be density perturbations, or rotational perturbations, or gravitational waves. However, in order to build a correct general picture, it is very important to know what kind of perturbations we are actually dealing with. Hopefully, this question can be answered in future observations, with the help, for example, of polarization measurements (for a recent paper on the subject, see [15]). So far, one can only rely on the theory. The quantum-mechanical generating mechanism, originally developed for gravitational waves, can also be applied, under certain conditions, to density perturbations and rotational perturbations. The contribution of each type of perturbations to the $\delta T/T$ can be calculated. According to the calculations of Ref. [16], if the observed large-angular-scale anisotropies are indeed caused by cosmological perturbations of quantum-mechanical origin, gravitational waves are at least as important as density perturbations and provide a somewhat larger contribution than that of density perturbations.

II. VARIOUS REPRESENTATIONS FOR $\delta T/T$

The quantity which appears naturally in the theory of the CMB anisotropies is a relative variation of the temperature seen in a given direction $\vec{e}$ on the sky: $\delta T/T(\vec{e})$. This quantity is a function of the angular coordinates on the celestial sphere:

$$\frac{\delta T}{T}(\vec{e}) \equiv \frac{\delta T}{T}(\theta, \varphi). \qquad (2.1)$$

It is convenient to define three different representations for this function:

$$\frac{\delta T}{T}(\theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} [a_{lm} Y_{lm}(\theta, \varphi) + a_{lm}^* Y_{lm}^*(\theta, \varphi)],$$

$$(2.2)$$

$$= \sum_{l=0}^{\infty} \left(b_{l0}^c \frac{Y_{l0}^c(\theta,\varphi)}{\sqrt{2}} + \sum_{m=1}^{l} [b_{lm}^c Y_{lm}^c(\theta,\varphi) \right.$$

$$\left. + b_{lm}^s Y_{lm}^s(\theta,\varphi)] \right), \tag{2.3}$$

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_{lm} Y_{lm}(\theta,\varphi), \tag{2.4}$$

where the orthonormal spherical harmonics, either complex Y_{lm}^c, or real $Y_{l0}^c/\sqrt{2}$, Y_{lm}^c, and Y_{lm}^s, are described in the Appendix. In what follows, the index l runs from 0 to ∞, and the index m runs either between $-l$ and $+l$ or between 1 and l, as will be explicitly specified.

Although the transitions between Eqs. (2.2), (2.3), and (2.4) are quite straightforward, each of the representations has its own advantages and we will use them below. Since every factor $\sqrt{2}$ can eventually prove to be very important, we need a rigorous, even if somewhat pedantic, description of these representations. The coefficients a_{lm} are complex and can be expressed in terms of their real and imaginary parts, $a_{lm} = a_{lm}^r + i a_{lm}^i$. In this a representation, the function $\delta T/T(\vec{e})$ is manifestly real, but the number of the a coefficients is larger than necessary. The b representation is a little cumbersome, but it has to be regarded as canonical in the sense that it contains only real and independent coefficients b_{lm}^A ($A = c,s$) and does not require any extra constraints. The properties of other representations will be derived from the properties of this one. Finally, the coefficients c_{lm} of the c representation are complex, and in order to have real $\delta T/T(\vec{e})$, they must satisfy the relationship $c_{lm}^* = c_{l,-m}$. They can be also written as $c_{lm} = c_{lm}^r + i c_{lm}^i$. Then, the last relationship implies $c_{lm}^r = c_{l,-m}^r$ and $c_{lm}^i = -c_{l,-m}^i$.

Let us now describe how these representations are related to one another.

The relationship between the b representation and the a representation is expressed through the equations

$$b_{l0}^c = 2a_{l0}^r, \tag{2.5}$$

$$b_{lm}^c = \sqrt{2}(a_{lm}^r + a_{l,-m}^r), \quad m \geq 1, \tag{2.6}$$

$$b_{lm}^s = -\sqrt{2}(a_{lm}^i - a_{l,-m}^i), \quad m \geq 1. \tag{2.7}$$

The link between the c representation and the a representation is given by

$$c_{lm} = a_{lm} + a_{l,-m}^*.$$

The link between the c representation and the b representation can be written as

$$c_{l0} = b_{l0}^c, \tag{2.8}$$

$$c_{lm} = \frac{1}{\sqrt{2}} (b_{lm}^c - i b_{lm}^s) \quad m \geq 1, \tag{2.9}$$

$$c_{lm} = \frac{1}{\sqrt{2}} (b_{l,-m}^c + i b_{l,-m}^s) \quad m \leq -1. \tag{2.10}$$

Using the previous equations it is easy to check that $c_{l,-m} = 1/\sqrt{2}(b_{lm}^c + i b_{lm}^s) = c_{lm}^*$. We can also express the real and imaginary parts of the coefficients c_{lm} in terms of the coefficients b_{lm}^A. Explicitly we have

$$c_{l0}^r = b_{l0}^c, \quad c_{l0}^i = 0,$$

$$c_{lm}^r = \frac{b_{lm}^c}{\sqrt{2}}, \quad m \geq 1,$$

$$c_{lm}^i = -\frac{b_{lm}^s}{\sqrt{2}}, \quad m \geq 1.$$

If $m \leq -1$, then b_{lm}^c and b_{lm}^s have to be replaced by $b_{l,-m}^c$ and $b_{l,-m}^s$, respectively. Finally, Eqs. (2.8)–(2.10) can be inverted, and one can express the coefficients b_{lm}^A in terms of the coefficients c_{lm}. One obtains

$$b_{l0}^c = c_{l0}, \tag{2.11}$$

$$b_{lm}^c = \frac{1}{\sqrt{2}} (c_{lm} + c_{lm}^*), \quad m \geq 1, \tag{2.12}$$

$$b_{lm}^s = \frac{i}{\sqrt{2}} (c_{lm} - c_{lm}^*), \quad m \geq 1. \tag{2.13}$$

III. THE PROBABILITY DENSITY FUNCTIONS, MEAN VALUES, AND VARIANCES

We need to formulate our statistical assumptions about the CMB temperature. We will start from the b representation. Our assumptions are as follows: (1) all the coefficients b_{l0}^c, b_{lm}^c, and b_{lm}^s are statistically independent random variables, (2) each individual variable is normally distributed with a zero mean, (3) all variables with the same index l have the same standard deviation σ_l. In other words, the probability density functions for the b coefficients are given by the expressions

$$f(b_{l0}^c) = \frac{1}{\sqrt{2\pi}\sigma_l} e^{-(b_{l0}^c)^2/2\sigma_l^2}, \tag{3.1}$$

$$f(b_{lm}^c) = \frac{1}{\sqrt{2\pi}\sigma_l} e^{-(b_{lm}^c)^2/2\sigma_l^2}, \quad m \geq 1, \tag{3.2}$$

$$f(b_{lm}^s) = \frac{1}{\sqrt{2\pi}\sigma_l} e^{-(b_{lm}^s)^2/2\sigma_l^2}, \quad m \geq 1. \tag{3.3}$$

The $\delta T/T$ taken in a given direction is a random variable, while the $\delta T/T$ treated as a function of θ,φ is a random (stochastic) process.

Having the PDF's one can calculate various useful expectation values. For the mean values of the b coefficients, one obtains

$$\langle b_{l0}^c \rangle = \langle b_{lm}^c \rangle = \langle b_{lm}^s \rangle = 0, \quad m \geq 1.$$

For the quadratic combinations, the result is

$$\langle b^c_{l_10}b^c_{l_20}\rangle = \sigma^2_{l_1}\delta_{l_1l_2},$$

$$\langle b^c_{l_1m_1}b^c_{l_2m_2}\rangle = \langle b^s_{l_1m_1}b^s_{l_2m_2}\rangle = \sigma^2_{l_1}\delta_{l_1l_2}\delta_{m_1m_2}, \quad m_1,m_2\geqslant 1,$$

$$\langle b^c_{l_1m_1}b^s_{l_2m_2}\rangle = \langle b^s_{l_1m_1}b^c_{l_2m_2}\rangle = 0, \quad m_1,m_2\geqslant 1. \quad (3.4)$$

In a similar manner, one can also determine the quartic combinations.

We can now deduce the statistical properties of the two other representations. For the a representation, all the coefficients a^r_{lm} and a^i_{lm} can be taken as statistically independent, and their PDF's can be written as

$$f(a^r_{lm}) = \frac{2}{\sqrt{2\pi}\sigma_l} e^{-2(a^r_{lm})^2/\sigma^2_l},$$

$$f(a^i_{lm}) = \frac{2}{\sqrt{2\pi}\sigma_l} e^{-2(a^i_{lm})^2/\sigma^2_l}.$$

To find the expectation values one can use these PDF's, and can also make a consistency check with the help of Eqs. (2.5)–(2.7) and (3.1)–(3.3). The mean values of a^r_{lm} and a^i_{lm} are obviously zero (and, therefore, this is also the case for a_{lm} and a^*_{lm}):

$$\langle a^r_{lm}\rangle = \langle a^i_{lm}\rangle = 0.$$

The quadratic combinations of a^r_{lm} and a^i_{lm} have the values

$$\langle a^r_{l_1m_1}a^r_{l_2m_2}\rangle = \langle a^i_{l_1m_1}a^i_{l_2m_2}\rangle = \frac{\sigma^2_{l_1}}{4}\delta_{l_1l_2}\delta_{m_1m_2},$$

$$\langle a^r_{l_1m_1}a^i_{l_2m_2}\rangle = \langle a^i_{l_1m_1}a^r_{l_2m_2}\rangle = 0,$$

from which one derives

$$\langle a_{l_1m_1}a_{l_2m_2}\rangle = 0, \quad \langle a_{l_1m_1}a^*_{l_2m_2}\rangle = \frac{\sigma^2_{l_1}}{2}\delta_{l_1l_2}\delta_{m_1m_2}.$$

Some of nonvanishing quartic combinations are given by the expressions

$$\langle a^r_{l_1m_1}a^r_{l_2m_2}a^r_{l_3m_3}a^r_{l_4m_4}\rangle = \frac{\sigma^2_{l_1}\sigma^2_{l_3}}{16}\delta_{l_1l_2}\delta_{m_1m_2}\delta_{l_3l_4}\delta_{m_3m_4}$$
$$+ \frac{\sigma^2_{l_1}\sigma^2_{l_2}}{16}\delta_{l_1l_3}\delta_{m_1m_3}\delta_{l_2l_4}\delta_{m_2m_4}$$
$$+ \frac{\sigma^2_{l_1}\sigma^2_{l_2}}{16}\delta_{l_1l_4}\delta_{m_1m_4}\delta_{l_2l_3}\delta_{m_2m_3},$$

$$\langle a^r_{l_1m_1}a^r_{l_2m_2}a^i_{l_3m_3}a^i_{l_4m_4}\rangle = \frac{\sigma^2_{l_1}\sigma^2_{l_3}}{16}\delta_{l_1l_2}\delta_{m_1m_2}\delta_{l_3l_4}\delta_{m_3m_4},$$

$$\langle a_{l_1m_1}a_{l_2m_2}a^*_{l_3m_3}a^*_{l_4m_4}\rangle = \frac{\sigma^2_{l_1}\sigma^2_{l_2}}{4}(\delta_{l_1l_3}\delta_{m_1m_3}\delta_{l_2l_4}\delta_{m_2m_4}$$
$$+ \delta_{l_1l_4}\delta_{m_1m_4}\delta_{l_2l_3}\delta_{m_2m_3}),$$

and other nonvanishing combinations can be obtained by permutting the indices r,i.

Finally, starting from the postulated distributions in the b representation, one can also establish the corresponding equations for the c representation. All the coefficients c^r_{l0}, c^r_{lm}, and c^i_{lm} ($m>0$) should be statistically independent, and their PDF's should be written as

$$f(c^r_{l0}) = \frac{1}{\sqrt{2\pi}\sigma_l} e^{-(c^r_{l0})^2/2\sigma^2_l}$$

and

$$f(c^r_{lm}) = \frac{1}{\sqrt{\pi}\sigma_l} e^{-(c^r_{lm})^2/\sigma^2_l},$$

$$f(c^i_{lm}) = \frac{1}{\sqrt{\pi}\sigma_l} e^{-(c^i_{lm})^2/\sigma^2_l}, \quad m\geqslant 1.$$

Note that the standard deviation for c^r_{l0} is different from those for c^r_{lm} and c^i_{lm}. Obviously, the mean values of the coefficients c^r_{l0}, c^r_{lm}, and c^i_{lm} vanish

$$\langle c^r_{l0}\rangle = \langle c^r_{lm}\rangle = \langle c^i_{lm}\rangle = 0.$$

The mean value of the quadratic combination of c^r_{l0} is given by

$$\langle c^r_{l_10}c^r_{l_20}\rangle = \sigma^2_{l_1}\delta_{l_1l_2}.$$

For other coefficients (where m_1 and m_2 are not both equal to zero), one obtains

$$\langle c^r_{l_1m_1}c^r_{l_2m_2}\rangle = \frac{\sigma^2_{l_1}}{2}\delta_{l_1l_2}\delta_{m_1m_2} + \frac{\sigma^2_{l_1}}{2}\delta_{l_1l_2}\delta_{m_1,-m_2},$$

$$\langle c^i_{l_1m_1}c^i_{l_2m_2}\rangle = \frac{\sigma^2_{l_1}}{2}\delta_{l_1l_2}\delta_{m_1m_2} - \frac{\sigma^2_{l_1}}{2}\delta_{l_1l_2}\delta_{m_1,-m_2},$$

$$\langle c^r_{l_1m_1}c^i_{l_2m_2}\rangle = \langle c^i_{l_1m_1}c^r_{l_2m_2}\rangle = 0.$$

This leads to

$$\langle c_{l_1m_1}c_{l_2m_2}\rangle = \sigma^2_{l_1}\delta_{l_1l_2}\delta_{m_1,-m_2},$$

$$\langle c_{l_1m_1}c^*_{l_2m_2}\rangle = \sigma^2_{l_1}\delta_{l_1l_2}\delta_{m_1m_2}. \quad (3.5)$$

The last equations are also valid for $m_1=m_2=0$.

One nonvanishing quartic combination is given by the expression (others can be obtained by the complex conjugation)

$$\langle c_{l_1 m_1} c_{l_2 m_2} c_{l_3 m_3} c_{l_4 m_4}\rangle = \sigma_{l_1}^2 \sigma_{l_2}^2 \delta_{l_1 l_3} \delta_{m_1, -m_3} \delta_{l_2 l_4} \delta_{m_2, -m_4}$$
$$+ \sigma_{l_1}^2 \sigma_{l_2}^2 \delta_{l_1 l_4} \delta_{m_1, -m_4} \delta_{l_2 l_3} \delta_{m_2, -m_3}$$
$$+ \sigma_{l_1}^2 \sigma_{l_3}^2 \delta_{l_1 l_2} \delta_{m_1, -m_2} \delta_{l_3 l_4} \delta_{m_3, -m_4}.$$
(3.6)

Let us now introduce new random variables which will play an important role in what follows. Let us define random variables a_l^2, b_l^2, and c_l^2 by the equations

$$a_l^2 \equiv \sum_{m=-l}^{l} a_{lm} a_{lm}^*,$$

$$b_l^2 \equiv (b_{l0}^c)^2 + \sum_{m=1}^{l} [(b_{lm}^c)^2 + (b_{lm}^s)^2],$$

$$c_l^2 \equiv \sum_{m=-l}^{l} c_{lm} c_{lm}^*.$$

Using Eqs. (2.11)–(2.13) it is easy to show that $b_l^2 = c_l^2$.

One can compute the mean values of these new random variables

$$2\langle a_l^2\rangle = \langle b_l^2\rangle = \langle c_l^2\rangle = (2l+1)\sigma_l^2$$

and their variances

$$\langle a_l^4\rangle - \langle a_l^2\rangle^2 = \frac{1}{2l+1} \langle a_l^2\rangle^2,$$
(3.7)

$$\langle b_l^4\rangle - \langle b_l^2\rangle^2 = \langle c_l^4\rangle - \langle c_l^2\rangle^2 = \frac{2}{2l+1} \langle c_l^2\rangle^2.$$
(3.8)

It is important to note that the above relationships are trivial consequences of the postulated distributions (3.1)–(3.3). These relationships are always true, regardless of what and how measured, and regardless of whether we have access to only one realization of the random process (only one sky or portion of sky) or to infinitely many. [But if one wants to use a ''cosmic'' word, one is free to call the relationships (3.7) and (3.8) the ''cosmic variance.'']

The original probability distributions dictate also the PDF's for these quadratic variables. They are the so-called χ^2 distributions. Denoting $\chi^2 = b_l^2/\sigma_l^2$ and $n=2l+1$, one can write [12]

$$f(\chi^2, n) = \frac{(\chi^2)^{(n-2)/2} e^{-\chi^2/2}}{(n/2-1)! 2^{n/2}},$$

and for the random variable b_l^2 we have

$$f(b_l^2) = \frac{(b_l^2)^{(n-2)/2} (\sigma_l^2)^{-n/2} e^{-b_l^2/2\sigma_l^2}}{(n/2-1)! 2^{n/2}}.$$
(3.9)

So far, we have been concerned with the statistical properties of the coefficients in the expansion of the random process $\delta T/T$ over the orthonormal spherical harmonics. We can now discuss some properties of the random process it-

self. No doubt, these properties follow from the properties of the coefficients. Obviously, the process is isotropic in the sense that the mean value of the $\delta T/T$ is one and the same number (zero) in every direction on the sky

$$\left\langle \frac{\delta T}{T}(\vec{e})\right\rangle = 0.$$
(3.10)

The process is also homogeneous in the sense that the angular correlation function depends only on the angle δ between two directions, but not on directions themselves. For each pair of vectors $\vec{e}_1$ and $\vec{e}_2$ separated by the angle δ, the angular correlation function takes the form

$$\left\langle \frac{\delta T}{T}(\vec{e}_1) \frac{\delta T}{T}(\vec{e}_2)\right\rangle = K(\delta)$$
$$= \frac{1}{4\pi} \sum_{l=0}^{\infty} \sigma_l^2 (2l+1) P_l(\cos\delta),$$
(3.11)

where $P_l(\cos\delta)$ are the Legendre polynomials.

The three-point correlation function [as well as all correlation functions containing an odd number of term $\delta T/T(\vec{e}_i)$] vanishes:

$$\left\langle \frac{\delta T}{T}(\vec{e}_1) \frac{\delta T}{T}(\vec{e}_2) \frac{\delta T}{T}(\vec{e}_3)\right\rangle = 0.$$

The four-point correlation function is given by the expression

$$\left\langle \frac{\delta T}{T}(\vec{e}_1) \frac{\delta T}{T}(\vec{e}_2) \frac{\delta T}{T}(\vec{e}_3) \frac{\delta T}{T}(\vec{e}_4)\right\rangle$$
$$= \frac{1}{(4\pi)^2} \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \sigma_l^2 \sigma_m^2 (2l+1)(2m+1)$$
$$\times [P_l(\cos\delta_{13}) P_m(\cos\delta_{24}) + P_l(\cos\delta_{14}) P_m(\cos\delta_{23})$$
$$+ P_l(\cos\delta_{12}) P_m(\cos\delta_{34})],$$

where the symbol δ_{ij} denotes the angle between vectors $\vec{e}_i$ and $\vec{e}_j$. In a similar manner one can derive the higher-order correlation functions and express them through the lower-order ones.

All the derived expressions are consequences of the postulated distribution functions (3.1)–(3.3). We do not possess a rigorous mathematical proof of the statement that there exists a one-to-one correspondence between Eqs. (3.1)–(3.3) and the fact that the relevant cosmological perturbations are placed in the squeezed vacuum quantum states. However, we believe this statement is indeed true. At any rate, the quantum-mechanical expectation values coincide with the corresponding ensemble averages if the appropriate identifications are made [6]. In particular, the quantum-mechanical expression for the angular correlation function

$$\left\langle 0 \left| \frac{\delta T}{T}(\vec{e}_1) \frac{\delta T}{T}(\vec{e}_2)\right| 0\right\rangle = \sum_{l=l_{\min}}^{\infty} C_l P_l(\cos\delta)$$

coincides with Eq. (3.11) if we identify

$$\frac{1}{4\pi}(2l+1)\sigma_l^2 = C_l. \qquad (3.12)$$

The quantity C_l explicitly contains the square of the Planck length. This quantity is calculable when the law of cosmological evolution and the sort of cosmological perturbations are specified. The value of the lowest multipole $l_{\min}$ is also determined by the sort of perturbations. In this sense, the abstract quantities σ_l^2, which completely characterize the random process (2.1), (3.1)–(3.3), are also calculable and are given by the expressions

$$\sigma_l^2 = \frac{4\pi}{2l+1} C_l.$$

IV. ERGODICITY OF RANDOM PROCESSES ON A LINE AND ON A SPHERE

Let us first recall the ergodic theorem [10,11] for a time-dependent random process $x(\xi,t)$ defined on an infinite t line. The symbol ξ indicates different possible realizations. Let us assume that the process is stationary, that is, its mean value does not depend on time,

$$\langle x(\xi,t)\rangle = \text{const} = m,$$

and its correlation function depends only on the time difference:

$$\langle x(\xi,t+\tau)x(\xi,t)\rangle = B(\tau).$$

To find the ensemble average of $x(\xi,t)$ at a fixed moment of time, one takes a large number N of different realizations and calculates the arithmetic mean of the observed values:

$$f = \frac{1}{N}\sum_{i=1}^{N} x(\xi_i,t).$$

In the limit of N going to infinity, the quantity f tends to the theoretical ensemble mean $\langle x(\xi,t)\rangle$ of the random process.

Let us now consider a situation in which we have access to only one realization $x(\xi_0,t)$ of the random process. What can we say about m and $B(\tau)$ on the grounds of this single realization? The ergodic theorem defines the conditions under which the ensemble averages can be replaced by the time averages, so that the m and $B(\tau)$ can be found from the time integrations of $x(\xi_0,t)$.

Introduce a random variable $x_T(\xi)$ defined by the equation

$$x_T(\xi) = \frac{1}{2T}\int_{-T}^{+T} x(\xi,t)dt. \qquad (4.1)$$

This variable is an unbiased estimator of m because $\langle x_T(\xi)\rangle = m$. However, we can say much more when we take the limit $T\to\infty$. If the process is such that

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{+T} B(\tau)d\tau = 0, \qquad (4.2)$$

then

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{+T} x(\xi,t)dt = m,$$

for every realization ξ. When condition (4.2) is satisfied, the process is called mean ergodic. The condition (4.2) can also be expressed as the requirement $\sigma_{x_T}^2 \to 0$ in the limit $T\to\infty$, where $\sigma_{x_T}^2$ is the variance of the random variable defined by Eq. (4.1). This explains why one is capable of deriving from a single realization a true parameter of the ergodic random process (in this case, the mean value m) with probability 1. Indeed, for every arbitrarily small ϵ, one has the Tchebysheff inequality

$$P(|x_T - m| < \epsilon) \geq 1 - \frac{\sigma_{x_T}^2}{\epsilon^2},$$

and the probability goes to 1 when $\sigma_{x_T}^2$ goes to 0. A sufficient condition for the validity of Eq. (4.2) is the vanishing of the correlations at large temporal separations: $\lim_{\tau\to\infty}B(\tau)=0$.

More stringent conditions should be satisfied for the process to be correlation ergodic, that is to have

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{+T} x(\xi,t+\tau)x(\xi,t)dt = B(\tau), \qquad (4.3)$$

for every ξ. Here, for simplicity, we will restrict ourselves to normal zero-mean ($m=0$) stationary processes. The equality (4.3) allows one to find the variance of the process from its single realization. This equality takes place if and only if the process is such that

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{+T} |B(\tau)|^2 d\tau = 0. \qquad (4.4)$$

For normal zero-mean stationary processes, and when the condition (4.4) is met, all the higher-order correlation functions can also be replaced by the time averages. Note that the integrand in Eq. (4.4) is a strictly positive function. The limit of the expression (4.4) is zero because the denominator goes to infinity in the limit $T\to\infty$.

We will now try to apply the notions formulated above to a random process on a sphere. The problem of our interest is the CMB temperature distributed over the sky. Strictly speaking, the quantum-mechanically generated cosmological perturbations form a nonstationary process: the squeezing makes the temporal correlation function a function of individual moments of time, and not only of the time difference. This property may turn out to be very important for the future observations of short gravitational waves, but is irrelevant for our discussion of very long-wavelength cosmological perturbations responsible for the microwave background anisotropies, since the time scale of variations is much much longer than the interval of time between possible missions for the CMB observations. Most importantly, the stationarity, a necessary (but not sufficient) condition for a time-dependent process to be ergodic, is replaced in our case by the analogous properties of isotropy and homogeneity of the process on a sphere, see Eqs. (3.10) and (3.11). So, at least

the necessary conditions for our process to be mean ergodic and correlation ergodic are satisfied.

To check the analogue of the condition (4.2), we will use $K(\delta)$ instead of $B(\tau)$ and will replace the time integral divided by T by the integral over a sphere divided by 4π, the surface area of a (unit radius) sphere. The result is

$$\frac{1}{4\pi}\int_{S^2}d\Omega K(\delta)=\frac{1}{4\pi}\sigma_0^2.$$

The right-hand side of this equation is zero when σ_0^2 is zero, that is when the monopole coefficient b_{00}^c in the expansion (2.3) is identically zero, see Eq. (3.4). In this case, our process is indeed mean ergodic since the integral over a given map

$$\frac{1}{4\pi}\int_{S^2}d\Omega\ \frac{\delta T}{T}\ (\vec{e})=\frac{1}{\sqrt{4\pi}}\ b_{00}^c$$

vanishes, and the average over the map coincides with the ensemble average (3.10).

What we really would like to have is the correlation ergodicity of our process. In this case, we would be able to replace the ensemble averaging by the integration over the sphere, and to find the $K(\delta)$ and hence all the σ_l^2 from a single map. Unfortunately, this is exactly what we cannot have on a sphere. The necessary and sufficient condition (4.4) translates into the requirement

$$\frac{1}{4\pi}\int_{S^2}d\Omega|K(\delta)|^2=0. \qquad (4.5)$$

The left-hand side of this equation can be calculated using Eq. (3.11) and the orthogonality properties of the Legendre polynomials. The resulting equation

$$\frac{1}{16\pi^2}\sum_{l=1}^{\infty}(2l+1)\sigma_l^4=0$$

can only be true if all the σ_l^2 are zero. In contrast with processes on an infinite line or in infinite space, we do not have here an infinite volume factor in the denominator of the left-hand side of Eq. (4.5) to enable it to vanish. We are bound to do the best what we can do with a single map, try and find out the best unbiased estimates for the parameters σ_l^2 and $K(\delta)$.

V. THE BEST UNBIASED ESTIMATOR FOR THE σ_l^2

Let us denote an estimator for the σ_l^2 by f_l. This is a random variable constructed from the original random process. One realization of this process is the observed map. The most general quadratic expression for f_l is given by

$$f_l=\int_{S^2}\int_{S^2}d\Omega_1 d\Omega_2 w_l(\vec{e}_1,\vec{e}_2)\ \frac{\delta T}{T}\ (\vec{e}_1)\ \frac{\delta T}{T}\ (\vec{e}_2), \qquad (5.1)$$

where $d\Omega=\sin\theta d\theta d\varphi$. The function $w_l(\vec{e}_1,\vec{e}_2)$ is a weight function to be determined from the requirements that the estimator f_l is unbiased and the minimum variance (the best). In this formulation, the problem was essentially solved in Ref. [17]. We refine and expand the arguments of Ref. [17].

An arbitrary weight function $w_l(\vec{e}_1,\vec{e}_2)$, being a function of two sets of angular coordinates, can be expanded over two sets of orthonormal spherical harmonics:

$$w_l(\vec{e}_1,\vec{e}_2)=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}d_{lij00}^{cc}\frac{Y_{i0}^c(\vec{e}_1)}{\sqrt{2}}\frac{Y_{j0}^c(\vec{e}_2)}{\sqrt{2}}+\sum_{i,j}\sum_{n=1}^{j}\left[d_{lijon}^{cc}\frac{Y_{i0}^c(\vec{e}_1)}{\sqrt{2}}\ Y_{jn}^c(\vec{e}_2)+d_{lijon}^{cs}\frac{Y_{i0}^c(\vec{e}_1)}{\sqrt{2}}\ Y_{jn}^s(\vec{e}_2)\right]$$

$$+\sum_{i,j}\sum_{m=1}^{i}\left[d_{lijmo}^{cc}Y_{im}^c(\vec{e}_1)\frac{Y_{j0}^c(\vec{e}_2)}{\sqrt{2}}+d_{lijmo}^{sc}Y_{im}^s(\vec{e}_1)\ \frac{Y_{j0}^c(\vec{e}_2)}{\sqrt{2}}\right]+\sum_{i,j}\sum_{m,n}[d_{lijmn}^{cc}Y_{im}^c(\vec{e}_1)Y_{jn}^c(\vec{e}_2)$$

$$+d_{lijmn}^{ss}Y_{im}^s(\vec{e}_1)Y_{jn}^s(\vec{e}_2)+d_{lijmn}^{cs}Y_{im}^c(\vec{e}_1)Y_{jn}^s(\vec{e}_2)+d_{lijmn}^{sc}Y_{im}^s(\vec{e}_1)Y_{jn}^c(\vec{e}_2)]. \qquad (5.2)$$

In this expression, all the coefficients d_{lijmn}^{AB} $(A,B=c,s)$ are real. The weight function may be asymmetric with respect to the interchange of $\vec{e}_1$ and $\vec{e}_2$, but the antisymmetric part of this function will not contribute to Eq. (5.1) anyway. To simplify calculations, we require this function to be explicitly symmetric, $w_l(\vec{e}_1,\vec{e}_2)=w_l(\vec{e}_2,\vec{e}_1)$. This means that the d coefficients must obey the relationship

$$d_{lijmn}^{AB}=d_{ljinm}^{BA}.$$

We will mostly use another representation for w_l defined by

$$w_l(\vec{e}_1,\vec{e}_2)=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{m=-i}^{i}\sum_{n=-j}^{j}d_{lijmn}Y_{im}(\vec{e}_1)Y_{jn}^*(\vec{e}_2). \qquad (5.3)$$

In this case, the coefficients d_{lijmn} are complex, and since the function $w_l(\vec{e}_1,\vec{e}_2)$ is real, they have the property

$$d_{lijmn}^*=d_{lij,-m,-n},$$

or, if we introduce the real and imaginary parts of d_{lijmn}, i.e., $d_{lijmn}=d_{lijmn}^r+id_{lijmn}^i$,

$$d_{lijmn}^r = d_{lij,-m,-n}^r, \quad d_{lijmn}^i = -d_{lij,-m,-n}^i. \quad (5.4)$$

In addition, the weight function is symmetric in this representation if

$$d_{lijmn} = d_{lji,-n,-m}.$$

The link between the two representations is expressed by the equations

$$d_{lij00} = d_{lij00}^{cc},$$

$$d_{lij0n} = \begin{cases} \dfrac{1}{\sqrt{2}}(d_{lij0n}^{cc} + i d_{lij0n}^{cs}), & n \geqslant 1, \\[3mm] \dfrac{1}{\sqrt{2}}(d_{lij0,-n}^{cc} - i d_{lij0,-n}^{cs}), & n \leqslant -1, \end{cases}$$

$$d_{lijm0} = \begin{cases} \dfrac{1}{\sqrt{2}}(d_{lijm0}^{cc} - i d_{lijm0}^{sc}), & m \geqslant 1, \\[3mm] \dfrac{1}{\sqrt{2}}(d_{lij,-m,0}^{cc} + i d_{lij,-m,0}^{sc}), & m \leqslant -1, \end{cases}$$

$$d_{lijmn} = \begin{cases} \dfrac{1}{2}(d_{lijmn}^{cc} + d_{lijmn}^{ss} - i d_{lijmn}^{sc} + i d_{lijmn}^{cs}), & m \geqslant 1,\ n \geqslant 1, \\[3mm] \dfrac{1}{2}(d_{lij,-m,-n}^{cc} + d_{lij,-m,-n}^{ss} + i d_{lij,-m,-n}^{sc} - i d_{lij,-m,-n}^{cs}), & m \leqslant -1,\ n \leqslant -1, \\[3mm] \dfrac{1}{2}(d_{lijm,-n}^{cc} - d_{lijm,-n}^{ss} - i d_{lijm,-n}^{sc} - i d_{lijm,-n}^{cs}), & m \geqslant 1,\ n \leqslant -1, \\[3mm] \dfrac{1}{2}(d_{lij,-mn}^{cc} - d_{lij,-mn}^{ss} + i d_{lij,-mn}^{sc} + i d_{lij,-mn}^{cs}), & m \leqslant -1,\ n \geqslant 1. \end{cases}$$

The angular integrals in Eq. (5.1) can be performed explicitly. This integration returns us from the random process $\delta T/T$ to the random variables, coefficients in the decomposition of the $\delta T/T$, and allows us to express the estimator f_l in terms of the general quadratic combination of these coefficients. As a consequence, we arrive at the following expression for the f_l in terms of the b coefficients:

$$f_l = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \left(d_{lij00}^{cc} b_{i0}^c b_{j0}^c + \sum_{m=1}^{i} (d_{lijm0}^{cc} b_{j0}^c b_{im}^c + d_{lijm0}^{sc} b_{j0}^c b_{im}^s) + \sum_{n=1}^{j} (d_{lij0n}^{cc} b_{i0}^c b_{jn}^c + d_{lij0n}^{cs} b_{i0}^c b_{jn}^s) \right.$$
$$\left. + \sum_{m=1}^{i} \sum_{n=1}^{j} (d_{lijmn}^{cc} b_{im}^c b_{jn}^c + d_{lijmn}^{cs} b_{im}^c b_{jn}^s + d_{lijmn}^{sc} b_{im}^s b_{jn}^c + d_{lijmn}^{ss} b_{im}^s b_{jn}^s) \right). \quad (5.5)$$

In the representation defined by Eqs. (5.3) and (2.4), the last equation takes the form

$$f_l = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \sum_{m=-i}^{i} \sum_{n=-j}^{j} d_{lijmn} c_{im}^* c_{jn}. \quad (5.6)$$

We have introduced the general expression for the estimator and can now subject it to the desired requirements. Let us start from the mean value of the estimator. Using Eqs. (5.7) and (3.5), we obtain

$$\langle f_l \rangle = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \sum_{m=-i}^{i} \sum_{n=-j}^{j} d_{lijmn} \langle c_{im}^* c_{jn} \rangle$$

$$= \sum_{i=0}^{\infty} \sigma_i^2 \sum_{m=-i}^{i} d_{liimm}.$$

Since the second set of equations (5.4) guarantees

$$\sum_{m=-i}^{i} d_{liimm}^i = -\sum_{m=-i}^{i} d_{liimm}^i = 0,$$

the mean value of f_l reduces to the manifestly real expression

$$\langle f_l \rangle = \sum_{i=0}^{\infty} \sigma_i^2 \sum_{m=-i}^{i} d_{liimm}^r .$$

We want our estimator to be unbiased, that is, we impose the condition $\langle f_l \rangle = \sigma_l^2$. This requirement can only be achieved if

$$\sum_{m=-i}^{i} d_{liimm}^r = \delta_{li} . \qquad (5.7)$$

Equation (5.8) form the first set of constraints on the weight function w_l and define the family of unbiased estimators.

The next step is to find, among the unbiased estimators, the one whose variance is minimal. The variance $\sigma_{f_l}^2$ of the random variable f_l,

$$\sigma_{f_l}^2 = \langle f_l^2 \rangle - \langle f_l \rangle^2 ,$$

can be calculated using the definition (5.6) and Eq. (3.6). The general expression for the variance reduces to the form

$$\sigma_{f_l}^2 = 2 \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \sum_{m=-i}^{i} \sum_{n=-j}^{j} d_{lijmn} d_{lijmn}^* \sigma_i^2 \sigma_j^2 . \qquad (5.8)$$

We have to minimize this expression taking into account the constraints (5.7). The expression (5.8) is the sum of strictly positive terms. To minimize this sum, we should set to zero as many terms as possible. First, we need to set to zero all the d coefficients which do not participate in the constraint (5.7) and whose presence in the sum only increases the variance. Thus, we require to vanish all the coefficients d_{lijmn}^i and those of d_{lijmn}^r which have indices $i \neq j$ and/or $m \neq n$. To minimize the remaining variance under the constraint (5.7), we introduce the Lagrange multipliers λ_i and write

$$\delta \left[2 \sum_{i=0}^{\infty} \sum_{m=-i}^{i} (d_{liimm}^r)^2 \sigma_i^4 + \sum_{i=0}^{\infty} \lambda_i \left(\sum_{m=-i}^{i} d_{liimm}^r - \delta_{li} \right) \right] = 0 .$$

Since the d_{liimm}^r are treated as independent variables, the variation of the previous expression provides us with

$$4 d_{liimm}^r \sigma_i^4 + \lambda_i = 0 . \qquad (5.9)$$

The sum over m of these equations together with Eq. (5.7) determines the quantities λ_i:

$$4 \sigma_i^4 \delta_{li} + (2i+1) \lambda_i = 0 . \qquad (5.10)$$

Using the expression (5.10) for the Lagrange multipliers λ_i in Eq. (5.9) allows us to write

$$d_{liimm}^r = \frac{1}{2i+1} \delta_{li} .$$

Thus, taking into account all relationships, we obtain the complete set of constraints on the weight function (5.3) which makes the estimator f_l unbiased and best:

$$d_{lijmn}^r = \frac{1}{2i+1} \delta_{li} \delta_{ij} \delta_{mn} , \quad d_{lijmn}^i = 0 . \qquad (5.11)$$

In the representation (5.2), this amounts to

$$d_{lij00}^{cc} = \frac{1}{2i+1} \delta_{li} \delta_{ij} , \qquad (5.12)$$

$$d_{lijmn}^{cc} = d_{lijmn}^{ss} = \frac{1}{2i+1} \delta_{li} \delta_{ij} \delta_{mn} , \qquad (5.13)$$

with all other coefficients being zero.

Having found all the d coefficients, we can write the weight function $w_l(\vec{e}_1, \vec{e}_2)$ explicitly. Using the definition (5.3) and the found expressions (5.11), we obtain

$$w_l(\vec{e}_1, \vec{e}_2)$$

$$= \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \sum_{m=-i}^{i} \sum_{n=-j}^{j} \frac{1}{2i+1} \delta_{li} \delta_{ij} \delta_{mn} Y_{im}(\vec{e}_1) Y_{jn}^*(\vec{e}_2)$$

$$= \frac{1}{2l+1} \sum_{m=-l}^{l} Y_{lm}(\vec{e}_1) Y_{lm}^*(\vec{e}_2) \qquad (5.14)$$

$$= \frac{1}{4\pi} P_l(\cos \delta_{12}), \qquad (5.15)$$

where, in the last step, the summation theorem for spherical harmonics has been used. Therefore, the best unbiased estimator for σ_l^2 can be written as

$$f_l = \frac{1}{4\pi} \int_{S^2} \int_{S^2} d\Omega_1 d\Omega_2 P_l(\cos \delta_{12}) \frac{\delta T}{T}(\vec{e}_1) \frac{\delta T}{T}(\vec{e}_2) . \qquad (5.16)$$

This formula answers the question what to do with a given map in order to get a concrete number, the best substitute for the true parameter σ_l^2. The answer is to perform with the map the integrations prescribed by this formula. In fact, the integrations can be further simplified.

The estimator (5.16) contains a double integral of the product of two functions $\delta T/T$ and, therefore, can be called a quadratic estimator. However, this estimator can be presented as a product of two linear estimators, i.e., a product of two appropriate single integrals of the function $\delta T/T$. Indeed, using the summation theorem, Eqs. (5.14) and (5.15), formula (5.16) can be written as

$$f_l = \frac{1}{2l+1} \sum_{m=-l}^{l} \int_{S^2} d\Omega_1 Y_{lm}(\vec{e}_1) \frac{\delta T}{T}(\vec{e}_1)$$

$$\times \int_{S^2} d\Omega_2 Y_{lm}^*(\vec{e}_2) \frac{\delta T}{T}(\vec{e}_2) .$$

This formula shows that it is sufficient to perform one appropriately weighted integration over the sphere with further multiplications and summations. Moreover, the remaining integrals define the c_{lm} coefficients. So, we obtain the following expression for the best unbiased estimator in terms of the original random coefficients:

$$f_l = \frac{1}{2l+1} \sum_{m=-l}^{l} c_{lm}^* c_{lm} = \frac{c_l^2}{2l+1}. \qquad (5.17)$$

Of course, this is the same expression which could be obtained by inserting Eq. (5.11) into Eq. (5.6) or by inserting Eqs. (5.12) and (5.13) into Eq. (5.5).

We have found the estimator with the smallest possible variance among all unbiased estimators. It is useful to write this minimal variance explicitly. This can be found either from Eqs. (5.8) and (5.11) or from Eqs. (5.17) and (3.8). The result is

$$\sigma_{f_l}^2 = \frac{2}{2l+1} \sigma_l^4 .$$

VI. THE BEST UNBIASED ESTIMATOR FOR THE $K(\delta)$

The best unbiased estimator for σ_l^2 is also the best unbiased estimator for the multipole moments C_l of the correlation function $K(\delta)$, see Eqs. (3.11) and (3.12). Since the parameter $K(\delta)$ is a combination of the parameters σ_l^2, it is

not surprising that the best unbiased estimator for $K(\delta)$ turns out to be the same combination of the best unbiased estimators for σ_l^2. It is interesting and instructive to follow this relationship in detail.

Let us denote an estimator of the $K(\delta)$ by $f(\delta)$. This is a random variable constructed from the random process $\delta T/T$. The most general (quadratic) expression for the $f(\delta)$ can be written as

$$f(\delta) = \int_{S^2} \int_{S^2} d\Omega_1 d\Omega_2 w(\vec{e}_1, \vec{e}_2, \delta) \frac{\delta T}{T}(\vec{e}_1) \frac{\delta T}{T}(\vec{e}_2),$$
$$(6.1)$$

where the δ is a fixed angle, whereas the angle between variable directions $\vec{e}_1$ and $\vec{e}_2$ will be denoted δ_{12}. The arbitrary weight function $w(\vec{e}_1, \vec{e}_2, \delta)$ can be expanded, without loss of generality, over the Legendre polynomials $P_l(\cos\delta)$:

$$w(\vec{e}_1, \vec{e}_2, \delta) = \frac{1}{4\pi} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\delta) w_l(\vec{e}_1, \vec{e}_2).$$

The estimator $f(\delta)$ takes the form

$$f(\delta) = \frac{1}{4\pi} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\delta) \int_{S^2} \int_{S^2} d\Omega_1 d\Omega_2 w_l(\vec{e}_1, \vec{e}_2) \frac{\delta T}{T}(\vec{e}_1) \frac{\delta T}{T}(\vec{e}_2) = \frac{1}{4\pi} \sum_{l=0}^{\infty} (2l+1) f_l P_l(\cos\delta).$$

Now, we want the $f(\delta)$ to be unbiased and best estimator of $K(\delta)$. The estimator $f(\delta)$ is unbiased if $\langle f_l \rangle = \sigma_l^2$, and it is the best if the variance of the f_l is the smallest one. In other words, we return to the solved problem (Sec. V) for the estimator f_l. Using the results of the previous section, we can write for the best unbiased estimator of the $K(\delta)$:

$$f(\delta) = \frac{1}{4\pi} \sum_{l=0}^{\infty} P_l(\cos\delta) c_l^2 . \qquad (6.2)$$

The weight function $w(\vec{e}_1, \vec{e}_2, \delta)$ is given, taking into account Eq. (5.15), by

$$w(\vec{e}_1, \vec{e}_2, \delta) = \frac{1}{(4\pi)^2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\delta) P_l(\cos\delta_{12}).$$
$$(6.3)$$

This last equation can also be written as

$$w(\vec{e}_1, \vec{e}_2, \delta) = \frac{1}{4\pi} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} P_l(\cos\delta) Y_{lm}(\vec{e}_1) Y_{lm}^*(\vec{e}_2),$$

showing that the double integral in Eq. (6.1) decays into the products and summations of the appropriately weighted single integrals. This form of the weight function permits an immediate recovery of the already known result (6.2). The variance of the best estimator (6.2) is

$$\sigma_{f(\delta)}^2 = \frac{1}{8\pi^2} \sum_{l=0}^{\infty} (2l+1) \sigma_l^4 P_l^2(\cos\delta).$$

The derived formulas answer the question what to do with a given map in order to derive the best unbiased estimate for the correlation function $K(\delta)$. The outlined prescription essentially goes through the derivation of the best unbiased estimate for σ_l^2. However, the weight function (6.3) allows also a different procedure for the derivation of the estimator and the estimate; the direct integration of the map, but with the help of the δ function.

Let us denote $\cos\delta = x$ and $\cos\delta_{12} = x_0$. Let us present (define) the δ function $\delta(x - x_0)$ as an expansion over the Legendre polynomials:

$$\delta(x - x_0) = \sum_{l=0}^{\infty} a_l P_l(x). \qquad (6.4)$$

To find the coefficients a_l, multiply both sides of Eq. (6.4) by $P_m(x)$ and integrate by x from -1 to 1. The result is

$$a_l = \frac{2l+1}{2} P_l(x_0)$$

and

$$\delta(x - x_0) = \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(x) P_l(x_0).$$

Thus, the weight function (6.3) can be written as

$$w(\vec{e}_1,\vec{e}_2,\delta)=\frac{1}{8\pi^2}\ \delta(\cos\delta-\cos\delta_{12}). \qquad (6.5)$$

Let us show that the integration in Eq. (6.1) with the weight function (6.5) does indeed provide us with the same result (6.2). The product of two $\delta T/T$ is the random process $v\equiv(\delta T/T)(\vec{e}_1)(\delta T/T)(\vec{e}_2)$. We have access to one realization of this process. To integrate the v over all directions $\vec{e}_1,\vec{e}_2$ on the sky separated by a fixed angle δ, one can proceed as follows. At the first step, rotate the vector $\vec{e}_2$ around the fixed direction defined by $\vec{e}_1$ and integrate the v over the circle traced by the vector $\vec{e}_2$ on the sphere. The result will depend only on (θ_1,φ_1), the coordinates of the vector $\vec{e}_1$. At the second step, integrate the result over all θ_1 and φ_1, letting the vector $\vec{e}_1$ to run over the whole sphere. The final result, taking into account also the factor $1/8\pi^2$ in Eq. (6.5), should be the random variable we are interested in. Let us do this computation in practice.

Every function on a sphere can be expanded in the basis of spherical harmonics. In particular, the function $Y_{lm}(\theta,\varphi)$ can be expanded in the basis $\{Y_{lr}(\theta',\varphi');l\geq0,-l\leq r\leq l\}$ according to the formula

$$Y_{lm}(\theta',\varphi')=\sum_{r=-l}^{l}Y_{lr}(\theta,\varphi)D_{rm}^l(\alpha,\beta,\gamma).$$

The coefficients of this expansion are called the Wigner D functions [18]. They depend on the Euler angles α, β, γ

describing the rotation which transforms the direction (θ,φ) into the direction (θ',φ'). Since the rotation specified by the angles α, $\beta=-\theta_1$, $\gamma=-\varphi_1$ brings the vector pointing out to the north pole to the direction defined by (θ_1,φ_1), we can write

$$Y_{lm}(\vec{e}_1)=\sum_{r=-l}^{l}Y_{lr}(0,-)D_{rm}^l(\alpha,-\theta_1,-\varphi_1). \qquad (6.6)$$

In the same manner, the $Y_{pq}(\vec{e}_2)$ can be expressed as

$$Y_{pq}(\vec{e}_2)=\sum_{s=-p}^{p}Y_{ps}(\delta,\chi)D_{sq}^p(\alpha,-\theta_1,-\varphi_1). \qquad (6.7)$$

Indeed, when the vector $\vec{e}_1$ points out to the north pole, the θ coordinate of $\vec{e}_2$ is simply δ.

Using the definition (2.4) and the formulas (6.6) and (6.7), we can present the random process v as

$$v=\sum_{lm}\sum_{pq}\sum_{rs}c_{lm}c_{pq}Y_{lr}(0,-)Y_{ps}(\delta,\chi)$$
$$\times D_{rm}^l(\alpha,-\theta_1,-\varphi_1)D_{sq}^p(\alpha,-\theta_1,-\varphi_1).$$

Let us now perform the two step integration procedure described above. The first step amounts to the integration of v over the angle χ from 0 to 2π. Using the explicit form of the spherical harmonics given in the Appendix, we get

$$\int_0^{2\pi}v d\chi=\sum_{lm}\sum_{pq}\sum_{rs}c_{lm}c_{pq}\left(\frac{2l+1}{4\pi}\right)^{1/2}\delta_{r0}\left(\frac{2p+1}{4\pi}\right)^{1/2}\left[\frac{(p-s)!}{(p+s)!}\right]P_{ps}(\cos\delta)D_{rm}^l(\alpha,-\theta_1,-\varphi_1)$$
$$\times D_{sq}^p(\alpha,-\theta_1,-\varphi_1)\int_0^{2\pi}e^{is\chi}d\chi.$$

In the last expression, the integral $\int_0^{2\pi}e^{is\chi}d\chi$ is simply $2\pi\delta_{s0}$. Using the relationship

$$\sqrt{\frac{2l+1}{4\pi}}\ D_{om}^l(\alpha,\beta,\gamma)=Y_{lm}(\beta,\gamma),$$

we obtain

$$\int_0^{2\pi}v d\chi=2\pi\sum_{lm}\sum_{pq}c_{lm}c_{pq}P_p(\cos\delta)Y_{lm}(\theta_1,\varphi_1)Y_{pq}(\theta_1,\varphi_1).$$

As expected, the result depends only on (θ_1,φ_1). In order to complete the procedure, we have to integrate this result over Ω_1. We find

$$\int d\Omega_1\int_0^{2\pi}v d\chi=2\pi\sum_{lm}\sum_{pq}c_{lm}c_{pq}P_p(\cos\delta)\int d\Omega_1 Y_{lm}(\theta_1,\varphi_1)Y_{pq}(\theta_1,\varphi_1)$$

$$=2\pi\sum_{l=0}^{\infty}P_l(\cos\delta)c_l^2.$$

Restoring the factor $1/8\pi^2$ from Eq. (6.5), we arrive at the best unbiased estimator (6.2). The same procedure performed over a given map provides us with the best unbiased estimate of the correlation function $K(\delta)$.

VII. BEST ESTIMATES AND THE ERROR BARS

We will denote the best unbiased estimate for the parameter σ_l^2 by $(\sigma_l^2)_{BU}$. Along with this one, there exist other estimates of the same parameter, for example, the maximum-likelihood estimate $(\sigma_l^2)_{ML}$. Not surprisingly, for the postulated distributions (3.1)–(3.3), these estimates coincide.

Apparently, the most ''naive'' evaluation of the σ_l^2, giving nevertheless the correct result, would be the following one. From a given map one derives the set of the observed coefficients $b_{lm}^{(map)}$ (that is to say, the set $\{b_{l0}^c, b_{lm}^c, b_{lm}^s\}$, $m \geq 1$). We know (postulate) that each of them is drawn from the normal zero-mean distribution

$$f(b_{lm}) = \frac{1}{\sqrt{2\pi}\sigma_l} \, e^{-b_{lm}^2/2\sigma_l^2}. \tag{7.1}$$

Each of the observed b_{lm} coefficients can be used for the maximum-likelihood evaluation of the corresponding σ_l^2. [We omit the label (map) when it is clear that we deal with the observed quantities.] One finds this estimate, denoted $\sigma_{l(m)}^2$, by assuming that the PDF (7.1) reaches its maximum at the observed b_{lm}. The result is known: $\sigma_{l(m)}^2 = b_{lm}^2$. Indeed,

$$\ln f = -\frac{1}{2}\ln(\sigma_l^2) - \frac{b_{lm}^2}{2\sigma_l^2} + C,$$

where C is a constant. Then, one gets

$$\frac{d \ln f}{d\sigma_l^2} = -\frac{1}{2\sigma_l^2} + \frac{b_{lm}^2}{2\sigma_l^4},$$

and the condition

$$\frac{d \ln f}{d\sigma_l^2} = 0 \tag{7.2}$$

leads to the stated result. Since for every l we have $2l+1$ independent b_{lm} coefficients and, hence, $2l+1$ independent evaluations, the estimate of the true σ_l^2 is given by

$$\frac{1}{2l+1}\sum_m \sigma_{l(m)}^2 = \frac{1}{2l+1}\sum_m b_{lm}^2 = \frac{b_l^2}{2l+1}.$$

This number coincides with the $(\sigma_l^2)_{BU}$ determined by Eq. (5.17).

A similar maximum-likelihood evaluation of σ_l^2 is based on the joint PDF for all coefficients b_{lm} (with the same index l) which is simply the product of the individual PDF's (7.1):

$$f(b_{l0}^c, b_{lm}^c, b_{lm}^s) = \frac{1}{(2\pi\sigma_l^2)^{(2l+1)/2}} \, e^{-b_l^2/2\sigma_l^2}.$$

Imposing the condition (7.2), we arrive at the same result

$$(\sigma_l^2)_{ML} = \frac{b_l^2}{2l+1} = (\sigma_l^2)_{BU}.$$

Finally, we can give the maximum-likelihood estimation based on the PDF (3.9) for the quantities b_l^2. Repeating the same steps, we come again to the result

$$(\sigma_l^2)_{ML} = \frac{b_l^2}{n}. \tag{7.3}$$

Thus, in the first approximation, we can write for the true value of σ_l^2: $\sigma_l^2 = (\sigma_l^2)_{BU}$. In the next approximation, we want to make this statement more accurate by assigning the error bars. This is the matter of definitions, and there are many ways of doing this. We will use the distribution function (3.9). This function attains its maximum at the measured b_l^2 and the estimated $(\sigma_l^2)_{ML}$, Eq. (7.3). The value of the f at the maximum is

$$f_{max} = \frac{(b_l^2)^{-1}e^{-n/2}}{(n/2-1)!(2/n)^{n/2}}.$$

When the σ_l^2, treated as a variable parameter, deviates from $(\sigma_l^2)_{ML}$, the value of the f decreases as compared with the f_{max}. We establish the error bars for σ_l^2 by requiring that the value of f does not drop below some confidence level

$$f = k f_{max}, \tag{7.4}$$

where k, $k < 1$, is a fixed number. Within the error box are included all σ_l^2 surrounding $(\sigma_l^2)_{ML}$ and up to the boundaries $(\sigma_l^2)_k$ determined by two solutions to Eq. (7.4).

Let us denote $x \equiv (\sigma_l^2)_{ML}/(\sigma_l^2)_k$. Equation (7.4) takes the form

$$\ln x - x = \frac{2}{n}\ln k - 1. \tag{7.5}$$

Obviously, $x = 1$ if $k = 1$. Let us now consider small deviations from this solution for $k < 1$. We write $x = 1 - y$, where $|y| \ll 1$. By expanding the $\ln x$ in terms of y and considering the first nonvanishing approximation to Eq. (7.5), we find $y^2 = -(4/n)\ln k$. That is, the two wanted solutions are

$$y = \pm\frac{2\sqrt{-\ln k}}{\sqrt{n}}.$$

The condition of their applicability is $-(4/n)\ln k \ll 1$. Thus, in this approximation, we can write the true σ_l^2 as

$$\sigma_l^2 = (\sigma_l^2)_{BU}\left(1 \pm \frac{2\sqrt{-\ln k}}{\sqrt{2l+1}}\right). \tag{7.6}$$

The choice of k is in our hands. If the distribution $f(z)$ were a normal zero-mean distribution, then a reasonable choice of k would be $k = e^{-1/2}$, because $f(z = \sigma) = e^{-1/2}f_{max}$. The χ^2 distribution (3.9) is not a normal one,

but approaches a normal distribution for large values of l. As a guidance, we will use $k = e^{-1/2}$ in Eq. (7.6). Then we get

$$\sigma_l^2 = (\sigma_l^2)_{BU}\left(1 \pm \sqrt{\frac{2}{2l+1}}\right).$$

This formula becomes progressively inaccurate for small l. Specifically, for $l = 2$ this formula would imply the error at the level ± 0.6. However, a direct derivation of the error bars from Eq. (7.5) (and assuming $k = e^{-1/2}$) gives

$$\sigma_2^2 = (\sigma_2^2)_{BU}(1 + \sigma),$$

where σ lies between $+1.0$ and -0.4. Note the asymmetry of the error interval: the larger than $(\sigma_2^2)_{BU}$ values are more tolerable than the smaller ones.

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APPENDIX

The complex spherical harmonics $Y_{lm}(\theta, \varphi)$ are defined by the expression

$$Y_{lm}(\theta, \varphi) = \frac{1}{\sqrt{2}}\left(\frac{2l+1}{2\pi}\frac{(l-|m|)!}{(l+|m|)!}\right)^{1/2} P_{l|m|}(\cos\theta) e^{im\varphi}.$$

In this expression, $l \geq 0$ and $-l \leq m \leq l$. The functions $Y_{lm}(\theta, \varphi)$ satisfy the relationship $Y_{lm}^* = Y_{l,-m}$. On the other hand, the real spherical harmonics are defined by the equations

$$Y_{lm}^c(\theta, \varphi) = \left(\frac{2l+1}{2\pi}\frac{(l-m)!}{(l+m)!}\right)^{1/2} P_{lm}(\cos\theta)\cos m\varphi,$$

$$Y_{lm}^s(\theta, \varphi) = \left(\frac{2l+1}{2\pi}\frac{(l-m)!}{(l+m)!}\right)^{1/2} P_{lm}(\cos\theta)\sin m\varphi,$$

where $l \geq 0$ but $0 \leq m \leq l$. The indices c, s indicate the presence of $\cos m\varphi$ or $\sin m\varphi$, respectively. The link between the complex and real spherical harmonics is given by

$$Y_{lm}^c = \frac{1}{\sqrt{2}}(Y_{lm} + Y_{lm}^*), \quad m \geq 0,$$

$$Y_{lm}^s = \frac{1}{i\sqrt{2}}(Y_{lm} - Y_{lm}^*), \quad m \geq 0.$$

The scalar product of two functions $f(\theta, \varphi)$ and $g(\theta, \varphi)$ on the sphere is defined by

$$(f, g) = \int_0^{2\pi} d\varphi \int_0^\pi d\theta \, \sin\theta f^*(\theta, \varphi) g(\theta, \varphi).$$

Then, we have the properties

$$(Y_{lm}, Y_{l'm'}) = \delta_{ll'}\delta_{mm'}, \quad -l \leq m \leq l,$$

$$\left(\frac{Y_{l0}^c}{\sqrt{2}}, \frac{Y_{l'0}^c}{\sqrt{2}}\right) = \delta_{ll'},$$

$$(Y_{lm}^A, Y_{l'm'}^B) = \delta_{ll'}\delta_{mm'}\delta^{AB}, \quad m \geq 1, \quad A, B = c, s.$$

The functions $Y_{l0}^c/\sqrt{2}$ ($l \geq 0$), Y_{lm}^c ($l \geq 1$, $l \geq m \geq 1$), Y_{lm}^s ($l \geq 1$, $l \geq m \geq 1$) form a complete orthonormal basis.

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