

Rapid separable analysis of higher order correlators in large-scale structureJ. R. Fergusson,¹ D. M. Regan,^{1,2} and E. P. S. Shellard¹¹*Centre for Theoretical Cosmology, DAMTP, University of Cambridge, Cambridge, CB3 0WA, United Kingdom*²*Department of Physics and Astronomy, University of Sussex, Brighton, BN1 9QH, United Kingdom*

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We present an efficient separable approach to the estimation and reconstruction of the bispectrum and the trispectrum from observational (or simulated) large-scale structure data. This is developed from general cosmic microwave background (poly)spectra methods that exploit the fact that the bispectrum and trispectrum in the literature can be represented by a separable mode expansion that converges rapidly (with $n_{\max} = \mathcal{O}(30)$ terms). The underlying methodology can encompass a wide variety of modal types, including polynomials, trigonometric functions, wavelets, and bins. With an effective grid resolution l_{\max} (number of particles/grid points $N = l_{\max}^3$), we present a bispectrum estimator that requires only $\mathcal{O}(n_{\max} \times l_{\max}^3)$ operations, along with a corresponding method for direct bispectrum reconstruction. This method is extended to the trispectrum revealing an estimator that requires only $\mathcal{O}(n_{\max}^{4/3} \times l_{\max}^3)$ operations. The complexity in calculating the trispectrum in this method is now involved in the original decomposition and orthogonalization process that need only be performed once for each model. However, for nondiagonal trispectra these processes present little extra difficulty and may be performed in $\mathcal{O}(l_{\max}^4)$ operations. A discussion of how the methodology may be applied to the quadspectrum is also given. An efficient algorithm for the generation of arbitrary non-Gaussian initial conditions for use in N-body codes using this separable approach is described. This prescription allows for the production of non-Gaussian initial conditions for arbitrary bispectra and trispectra. A brief outline of the key issues involved in parameter estimation, particularly in the nonlinear regime, is also given.

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I. INTRODUCTION

In previous work [1–3] we developed and implemented a methodology for the efficient and general analysis of non-Gaussianity in the cosmic microwave sky. Our purpose here is to apply these separable mode methods to large-scale structure, making tractable a fast general analysis of all bispectra and trispectra, rather than the few special cases studied to date. Calculation of the three-point correlator or bispectrum $\langle \delta_{\mathbf{k}_1} \delta_{\mathbf{k}_2} \delta_{\mathbf{k}_3} \rangle$ using 3D large-scale structure data naively appears to require a computationally intensive l_{\max}^6 operation, or l_{\max}^9 for the trispectrum, where l_{\max} is the effective observational or simulated grid resolution (i.e. the volume sidelength L over the averaged galaxy or grid spacing Δx , giving a particle number $N \approx l_{\max}^3$). However, if—as in the cosmic microwave background (CMB)—predicted non-Gaussianity can be described by rapidly convergent and separable mode expansions, then there is a dramatic reduction to only $\mathcal{O}(n_{\max} \times l_{\max}^3)$ operations for estimating any bispectrum, where n_{\max} is the (small) number of modes required for an accurate representation ($n_{\max} \approx 30$ for WMAP analysis [2]). The relative impact on trispectrum estimation is even more dramatic, reducing again to $\sim \mathcal{O}(n_{\max}^{4/3} \times l_{\max}^3)$ operations. Direct reconstruction of the bispectrum today then allows for the decomposition into its constituent and independent shapes, including contributions directly from the primordial bispectrum, from next-to-leading order terms in nonlinear gravitational collapse, from the con-

volved primordial trispectrum, etc. These methods equally can be applied to generating simulation initial conditions with arbitrary given bispectrum and trispectrum, again using a simple separable mode algorithm requiring only $\mathcal{O}(n_{\max} \times l_{\max}^3)$ or $\mathcal{O}(n_{\max}^{4/3} \times l_{\max}^3)$ operations, respectively. It should be noted that, while an application of the methodology to real data sets such as the Sloan Digital Sky Survey (SDSS) [4] would necessitate an analysis of complications such as galaxy bias, redshift space distortions, etc., the methods described here may be most straightforwardly applied to simulated dark matter distributions as formed using N-body codes.

Our purpose here is not to review the many important contributions made to the study of higher order correlators in large-scale structure, for which there are some comprehensive recent reviews available [5,6]; however, we note that the field is well-motivated because non-Gaussianity is recognized as a critical test of the simplest standard inflationary scenario. Moreover, there are a growing number of alternative inflationary scenarios where deviations from non-Gaussianity can be large (see [7] for a review). The most stringent constraints on primordial non-Gaussianity so far have come from CMB bispectrum measurements (e.g. [2,8], see [5]) with relatively weak constraints coming from the large-scale structure galaxy bispectrum [9] due to complications in dealing with nonlinear evolution. While it appears to be possible also to derive competitive constraints using the abundance of rare objects or scale-dependent bias (e.g. [10]), these complementary

approaches generally assume a local-type non-Gaussianity (see the review [11]). With improving galaxy and other surveys covering a growing fraction of the sky, it is reasonable to expect measurements of higher order correlators from this three-dimensional data to provide the best and most comprehensive information about non-Gaussianity. These large-scale structure (poly)spectra should allow us to discriminate between different non-Gaussian shapes, notably between primordial and late-time sources, ultimately complementing CMB measurements and exceeding them in precision.

In this paper we present a method for quickly calculating the bispectrum from a given density perturbation in Sec. II. Next we show how to extend this analysis to the trispectrum in Sec. III. As any estimator would require non-Gaussian simulations for testing and error analysis, we present an approach in Sec. IV for including a general bispectrum and trispectrum in the initial conditions for N -body simulations. We then go on to show in Sec. V how a general estimator for constraining primordial non-Gaussianity can be constructed, when the bispectrum can be approximated using a simple ansatz, and in the completely general case. Finally we present our concluding remarks.

II. LARGE-SCALE STRUCTURE BISPECTRUM CALCULATION

A. General bispectrum estimator

Higher order correlators of the galaxy or matter density distribution can be expected to exhibit a low signal-to-noise ratio for individual combinations of wave numbers (as for multipoles in the CMB). A useful strategy for the comparison between observations and theoretical models (or simulated numerical models) is the use of an estimator that tests for consistency by summing over all multipoles using an optimal signal-to-noise weighting. The general estimator for the galaxy or density bispectrum, when searching for a given theoretical three-point correlator $\langle \delta_{\mathbf{k}_1} \delta_{\mathbf{k}_2} \delta_{\mathbf{k}_3} \rangle$, is

$$\begin{aligned} \mathcal{E} &= \int \frac{d^3 k_1}{(2\pi)^3} \frac{d^3 k_2}{(2\pi)^3} \frac{d^3 k_3}{(2\pi)^3} \langle \delta_{\mathbf{k}_1} \delta_{\mathbf{k}_2} \delta_{\mathbf{k}_3} \rangle \\ &\times [C^{-1}(\delta_{\mathbf{k}_1}^{\text{obs}})C^{-1}(\delta_{\mathbf{k}_2}^{\text{obs}})C^{-1}(\delta_{\mathbf{k}_3}^{\text{obs}}) \\ &- 3C^{-1}(\delta_{\mathbf{k}_1}^{\text{obs}} \delta_{\mathbf{k}_2}^{\text{obs}})C^{-1}(\delta_{\mathbf{k}_3}^{\text{obs}})], \end{aligned} \quad (1)$$

where $\delta_{\mathbf{k}}^{\text{obs}}$ represents a noisy measurement of the galaxy or density perturbation with signal plus noise covariance C given by

$$C^{-1}(\delta_{\mathbf{k}}^{\text{obs}}) = \int \frac{d^3 k'}{(2\pi)^3} \langle \delta_{\mathbf{k}} \delta_{\mathbf{k}'} \rangle^{-1} \delta_{\mathbf{k}'}^{\text{obs}}. \quad (2)$$

We will discuss the normalization necessary for parameter estimation in Sec. V. Here, we have added a linear term to the cubic estimator in order to account for inhomogeneous

effects from incomplete survey coverage (e.g. due to dust extinction), sampling bias, shot noise, and other known systematics, which together can substantially increase the experimental variance.

If we assume that the density field is statistically isotropic, as it is in most well-motivated theoretical models, then the bispectrum $B(k_1, k_2, k_3)$ is defined by

$$\langle \delta_{\mathbf{k}_1} \delta_{\mathbf{k}_2} \delta_{\mathbf{k}_3} \rangle = (2\pi)^3 \delta_D(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) B(k_1, k_2, k_3), \quad (3)$$

where $\delta_D(\mathbf{k})$ is the three-dimensional Dirac δ function enforcing a triangle condition on the wave vectors \mathbf{k}_i , for which it is sufficient to use only the wave numbers $k_i = |\mathbf{k}_i|$. For simplicity, let us suppose we are only in a mildly nonlinear regime with good observational coverage over a modest redshift range, so that we can make the approximation that the covariance matrix is nearly diagonal $C^{-1}(\delta_{\mathbf{k}}^{\text{obs}}) \approx \delta_{\mathbf{k}}^{\text{obs}}/P(k)$. With these replacements, the estimator (1) becomes

$$\begin{aligned} \mathcal{E} &= \int \frac{d^3 k_1}{(2\pi)^3} \frac{d^3 k_2}{(2\pi)^3} \frac{d^3 k_3}{(2\pi)^3} \\ &\times \frac{(2\pi)^3 \delta_D(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) B(k_1, k_2, k_3)}{P(k_1)P(k_2)P(k_3)} \\ &\times [\delta_{\mathbf{k}_1}^{\text{obs}} \delta_{\mathbf{k}_2}^{\text{obs}} \delta_{\mathbf{k}_3}^{\text{obs}} - 3\langle \delta_{\mathbf{k}_1}^{\text{sim}} \delta_{\mathbf{k}_2}^{\text{sim}} \rangle \delta_{\mathbf{k}_3}^{\text{obs}}], \end{aligned} \quad (4)$$

where $\delta_{\mathbf{k}}^{\text{sim}}$ represents simulated data with the known inhomogeneous systematic effects included, while we also assume that shot noise is incorporated in the power spectrum $P + N \rightarrow \tilde{P}$, along with incomplete sample coverage (though we will drop the tilde). We note that, although this galaxy estimator with a linear term (4) has not been given in this form explicitly before, the bispectrum scaling and signal-to-noise ratios here and in what follows are consistent with the pioneering discussions in Refs. [9,12] (see also the analogous CMB bispectrum estimator discussed in Ref. [13] and elsewhere). In any case, this large-scale structure bispectrum estimator (4) does not appear to be particularly useful because its brute force evaluation would require at least I_{max}^6 operations for a single measurement (after imposing the triangle condition). The problem is compounded by the many simulated realizations of the observational setup that are required to obtain an accurate linear term in (4). In fact, if the theoretical bispectrum $B(k_1, k_2, k_3)$ is computed numerically, then this is even more computationally intensive, since it requires many N -body simulations and bispectrum evaluations to achieve statistical precision.

Nevertheless, let us now suppose that we have a large set of simulated non-Gaussian realizations $\delta_{\mathbf{k}}^{\text{obs}}$ generated with the same theoretical bispectrum $B(k_1, k_2, k_3)$ [and the same power spectrum $P(k)$]. If we take the expectation value of the estimator (4) by summing over these realizations, then we find the average to be

$$\begin{aligned}
 \langle \mathcal{E} \rangle &= \int \frac{d^3 k_1}{(2\pi)^3} \frac{d^3 k_2}{(2\pi)^3} \frac{d^3 k_3}{(2\pi)^3} (2\pi)^6 \delta_D^2(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) \\
 &\quad \times \frac{B^2(k_1, k_2, k_3)}{P(k_1)P(k_2)P(k_3)} \\
 &= \frac{V}{8\pi^4} \int_{\mathcal{V}_B} dk_1 dk_2 dk_3 \frac{k_1 k_2 k_3 B^2(k_1, k_2, k_3)}{P(k_1)P(k_2)P(k_3)}, \quad (5)
 \end{aligned}$$

where \mathcal{V}_B is the tetrahedral region allowed by the triangle condition. The averaged estimator (5) is an important expression, so it is instructive for subsequent calculations to outline the explicit steps that take us between these two lines. First, the second Dirac δ function contributes only a volume factor $\delta(\mathbf{0}) = V/(2\pi)^3$. Second, we complete the angular integration by expanding the integral form of the remaining δ function in spherical Bessel functions and harmonics,

$$\delta_D(\mathbf{k}) = \frac{1}{(2\pi)^3} \int d^3 x e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (6)$$

$$e^{i\mathbf{k}\cdot\mathbf{x}} = 4\pi \sum_{lm} i^l j_l(kx) Y_{lm}(\hat{\mathbf{k}}) Y_{lm}^*(\hat{\mathbf{x}}). \quad (7)$$

Third, each $\hat{\mathbf{k}}_i$ integration involves just a single spherical harmonic and contributes a factor $2\sqrt{\pi}\delta_{l0}\delta_{m0}$, so we end up with only a constant term from the Gaunt integral $G_{000}^{000} = 1/2\sqrt{\pi}$ [i.e. the integration over the three remaining $Y_{lm}(\mathbf{x})$]. Finally, the last integral over the three Bessel functions $j_0(k_1 x)j_0(k_2 x)j_0(k_3 x)$ yields $\pi/(4k_1 k_2 k_3)$ and simultaneously imposes a triangle condition on k_1, k_2, k_3 that we denote by the restricted domain of integration \mathcal{V}_B .

The estimator average (5) leads naturally to a weighted cross correlator or inner product between two different bispectra $B_i(k_1, k_2, k_3)$ and $B_j(k_1, k_2, k_3)$, that is,

$$\mathcal{C}(B_i, B_j) = \frac{\langle B_i, B_j \rangle}{\sqrt{\langle B_i, B_i \rangle \langle B_j, B_j \rangle}}, \quad (8)$$

where

$$\begin{aligned}
 \langle B_i, B_j \rangle &\equiv \frac{V}{8\pi^4} \int_{\mathcal{V}_B} dk_1 dk_2 dk_3 \\
 &\quad \times \frac{k_1 k_2 k_3 B_i(k_1, k_2, k_3) B_j(k_1, k_2, k_3)}{P(k_1)P(k_2)P(k_3)}. \quad (9)
 \end{aligned}$$

The estimator (4) is thus proportional to the Fisher matrix of the bispectrum, $F_{ij} = \mathcal{C}(B_i, B_j)/6\pi$ (see Ref. [9]).

The fiducial model for non-Gaussianity is the $f_{\text{NL}} = 1$ local model. For the CMB, where the final CMB bispectrum $B_{l_1 l_2 l_3}$ is linearly related to the primordial bispectrum $B_0(k_1, k_2, k_3)$, it is straightforward to define a normalization that yields a universal F_{NL} , representing the total integrated bispectrum for a particular theoretical model relative to that from the $f_{\text{NL}} = 1$ local model (see Ref. [2]). However, with bispectrum contributions from

gravitational collapse and nonlinear bias arising even with Gaussian initial conditions, a universal normalization is a more subtle issue that we will defer to Sec. V.

Finally, we point out that the bispectrum estimator (1) can be applied in any three-dimensional physical context where we wish to test for a particular non-Gaussian model. It can be applied at primordial times, with potential fluctuations (i.e. replacing $\delta_{\mathbf{k}} \rightarrow \Phi_{\mathbf{k}}$), in the late-time linear regime on large scales where the density perturbation is simply related by a transfer function $\delta_{\mathbf{k}} = T(k, z)\Phi_{\mathbf{k}}$ (as in the CMB), in the mildly nonlinear regime where next-to-leading order corrections are known, or deep in the nonlinear regime on small scales where we must rely on N -body and hydrodynamic simulations. However, for a useful implementation, we must rewrite (1) in a separable form.

B. Separable mode expansions and bispectrum reconstruction

The averaged estimator (5) gives a natural measure for defining separable mode functions

$$\begin{aligned}
 Q_n(k_1, k_2, k_3) &= \frac{1}{6} [q_r(k_1)q_s(k_2)q_t(k_3) + 5 \text{ perms}] \\
 &\equiv q_{\{r}(k_1)q_s(k_2)q_{\{t}(k_3), \quad (10)
 \end{aligned}$$

which we can use to decompose an arbitrary bispectrum (here, for convenience, the label n , denotes a linear ordering of the 3D products $n \leftrightarrow \{rst\}$). We choose to expand the bispectrum $B(k_1, k_2, k_3)$ in its noise-weighted form (see Ref. [1]),

$$\frac{B(k_1, k_2, k_3)v(k_1)v(k_2)v(k_3)}{\sqrt{P(k_1)P(k_2)P(k_3)}} = \sum \alpha_n^Q Q_n(k_1, k_2, k_3), \quad (11)$$

where we have used the freedom to introduce a separable modification to the weight function $w(k_1, k_2, k_3) = k_1 k_2 k_3 / v^2(k_1)v^2(k_2)v^2(k_3)$ in (5). Series convergence usually can be improved with scale invariance, suggesting the choice $v(k) = \sqrt{k}$. The exact form of the one-dimensional basis functions $q_r(k)$ is not important, except that they should be bounded and well behaved on the bispectrum domain \mathcal{V}_B . Some $q_r(k)$ examples that are orthogonal on \mathcal{V}_B were given explicitly in Ref. [1]. In particular, these are analogues of Legendre polynomials $P_n(k)$. However, it is important to note that the modes employed in these separable products can be polynomials, trigonometric functions, wavelets, or bins. The choice depends on utility and the modes can be tailored for specific classes of theoretical models under investigation.

The product functions Q_n are independent but not necessarily orthogonal, so it is convenient from these to generate an orthonormal set of mode functions \mathcal{R}_n , such that, $\langle \mathcal{R}_n, \mathcal{R}_m \rangle = \delta_{nm}$ (achieved using Gram-Schmidt orthogonalization with the inner product (8) or other methods such

as Cholesky decomposition). We distinguish the expansion coefficients α_n^Q and α_n^R by the superscripts for the separable “ Q ” and orthonormal “ R ” modes, respectively; these are related to each other by a rotation involving the matrices $\langle Q_m, Q_n \rangle$ and $\langle Q_m, R_n \rangle$ (see Ref. [1]). The orthonormal modes R_n are convenient for finding the expansion coefficients of an arbitrary bispectrum $B(k_1, k_2, k_3)$ from the inner product (8) through $\alpha_n^R = \langle B, R_n \rangle$ that are then rotated to the more explicitly separable form α_n^Q . Of course, there is some computational effort $\mathcal{O}(n_{\max} \times l_{\max}^3)$ to achieve this orthogonalization and decomposition, but it is a modest initial computation that creates a framework for the subsequent data and error analysis.

Now consider the effect of substituting the expansion (11) into the bispectrum estimator (4). It collapses to the simple summation

$$\mathcal{E} = \sum_n \alpha_n^Q \beta_n^Q, \quad (12)$$

where the observed β_n^Q coefficients are defined by

$$\beta_n^Q = \int d^3x M_r(\mathbf{x}) M_s(\mathbf{x}) M_t(\mathbf{x}), \quad (13)$$

with $M_r(\mathbf{x})$ the observed density perturbation multiplied in Fourier space with the mode functions $q_r(k)$, that is,

$$M_p(\mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} \frac{\delta_{\mathbf{k}}^{\text{obs}} q_r(k) e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{kP(k)}}. \quad (14)$$

Including the linear term in (4) to account for systematic inhomogeneous effects, we have

$$\beta_n^Q = \int d^3x (M_r(\mathbf{x}) M_s(\mathbf{x}) M_t(\mathbf{x}) - [\langle M_r(\mathbf{x}) M_s(\mathbf{x}) \rangle M_t(\mathbf{x}) + 2 \text{ perms}]). \quad (15)$$

Furthermore, rotating to the orthonormal frame with R_n , it is straightforward to demonstrate that the averaged observed coefficient will be $\alpha_n^R = \langle \beta_n^R \rangle$, given a set of realizations with the bispectrum $B(k_1, k_2, k_3)$ in (11). Thus we can directly reconstruct the bispectrum from a single realization (with a sufficient single-to-noise ratio) using

$$B(k_1, k_2, k_3) = \frac{\sqrt{P(k_1)P(k_2)P(k_3)}}{\sqrt{k_1 k_2 k_3}} \sum_n \beta_n^R R_n(k_1, k_2, k_3). \quad (16)$$

This reconstruction yields the full bispectrum shape in a model-independent manner. One can also consider a model-independent measure of the total integrated non-Gaussian signal, using Parseval’s theorem in the orthonormal frame (see Ref. [2] for a discussion of the quantity $\bar{F}_{\text{NL}}^2 = \sum_n \beta_n^R{}^2$). However, the bispectrum estimator (12)

provides an immediate means to determine the significance of an observation of a particular type of non-Gaussianity with specific coefficients α_n^Q , e.g. by comparison with the β_n^R extracted from Gaussian simulations. We note that an initial implementation of the bispectrum reconstruction method (16) indicates its efficacy in recovering local non-Gaussianity.

We emphasize that the bispectrum reconstruction (16) provides an extremely efficient method for calculating the bispectrum from any given density field $\delta_{\mathbf{k}}$ with optimum noise weighting. Moreover, these separable mode expansion methods have been thoroughly tested in a CMB context [2]. In essence, the l_{\max}^6 operations required with the original estimator (or for a direct bispectrum calculation such as that described in Ref. [12]) have been reduced to a series of l_{\max}^3 integrations given by (14). Of course, the number of mode coefficients depends on the rate of convergence of the expansion (11) that is usually remarkably rapid. For the CMB, a comprehensive survey of most theoretical bispectra in the literature required only 30 eigenmodes for an accurate description at WMAP resolution [2]. Even for a separable bispectrum in the linear regime (i.e. a terminating sum), we shall explain the advantages of using the well-behaved mode expansion (11). The form of the next-to-leading order corrections for large-scale structure show no obvious pathologies that would alter this convergence significantly in the mildly nonlinear regime (see later), and substantial efficiencies will remain even in highly nonlinear contexts. This reconstruction approach (16) is ideally suited for N -body simulations where the bispectrum can be predicted at high precision by efficiently extracting it from multiple realizations using both Gaussian and non-Gaussian initial conditions (see later). In an observational context, sparse sampling or poor survey strategies could reduce the effectiveness of the estimator (4) in Fourier space, so care must be taken in a large-scale structure survey design to ensure good coverage so that higher order correlator measurements exploit these efficiencies.

III. EXTENSION TO THE TRISPECTRUM AND BEYOND

A. General trispectrum estimator

In [3] we discussed general CMB estimators for the trispectrum, where the decomposition of a planar trispectrum (nondiagonal or single diagonal) is sufficient to study the majority of cases described in the literature. While this projection depends explicitly on five parameters (or four in the nondiagonal case), in order to study other probes of non-Gaussianity, particularly for nonlinear large-scale structure, it may be necessary to consider the general trispectrum depending on the full six parameters. This is further motivated by the study of the galaxy bispectrum, which may contain an enhanced contribution due to the

trispectrum (see, e.g., Ref. [14]). Clearly, then, we should also include a nonzero trispectrum to obtain non-Gaussian initial conditions suitable for a general bispectrum analysis using N -body codes.

The form of the general trispectrum estimator, for the connected part of a given four-point correlator $\langle \delta_{\mathbf{k}_1} \delta_{\mathbf{k}_2} \delta_{\mathbf{k}_3} \delta_{\mathbf{k}_4} \rangle_c$, is directly analogous to that presented already in Ref. [3] for the CMB:

$$\mathcal{E} = \frac{\int \frac{d^3 \mathbf{k}_1}{(2\pi)^3} \frac{d^3 \mathbf{k}_2}{(2\pi)^3} \frac{d^3 \mathbf{k}_3}{(2\pi)^3} \frac{d^3 \mathbf{k}_4}{(2\pi)^3} (\delta_{\mathbf{k}_1}^{\text{obs}} \delta_{\mathbf{k}_2}^{\text{obs}} \delta_{\mathbf{k}_3}^{\text{obs}} \delta_{\mathbf{k}_4}^{\text{obs}} - 6 \langle \delta_{\mathbf{k}_1}^{\text{sim}} \delta_{\mathbf{k}_2}^{\text{sim}} \rangle \delta_{\mathbf{k}_3}^{\text{obs}} \delta_{\mathbf{k}_4}^{\text{obs}} + 3 \langle \delta_{\mathbf{k}_1}^{\text{sim}} \delta_{\mathbf{k}_2}^{\text{sim}} \rangle \langle \delta_{\mathbf{k}_3}^{\text{sim}} \delta_{\mathbf{k}_4}^{\text{sim}} \rangle) \langle \delta_{\mathbf{k}_1} \delta_{\mathbf{k}_2} \delta_{\mathbf{k}_3} \delta_{\mathbf{k}_4} \rangle_c}{P(k_1)P(k_2)P(k_3)P(k_4)}, \quad (17)$$

where the notation $\langle \cdot \cdot \cdot \rangle_c$ denotes the connected component of the correlator. Note that this formula includes the quadratic term necessary to generalize to the case of incomplete sample coverage and inhomogeneous noise in a similar fashion to the CMB trispectrum estimator [see the discussion after (4)]. We omit the covariance-weighted version of the expression that is obvious from a comparison with (1). Imposing the δ function appears to leave an intractable l_{max}^9 operation for a full trispectrum estimator

evaluation, but, as with the bispectrum, this can be reduced dramatically using a separable approach.

Assuming statistical isotropy, we can choose to parametrize the trispectrum using the lengths of four of its sides and two of its diagonals. In particular, we can exhibit these dependencies explicitly by representing the δ function imposing the quadrilateral condition, as a product of triangle conditions using the diagonals:

$$\langle \delta_{\mathbf{k}_1} \delta_{\mathbf{k}_2} \delta_{\mathbf{k}_3} \delta_{\mathbf{k}_4} \rangle_c = (2\pi)^3 \delta_D(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4) T(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) \quad (18)$$

$$= (2\pi)^3 \int d^3 \mathbf{K}_1 d^3 \mathbf{K}_2 \delta_D(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{K}_1) \delta_D(\mathbf{k}_3 + \mathbf{k}_4 + \mathbf{K}_1) \delta_D(\mathbf{k}_1 + \mathbf{k}_4 - \mathbf{K}_2) T(k_1, k_2, k_3, k_4, K_1, K_2). \quad (19)$$

The decomposition of the trispectrum $T(k_1, k_2, k_3, k_4, K_1, K_2)$ is similar to that described in [3], but in which the trispectrum is assumed to depend on the first five parameters only. In the interest of completeness we evaluate a suitable weight function necessary for evaluation of

the more general decomposition from the expectation value of the estimator (17). Similarly to the case of the bispectrum (5), the expectation value for the estimator is found to take the following simple form:

$$\langle \mathcal{E} \rangle = \frac{V}{(2\pi)^3} \int \frac{d^3 \mathbf{k}_1}{(2\pi)^3} \frac{d^3 \mathbf{k}_2}{(2\pi)^3} \frac{d^3 \mathbf{k}_3}{(2\pi)^3} \frac{d^3 \mathbf{k}_4}{(2\pi)^3} \frac{(2\pi)^6 \delta_D(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4) T^2(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4)}{P(k_1)P(k_2)P(k_3)P(k_4)} \quad (20)$$

$$= \frac{V}{(2\pi)^3} \frac{1}{2\pi^4} \int_{\mathcal{V}_T} dk_1 dk_2 dk_3 dk_4 dK_1 dK_2 \frac{k_1 k_2 k_3 k_4 K_1 K_2}{\sqrt{g_1}} \frac{T^2(k_1, k_2, k_3, k_4, K_1, K_2)}{P(k_1)P(k_2)P(k_3)P(k_4)}, \quad (21)$$

where the function g_1 is given by the expression

$$g_1 = K_1^2 K_2^2 \left(\sum_i k_i^2 - K_1^2 - K_2^2 \right) - K_1^2 \kappa_{23} \kappa_{14} + K_2^2 \kappa_{12} \kappa_{34} - (k_1^2 k_3^2 - k_2^2 k_4^2) (\kappa_{12} + \kappa_{34}), \quad (22)$$

and we denote $\kappa_{ij} = k_i^2 - k_j^2$. For clarity, we omit the many calculational steps required in the derivation and present them in the Appendix. Here, we note that \mathcal{V}_T is the region allowed by the quadrilateral condition that is described in some detail in [3], noting the different ranges for the wave numbers $k_i < k_{\text{max}}$ and diagonals $K_i < 2k_{\text{max}}$. By considering two different trispectra $T^2 \rightarrow T_i T_j$ in the estimator average (20), we can use this expression to define

a noise-weighted cross correlator and inner product [or Fisher matrix, see the discussion after (5)].

B. Separable mode expansions and the trispectrum estimator

Using the weight (20), a simple extension of the argument outlined in [3] to include two diagonals instead of one, we find a similar eigenmode to the case of the

bispectrum. In particular, we could expand the trispectrum as $\omega T(k_1, k_2, k_3, k_4, K_1, K_2) = \sum_n \alpha_n \mathcal{Q}_n(k_1, k_2, k_3, k_4, K_1, K_2)$ where $\mathcal{Q}_n = q_{\{r}(k_1)q_s(k_2)q_t(k_3)q_u\}(k_4)r_v(K_1)r_w(K_2)$, n represents $\{rstuvw\}$ ¹ and ω , here and subsequently, is shorthand for an appropriate separable weighting. As we will see in the estimator below, however, it is simpler to achieve a separable form by parametrizing our bispectrum using angles rather than diagonals. To achieve this, we may make a coordinate transformation from $(K_1, K_2) \rightarrow (\mu = \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2, \nu = \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_4)$ where we use $K_1 = \sqrt{k_1^2 + k_2^2 + 2k_1k_2\mu}$ and $K_2 = \sqrt{k_1^2 + k_4^2 + 2k_1k_4\nu}$. The Jacobian of this transformation is $k_1^2k_2k_4/(K_1K_2)$. Thus (20) becomes

$$\langle \mathcal{E} \rangle = \frac{V}{(2\pi)^3} \frac{1}{2\pi^4} \int_{\mathcal{V}_T} dk_1 dk_2 dk_3 dk_4 d\mu d\nu \times \frac{k_1^3 k_2^3 k_3^3 k_4^3}{\sqrt{g_1}} \frac{T^2(k_1, k_2, k_3, k_4, \mu, \nu)}{P(k_1)P(k_2)P(k_3)P(k_4)}, \quad (23)$$

where g_1 is given by Eq. (22) but now must be expressed in terms of μ, ν . We may use this weight to form an eigenmode expansion of the trispectrum where we use Legendre

polynomials to describe the angular part. Explicitly we may expand the trispectrum in a noise-weighted form as

$$\frac{v(k_1)v(k_2)v(k_3)v(k_4)}{\sqrt{P(k_1)P(k_2)P(k_3)P(k_4)}} T(k_1, k_2, k_3, k_4, \mu, \nu) = \sum_{n_{l_1 l_2}} \alpha_{n_{l_1 l_2}} \mathcal{Q}_n(k_1, k_2, k_3, k_4) P_{l_1}(\mu) P_{l_2}(\nu), \quad (24)$$

where $n = \{r, s, t, u\}$ and $\mathcal{Q}_n(k_1, k_2, k_3, k_4) = q_{\{r}(k_1)q_s(k_2)q_t(k_3)q_u\}(k_4)$ in an analogous manner to Eq. (10). Scale invariance suggests the choice $v(k) = k^{3/4}$. In order to make this expression separable in terms of the vectors \mathbf{k}_i , we note the following expansion of the Legendre polynomials

$$P_l(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2) = \frac{4\pi}{2l+1} \sum_{m=-l}^l Y_{lm}(\hat{\mathbf{k}}_1) Y_{lm}^*(\hat{\mathbf{k}}_2). \quad (25)$$

Using Eqs. (6) and (7) we can now write the estimator as expressed in (17) in the form

$$\mathcal{E} = \sum_{n_{l_1 l_2}} \bar{\alpha}_{n_{l_1 l_2}}^{\mathcal{Q}} \bar{\beta}_{n_{l_1 l_2}}^{\mathcal{Q}}, \quad (26)$$

where the extracted trispectrum coefficients are given by

$$\bar{\beta}_{n_{l_1 l_2}}^{\mathcal{Q}} = \frac{(4\pi)^2}{(2l_1+1)(2l_2+1)} \sum_{m_1 m_2} \int d^3 \mathbf{x} [M_{r_{l_1 l_2}}^{m_1 m_2}(\mathbf{x}) M_{s_{l_1}^*}^{m_1^*}(\mathbf{x}) M_t(\mathbf{x}) M_{u_{l_2}^*}^{m_2^*}(\mathbf{x}) - (M_{r_{l_1 l_2}}^{m_1 m_2}(\mathbf{x}) M_{s_{l_1}^*}^{m_1^*}(\mathbf{x}) \langle M_t(\mathbf{x}) M_{u_{l_2}^*}^{m_2^*}(\mathbf{x}) \rangle + 5 \text{ perms}) + (\langle M_{r_{l_1 l_2}}^{m_1 m_2}(\mathbf{x}) M_{s_{l_1}^*}^{m_1^*}(\mathbf{x}) \rangle \langle M_t(\mathbf{x}) M_{u_{l_2}^*}^{m_2^*}(\mathbf{x}) \rangle + 2 \text{ perms})], \quad (27)$$

where the permutations are with respect to the indices $\{r, s, t, u\}$. In the above we define the filtered density perturbations M_{\dots} by

$$M_{r_{l_1 l_2}}^{m_1 m_2}(\mathbf{x}) = \int \frac{d^3 \mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{x}} \frac{q_r(k) \delta_{\mathbf{k}}^{\text{obs}}}{\sqrt{P(k)} k^{3/4}} Y_{l_1 m_1}(\hat{\mathbf{k}}) Y_{l_2 m_2}(\hat{\mathbf{k}}), \quad M_{s_{l_1}^*}^{m_1^*}(\mathbf{x}) = \int \frac{d^3 \mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{x}} \frac{q_s(k) \delta_{\mathbf{k}}^{\text{obs}}}{\sqrt{P(k)} k^{3/4}} Y_{l_1 m_1}^*(\hat{\mathbf{k}}), \quad (28)$$

$$M_t(\mathbf{x}) = \int \frac{d^3 \mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{x}} \frac{q_t(k) \delta_{\mathbf{k}}^{\text{obs}}}{\sqrt{P(k)} k^{3/4}},$$

with a $*$ denoting a filtered map using Y_{lm}^* .

The algorithm (26) provides a highly efficient method for estimating any trispectrum from a given density field. It requires only $\mathcal{O}(n_{\text{max}}^{4/3} \times l_{\text{max}}^3)$ operations, which makes feasible the intractable naive brute force calculation requiring $\mathcal{O}(l_{\text{max}}^9)$ operations. In making this rough numerical estimate, we assume that the number of modes in each of the six dimensions is equal (and small), while noting that we have to perform a double summation for the two angle parameters μ, ν over the indices l_1, m_1, l_2, m_2 .

As for the bispectrum, it is possible from the separable $\bar{\mathcal{Q}}_{n_{l_1 l_2}}$ modes to create a set of orthonormal $\bar{\mathcal{R}}_{n_{l_1 l_2}}$ modes

using the inner product (23). Like the original decomposition of a theoretical trispectrum (24), orthogonalization is a computationally intensive task requiring up to $\mathcal{O}(l_{\text{max}}^6)$ operations. However, it need only be performed once at the outset to set up the calculation framework, with the resulting rotation matrices being available for all the repetitive subsequent analysis ($\sim l_{\text{max}}^3$ operations). We can realistically envisage, then, reconstructing the complete trispectrum directly from the observational data using the rotated $\bar{\beta}_{n_{l_1 l_2}}^{\mathcal{Q}}$ coefficients [as in (16)]. It is interesting to note that almost all theoretical trispectra presented to date in the literature are ‘‘planar,’’ that is, either depending on only one diagonal or none. We treat the latter special case below, but we leave the simplifications arising from the single diagonal case for discussion elsewhere [15].

¹The diagonals and the wave numbers are described by different eigenmodes due to their differing range, i.e. $k_i < k_{\text{max}}$ while $K_i < 2k_{\text{max}}$.

C. Nondiagonal trispectrum and quadspectrum estimation

In the case that the trispectrum is independent of the diagonals K_1, K_2 (or angles μ, ν) we get a simpler expression for the averaged estimator (17):

$$\langle \mathcal{E} \rangle = \frac{V}{(2\pi)^6} \int_{\mathcal{V}_T} dk_1 dk_2 dk_3 dk_4 k_1 k_2 k_3 k_4 \left(\sum_i k_i - |\tilde{k}_{34}| - |\tilde{k}_{24}| - |\tilde{k}_{23}| \right) \frac{T^2(k_1, k_2, k_3, k_4)}{P(k_1)P(k_2)P(k_3)P(k_4)}, \quad (29)$$

where $\tilde{k}_{34} = k_1 + k_2 - k_3 - k_4$, etc. We may use the weighting this suggests to decompose the trispectrum into the form $\omega T = \sum_n \alpha_n Q_n$ where $Q_n = q_{\{r,s,t,u\}}$. The estimator is simpler to calculate since there are no cross terms between integrals. We find the extracted observational coefficients simplify to

$$\beta_n = \int d^3 \mathbf{x} [M_r(\mathbf{x}) M_s(\mathbf{x}) M_t(\mathbf{x}) M_u(\mathbf{x}) - (M_r(\mathbf{x}) M_s(\mathbf{x}) \langle M_t(\mathbf{x}) M_u(\mathbf{x}) \rangle + 5 \text{ perms}) + (\langle M_r(\mathbf{x}) M_s(\mathbf{x}) \rangle \langle M_t(\mathbf{x}) M_u(\mathbf{x}) \rangle + 2 \text{ perms})], \quad (30)$$

where M_i was defined in (28). Here, we see that the trispectrum estimation scales once again as only $\mathcal{O}(n_{\max} \times l_{\max}^3)$ operations. The extraction of expansion coefficients $\tilde{\alpha}^Q$ from a given nonseparable theoretical trispectrum appears to require up to l_{\max}^4 operations, but it is a one-off calculation amenable to many shortcuts. A practical implementation reveals that nondiagonal trispectra given in the literature require only $n_{\max} \approx \mathcal{O}(10)$ modes for accurate representation. As an example, even the pathological local model with diverging squeezed states requires only $n_{\max} = 20$ for the expansion (24) to achieve a 95% correlation with the primordial shape. It is clear that there is no inherent impediment to direct estimation and evaluation of trispectra from survey data of adequate quality.

This separable methodology can be applied to correlators beyond the trispectrum, such as the quadspectrum $\tilde{Q}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4, \mathbf{k}_5)$ defined from

$$\langle \delta_{\mathbf{k}_1} \delta_{\mathbf{k}_2} \delta_{\mathbf{k}_3} \delta_{\mathbf{k}_4} \delta_{\mathbf{k}_5} \rangle = (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4 + \mathbf{k}_5) \times \tilde{Q}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4, \mathbf{k}_5). \quad (31)$$

For simplicity, however, we restrict attention here to quadspectra that are nondiagonal, depending only on the wave numbers k_1, \dots, k_5 , that is, $\tilde{Q}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4, \mathbf{k}_5) = \tilde{Q}(k_1, k_2, k_3, k_4, k_5)$. The expectation value of the quad-spectrum estimator is then given by

$$\begin{aligned} \langle \mathcal{E} \rangle &= \frac{V}{(2\pi)^3} \int \left(\prod_{i=1}^5 \frac{d^3 \mathbf{k}_i}{(2\pi)^3} \right) \\ &\times \frac{(2\pi)^6 \delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4 + \mathbf{k}_5) \tilde{Q}^2(k_1, k_2, k_3, k_4, k_5)}{P(k_1)P(k_2)P(k_3)P(k_4)P(k_5)} \\ &= \frac{V}{(2\pi^3)^3} \int dk_1 dk_2 dk_3 dk_4 dk_5 (k_1 k_2 k_3 k_4 k_5)^2 \\ &\times \left(\int dx x^2 j_0(k_1 x) j_0(k_2 x) j_0(k_3 x) j_0(k_4 x) j_0(k_5 x) \right) \\ &\times \frac{\tilde{Q}^2(k_1, k_2, k_3, k_4, k_5)}{P(k_1)P(k_2)P(k_3)P(k_4)P(k_5)}, \quad (32) \end{aligned}$$

where the integral over the five spherical Bessel functions serves also to define the allowed quadspectrum domain \mathcal{V}_Q . The expression (32) may be used to derive a weight to decompose the quadspectrum in the form $[\prod_{i=1}^5 v(k_i) / \sqrt{P(k_i)}] \tilde{Q}(k_1, k_2, k_3, k_4, k_5) = \sum_n \alpha_n Q_n(k_1, k_2, k_3, k_4, k_5)$ where $n \leftrightarrow \{r, s, t, u, v\}$ and $Q_n(k_1, k_2, k_3, k_4, k_5) = q_{\{r\}}(k_1) q_{\{s\}}(k_2) q_{\{t\}}(k_3) q_{\{u\}}(k_4) q_{\{v\}}(k_5)$, and where imposing scale invariance sets $v(k) = k^{9/10}$. The resulting separable estimator is directly analogous to that for the nondiagonal trispectrum (30), but for brevity we will only discuss initial conditions with a nontrivial quadspectrum.

IV. EFFICIENT GENERATION OF ARBITRARY NON-GAUSSIAN INITIAL CONDITIONS

The generation of non-Gaussian initial conditions for N-body simulations with a given primordial bispectrum has been achieved to date only for bispectra that have a simple separable form (see, e.g., [16–19]). For N-body codes to efficiently produce non-Gaussian initial conditions for an arbitrary nonseparable bispectrum, a well-behaved separable mode decomposition will be required, as achieved for CMB map simulations in Ref. [1]. However, we can do even better by simulating initial data given both an arbitrary bispectrum and trispectrum, as shown for the CMB in [3]. As we have discussed already, this is of particular interest for measurements of the large-scale structure bispectrum, because of nonlinear contributions expected from the trispectrum. We describe the non-Gaussian primordial potential perturbation as

$$\Phi = \Phi^G + \frac{1}{2} F_{\text{NL}} \Phi^B + \frac{1}{6} G_{\text{NL}} \Phi^T, \quad (33)$$

where Φ^G is a Gaussian random field with the required power spectrum $P(k)$. It should be noted that this definition introduces two trispectrum terms of the form $\langle \Phi^T \Phi^G \Phi^G \Phi^G \rangle$ and $\langle \Phi^B \Phi^B \Phi^G \Phi^G \rangle$ (similar to the local trispectrum terms with coefficients g_{NL} and τ_{NL} , respectively). Therefore, it may be desirable to cancel this extra contribution. This issue will be addressed at the end of the section. Following Ref. [1] for the primordial bispectrum $B(k_1, k_2, k_3)$ with separable expansion

$$\begin{aligned} & \frac{B(k, k', k'')}{P(k')P(k'') + P(k)P(k') + P(k)P(k'')} \\ &= \sum_n \alpha_n^Q Q_n(k, k', k''), \end{aligned} \quad (34)$$

the bispectrum contribution to the primordial perturbation Φ becomes simply

$$\begin{aligned} \Phi^B(\mathbf{k}) &= \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \frac{d^3\mathbf{k}''}{(2\pi)^3} \\ &\times \frac{(2\pi)^3 \delta(\mathbf{k} + \mathbf{k}' + \mathbf{k}'') B(k, k', k'') \Phi^G(\mathbf{k}') \Phi^G(\mathbf{k}'')}{P(k')P(k'') + P(k)P(k') + P(k)P(k'')} \end{aligned} \quad (35)$$

$$= \sum_n \alpha_n q_r(k) \int d^3\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}} M_s(\mathbf{x}) M_{t_j}(\mathbf{x}), \quad (36)$$

where the filtered density perturbations $M_s(\mathbf{x})$ are now defined by

$$M_s(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \Phi^G(\mathbf{k}) q_s(k) e^{i\mathbf{k}\cdot\mathbf{x}}. \quad (37)$$

We note that the modal bispectrum algorithm in Ref. [1] used here is a generalization of the separable CMB bispectrum simulation method presented in Ref. [20]. Here, in 3D, the intermediate expression [(35) was first presented in

convolved form; see (49) below] in Refs. [19,21]. It should be noted that, with this prescription, the definition agrees identically with the expansion $\Phi = \Phi^G + F_{\text{NL}} \Phi^G * \Phi^G$ in the case of the local model. Of course, we normalize $B(k_1, k_2, k_3)$ such that it has $F_{\text{NL}} = 1$. Like the estimator, this requires only $\mathcal{O}(n_{\text{max}} \times l_{\text{max}}^3)$ operations for every realization of new initial conditions, as opposed to a brute force approach that requires l_{max}^6 . Note also that once the n_{max} filtered density perturbations $\int d^3\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}} M_s(\mathbf{x}) M_t(\mathbf{x})$ have been obtained for a given Φ^G , they can be applied to an arbitrary number of differently shaped bispectra represented by α_n^Q s.

We can similarly find a relatively simple and highly efficient expression to compute initial conditions for the trispectrum Φ^T . Following [3], the primordial trispectrum $T(k_1, k_2, k_3, k_4, \mu, \nu)$ is represented and expanded using wave number $q_r(k)$ and angle $P_u(\mu)$ modes in a similar fashion to Eq. (24),

$$\begin{aligned} & \frac{T(k_1, k_2, k_3, k_4, \mu, \nu)}{P(k_1)P(k_2)P(k_3)P(k_4) + 3 \text{ perms}} \\ &= \sum_{nl_1l_2} \alpha_{nl_1l_2} Q_n(k_1, k_2, k_3, k_4) P_{l_1}(\mu) P_{l_2}(\nu). \end{aligned} \quad (38)$$

The trispectrum contribution to Φ then becomes

$$\Phi^T(\mathbf{k}) = \int \frac{d^3\mathbf{k}' d^3\mathbf{k}'' d^3\mathbf{k}'''}{(2\pi)^6} \frac{\delta(\mathbf{k} + \mathbf{k}' + \mathbf{k}'' + \mathbf{k}''') T(\mathbf{k}, \mathbf{k}', \mathbf{k}'', \mathbf{k}''') \Phi^G(\mathbf{k}') \Phi^G(\mathbf{k}'') \Phi^G(\mathbf{k}''')}{P(k')P(k'')P(k''') + 3 \text{ perms}} \quad (39)$$

$$= \sum_{nl_1l_2nl_1l_2} \tilde{\alpha}_{nl_1l_2}^Q \frac{(4\pi)^2}{(2l_1 + 1)(2l_2 + 1)} \sum_{m_1m_2} Y_{l_1m_1}(\hat{\mathbf{k}}) Y_{l_2m_2}(\hat{\mathbf{k}}) q_r(k) \int d^3\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}} M_{sl_1}^{m_1*}(\mathbf{x}) M_t(\mathbf{x}) M_{ul_2}^{m_2*}(\mathbf{x}), \quad (40)$$

where the filtered density perturbations $M_{sl_1}^{m_1*}$ and M_t are now given by

$$\begin{aligned} M_{sl_1}^{m_1*}(\mathbf{x}) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} q_s(k) \Phi^G(\mathbf{k}) Y_{l_1m_1}^*(\hat{\mathbf{k}}), \\ M_t(\mathbf{x}) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} q_t(k) \Phi^G(\mathbf{k}). \end{aligned} \quad (41)$$

For the particular case that the trispectrum is independent of the angles μ, ν (or diagonals K_1, K_2) the decomposition is somewhat simpler:

$$\Phi^T(\mathbf{k}) = \sum_{nn} \tilde{\alpha}_n^Q q_r(k) \int d^3\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}} M_s(\mathbf{x}) M_t(\mathbf{x}) M_u(\mathbf{x}). \quad (42)$$

This applies to many cases in the literature, including constant, local, and equilateral models. This simplification

will also apply to initial conditions with nondiagonal quadspectra. The expression for quadspectrum perturbation $\Phi^{\tilde{Q}}$ is very similar to the expressions above with

$$\Phi^{\tilde{Q}} = \sum_n \tilde{\alpha}_n^Q q_r(k) \int d^3\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}} M_s(\mathbf{x}) M_t(\mathbf{x}) M_u(\mathbf{x}) M_v(\mathbf{x}). \quad (43)$$

It is clear that it is possible, given separable expansions of an arbitrary bispectrum and trispectrum, to efficiently generate multitudes of realizations, with each requiring only $\mathcal{O}(n_{\text{max}} \times l_{\text{max}}^3)$ operations.

It should be noted that since the bispectrum (35) and trispectrum (39) contributions are not independent, it may be necessary to subtract out an unwanted ‘‘bispectrum’’ contribution to the trispectrum. The bispectrum contribution induces a trispectrum given by

$$\begin{aligned}
 \langle \Phi(\mathbf{k}_1)\Phi(\mathbf{k}_2)\Phi(\mathbf{k}_3)\Phi(\mathbf{k}_4) \rangle_c &= (2\pi)^3 F_{\text{NL}}^2 \int d^3\mathbf{K} [\tilde{T}(k_1, k_2, k_3, k_4, K) \delta_D(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{K}) \delta_D(\mathbf{k}_3 + \mathbf{k}_4 + \mathbf{K}) \\
 &+ \tilde{T}(k_1, k_3, k_2, k_4, K) \delta_D(\mathbf{k}_1 + \mathbf{k}_3 - \mathbf{K}) \delta_D(\mathbf{k}_2 + \mathbf{k}_4 + \mathbf{K}) \\
 &+ \tilde{T}(k_1, k_4, k_2, k_3, K) \delta_D(\mathbf{k}_1 + \mathbf{k}_4 - \mathbf{K}) \delta_D(\mathbf{k}_2 + \mathbf{k}_3 + \mathbf{K})], \quad (44)
 \end{aligned}$$

where

$$\begin{aligned}
 \tilde{T}(k_1, k_2, k_3, k_4, K) &= \frac{B(k_1, k_2, K)}{P(k_1)P(k_2) + 2 \text{ perms}} \frac{B(k_3, k_4, K)}{P(k_3)P(k_4) + 2 \text{ perms}} P(K)(P(k_1)P(k_3) \\
 &+ P(k_1)P(k_4) + P(k_2)P(k_3) + P(k_2)P(k_4)). \quad (45)
 \end{aligned}$$

Cancellation of this spurious ‘‘trispectrum’’ may be achieved by altering the algorithm given by Eq. (33) to the form

$$\Phi = \Phi^G + \frac{1}{2} F_{\text{NL}} + \frac{1}{6} G_{\text{NL}} \Phi^T - \frac{1}{2} F_{\text{NL}}^2 \tilde{\Phi}^T, \quad (46)$$

where

$$\begin{aligned}
 \tilde{\Phi}^T(\mathbf{k}) &= \int \frac{d^3\mathbf{k}_2}{(2\pi)^3} \frac{d^3\mathbf{k}_3}{(2\pi)^3} \frac{d^3\mathbf{k}_4}{(2\pi)^3} d^3\mathbf{K} (2\pi)^3 \delta_D(\mathbf{k} + \mathbf{k}_2 - \mathbf{K}) \\
 &\times \delta_D(\mathbf{k}_3 + \mathbf{k}_4 + \mathbf{K}) \frac{\tilde{T}(k, k_2, k_3, k_4, K)}{P(k)P(k_2)P(k_3) + 3 \text{ perms}} \\
 &\times \Phi^G(\mathbf{k}_2)\Phi^G(\mathbf{k}_3)\Phi^G(\mathbf{k}_4). \quad (47)
 \end{aligned}$$

With this prescription it is found that

$$\begin{aligned}
 \langle \Phi(\mathbf{k}_1)\Phi(\mathbf{k}_2)\Phi(\mathbf{k}_3) \rangle &= (2\pi)^3 \delta_D(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) \\
 &\times B(k_1, k_2, k_3), \\
 \langle \Phi(\mathbf{k}_1)\Phi(\mathbf{k}_2)\Phi(\mathbf{k}_3)\Phi(\mathbf{k}_4) \rangle_c &= (2\pi)^3 \delta_D(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4) \\
 &\times T(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4), \quad (48)
 \end{aligned}$$

as desired. We shall leave a detailed analysis of this issue to a future work.

Recently, Refs. [19,21] proposed an alternative approach to creating non-Gaussian initial conditions from bispectra by integrating directly the convolution expression

$$\begin{aligned}
 \Phi^B(\mathbf{k}) &= \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \\
 &\times \frac{B(k, k', |\mathbf{k} + \mathbf{k}'|) \Phi^G(\mathbf{k}') \Phi^G(\mathbf{k} + \mathbf{k}')}{P(k')P(|\mathbf{k} + \mathbf{k}'|) + P(k)P(k') + P(k)P(|\mathbf{k} + \mathbf{k}'|)}. \quad (49)
 \end{aligned}$$

Originally in Ref. [19] the denominator only had a $P(k')P(|\mathbf{k} + \mathbf{k}'|)$ term, so for explicitly separable bispectra, using convolutions, they were able to exploit the same efficiencies described above to reduce the problem from $\mathcal{O}(l_{\text{max}}^6)$ to $\mathcal{O}(l_{\text{max}}^3)$ operations. However, this procedure leads in general to a nontrivial and spurious non-Gaussian contribution to the power spectrum, so the above expression with a symmetrized denominator was advocated instead [21]. The key difficulty with this modifica-

tion, however, is that the denominator becomes nonseparable, so the method can no longer exploit separability in evaluating the convolution (except in the trivial local case where the integrand is unity). For models other than local, a highly inefficient brute force analysis was pursued. We contrast this with the modal approach where the problem of separable efficiency is already solved in general. The modal decomposition does not require the bispectrum $B(k_1, k_2, k_3)$ to be separable, so the form of the denominator in (34) presents no additional difficulty. In addition, we note that even in the separable bispectra, the CMB modal initial conditions prescription had other beneficial effects because of the well-behaved bounded mode functions employed; these may carry over to this three-dimensional case.

V. NON-GAUSSIAN PARAMETER ESTIMATION

Fast separable methods for estimating arbitrary bispectra or trispectra in large-scale structure observations or simulated data greatly improve the prospect of using higher order correlators as an important cosmological diagnostic. This is particularly pertinent for testing the Gaussian hypothesis of the inflationary scenario. The complication is that even Gaussian initial fluctuations receive non-Gaussian contributions through late-time gravitational collapse (see reviews [5,22] and the references therein). Here, we briefly sketch some key issues facing parameter estimation in this context.

There has been much recent progress describing next-to-leading order contributions to non-Gaussianity from gravity. A simple example of this is the matter density power spectrum which contains several contributions, including those from an enhanced primordial bispectrum $F_{\text{NL}} B_0(k_1, k_2, k_3)$ [23]:

$$\begin{aligned}
 P^B(k) &= \frac{F_{\text{NL}}}{(2\pi)^3} \int d^3\mathbf{y} B_0(\mathbf{k}, \mathbf{y}, \mathbf{k} - \mathbf{y}) F_2(\mathbf{y}, \mathbf{k} - \mathbf{y}) \\
 &= \frac{F_{\text{NL}}}{(2\pi)^3} \int d^3\mathbf{y} d^3\mathbf{k}_2 \delta(\mathbf{k}_2 - \mathbf{k} + \mathbf{y}) \\
 &\times B_0(k, y, k_2) F_2(\mathbf{y}, \mathbf{k}_2), \quad (50)
 \end{aligned}$$

where the gravitational kernel for this convolution is given by

$$F_2(\mathbf{y}, \mathbf{k}_2) = \frac{17}{21} + P_1(\mu) \left(\frac{y}{k_2} + \frac{k_2}{y} \right) + \frac{4}{21} P_2(\mu). \quad (51)$$

Taking the separable expansion (11) for $B_0(k_1, k_2, k_3)$ and substituting into Eq (50), we find the simple integral over the mode functions $q_r(k)$:

$$\begin{aligned} P^B(k) = F_{\text{NL}} \sum_n \frac{\alpha_n}{2\pi^2} \frac{q_r(k) \sqrt{P(k)}}{k^{3/2}} \int_{\mathcal{V}_B} dy dk_2 \sqrt{y P(y)} q_s(y) \\ \times \sqrt{k_2 P(k_2)} q_t(k_2) \left[\frac{5}{7} + \frac{2}{7} \left(\frac{k_2^2 + y^2 - k^2}{2k_2 y} \right)^2 \right. \\ \left. - \left(\frac{y}{k_2} + \frac{k_2}{y} \right) \left(\frac{k_2^2 + y^2 - k^2}{2k_2 y} \right) \right], \quad (52) \end{aligned}$$

$$\begin{aligned} B(k_1, k_2, k_3) = [2F_2(\mathbf{k}_1, \mathbf{k}_2) P_0(k_1) P_0(k_2) + 2\text{perms}] + F_{\text{NL}} B_0(k_1, k_2, k_3) \\ + \frac{\tau_{\text{NL}}}{(2\pi)^3} \int d^3 T_0(\mathbf{k}_1, \mathbf{k}_2, \mathbf{y}, \mathbf{k}_3 - \mathbf{y}) F_2(\mathbf{y}, \mathbf{k}_3 - \mathbf{y}) + 2\text{perms} \\ \equiv B^G(k_1, k_2, k_3) + F_{\text{NL}} B_0(k_1, k_2, k_3) + \tau_{\text{NL}} B^T(k_1, k_2, k_3). \quad (53) \end{aligned}$$

In Appendix B, we substitute the separable expansion for the trispectrum (24) into (53) to find integral expressions for the resulting bispectrum. For nondiagonal trispectra, the result is simple and very similar to the power spectrum modification (52). The result is three distinct contributions to the late-time bispectrum $\omega B(k_1, k_2, k_3) = \sum_n \alpha_n Q_n$ with the bispectrum approximated as in separable form as

$$\omega B(k_1, k_2, k_3) = \sum_n (\alpha_n^G + \alpha_n^B + {}_{\text{NL}} \alpha_n^T) \mathcal{R}_n(k_1, k_2, k_3), \quad (54)$$

with the coefficients α_n^i representing distinct shapes in the orthonormal frame. Here, the primordial α^B coefficients are normalized such that in the initial conditions $F_{\text{NL}} = 1$, and similarly for the primordial trispectrum $\tau_{\text{NL}} = 1$.

Setting aside the trispectrum contribution, if we can remove the Gaussian part from α_n , β_n then we have an optimal estimator for the non-Gaussianity parameter F_{NL} ,

$$\mathcal{E} = \frac{1}{N^2} \sum \alpha_n^B \beta_n^B, \quad (55)$$

where we have defined the predicted α_n^B and measured α_n^B by

$$\alpha_n^B = \alpha_n - \bar{\alpha}_n^G, \quad \beta_n^B = \beta_n - \bar{\beta}_n^G, \quad N^2 = \sum \alpha_n^{B^2}. \quad (56)$$

Here $\bar{\alpha}_n^G$ refers to the decomposition coefficients for Gaussian initial conditions, calculated either from theory [as above in (53)] or obtained from N-body simulations (note $\bar{\alpha}_n^G = \bar{\beta}_n^G$) and the n are calculated from initial conditions with $F_{\text{NL}} = 1$. The variance of the estimator can then be calculated by applying it to a large set of Gaussian 12 simulations. This is directly analogous to

where \mathcal{V}_B represents the domain for which the triangle condition holds for the wave numbers (k_2, y, k) . Note that this integral breaks down into products of one-dimensional integrals over y and k_2 , which can be evaluated easily. Here, the calculation steps leading to (52) are very similar to those used to obtain (5).

In the mildly nonlinear regime, the matter density bispectrum similarly contains nonlinear contributions from gravitational collapse, from the primordial bispectrum $F_{\text{NL}} B_0$, and from the primordial trispectrum $\tau_{\text{NL}} T_0$ [14,24]:

the CMB estimator used in [1] (where of course $\bar{\alpha}_n^G = 0$). It should be noted that in the study of real data sets, such as from SDSS, it is necessary to account for complications such as redshift space distortions, survey geometry, galaxy bias, etc. This requires that the decomposition coefficients, $\bar{\alpha}_n^G$, include these effects. The usual method employed to carry out such an analysis is to create a mock data set that includes such systematics. These are generally created using large suites of N-body simulations. However, in [25] an alternative approach using second order Lagrangian perturbation theory that is accurate on large scales (between 30 and 80 h^{-1} Mpc) was described. We defer the important study of real three-dimensional data using the modal approach to a future publication.

In the nonlinear regime, and with significant bias affecting the galaxy distribution, it may not be possible to approximate non-Gaussianity using (55). We need to approach parameter estimation for F_{NL} (or τ_{NL}) quite differently. The estimator (55) can be thought of as a least squares fit of the theory to the data. As the relative size of the individual α_n^B are constant, we can only change the amplitude, F_{NL} . Therefore, we must simply choose an F_{NL} that minimizes

$$\mathcal{E} = \sum (\alpha_n^B F_{\text{NL}} - \beta_n^B)^2 \quad (57)$$

for a given form of α_n^B . In the general case we expect the ratios of the individual coefficients to change as we change F_{NL} . As a result we must consider the α_n^B to be an arbitrary function of F_{NL} and so we now wish to minimize

$$\mathcal{E}(F_{\text{NL}}) = \sum (\alpha_n^B(F_{\text{NL}}) - \beta_n^B)^2 \quad (58)$$

with respect to F_{NL} . We will assume that it will not be possible in general to determine $\alpha_n(F_{\text{NL}})$ analytically so that we could then try to solve $\partial\mathcal{E}/\partial F_{\text{NL}} = 0$. This means that to minimize \mathcal{E} requires extracting the α_n from sets of N-body simulations each with different non-Gaussian initial conditions that correspond to a particular F_{NL} . We then reconstruct the dependence of \mathcal{E} on F_{NL} and find the best-fit F_{NL} for the given observations. One also must be careful calculating the variance on such a measurement of F_{NL} . In general this would entail applying the same approach to each density distribution in the set of simulations with the estimated F_{NL} , \hat{F}_{NL} , and then determining the distribution of the recovered $F_{\text{NL}}^{\text{sim}}$, $P[F_{\text{NL}}^{\text{sim}}; F_{\text{NL}} = \hat{F}_{\text{NL}}]$. Of course, Gaussian simulations may be substituted if F_{NL} is sufficiently small that the effect on the error bars is negligible, i.e. such that the probability distribution function may be approximated as $P[F_{\text{NL}}^{\text{sim}}; F_{\text{NL}} = \hat{F}_{\text{NL}}] = 0$. Of course, generating enough N-body simulations to reliably produce this probability distribution function is an onerous task. We may instead attempt to analytically calculate the quantities $\alpha_n(F_{\text{NL}})$ by extending the tree-level approach [see, for example, Eq. (53)] to include higher order loop corrections. Work in this direction has been carried out in [26–30]. A study of the domain of validity of these perturbation theory formulas is, therefore, an extremely worthwhile task.

Finally, we note that in general the galaxy bispectrum will take contributions from both the bispectrum and trispectrum of the curvature perturbation [14] (which is why we cannot in general connect F_{NL} with its CMB counterpart in a simple way). The amplitudes of F_{NL} and τ_{NL} can be determined by consistency conditions for certain models or they can vary independently. In this case we must constrain the amplitude of both F_{NL} and τ_{NL} contributions marginalizing over these two parameters. Such a computationally intensive analysis becomes much more feasible with an efficient bispectrum extraction method (16) and with non-Gaussian initial conditions that include the specification of the trispectrum (33).

VI. CONCLUSION

While the CMB is an ideal observable for tests of primordial non-Gaussianity since the perturbations remain in the linear regime, there are encouraging prospects for achieving comparable, and ultimately superior, constraints on non-Gaussianity because of forthcoming galaxy surveys. In this paper we have described how methods developed for the analysis of non-Gaussianity in the CMB may be applied to the study of N-body simulations and surveys of large-scale structure. These methods are based on mode expansions (whether polynomials, wavelets, or bins), exploiting a complete orthonormal eigenmode basis to efficiently decompose arbitrary polyspectra into a separable polynomial expansion.

Applying the methodology to the bispectrum reveals a vast improvement in computational speed for finding a

general estimator and correlator, reducing complexity from $\mathcal{O}(l_{\text{max}}^6)$ to $\mathcal{O}(n_{\text{max}} \times l_{\text{max}}^3)$. As we use a complete orthonormal basis we are also able to efficiently calculate the bispectrum from simulations and, assuming a sufficient signal-to-noise ratio, observations. Of particular interest is the application to the generation of non-Gaussian initial conditions for N-body codes. The approach can be used to create initial conditions with arbitrary independent polyspectra. With this method, calculation of the bispectrum contribution requires a similar number of operations as decomposition. This improvement to the brute force approach opens up the opportunity of investigating a far wider range of models using large-scale structure than has hitherto been considered.

The extension of the approach to the trispectrum has also been described in some detail. As with the bispectrum, computational speed is vastly improved using the separable method. However, for trispectra that depend on the diagonals as well as the wave numbers, the decomposition into separable modes is still a computationally intensive operation requiring up to $\mathcal{O}(l_{\text{max}}^6)$ operations. Nonetheless, this decomposition need only be performed once for each model. In the particular case that the trispectra is independent of the diagonals, the decomposition process may be performed efficiently in $\mathcal{O}(l_{\text{max}}^4)$ operations. It should also be noted that the general trispectrum may be divided into contributions denoted as “reduced” trispectra. Since, for almost all theoretical trispectra presented to date in the literature, the reduced trispectra depends on five parameters (i.e. the four wave numbers and one diagonal), a reduction in complexity for this wide range of models may also be achieved. This class of models will be discussed in a subsequent article [15].

As in the case of the bispectrum, this approach can also be used to recover trispectra from simulations and produce non-Gaussian initial conditions with arbitrary trispectra for N-body codes. Once the trispectrum has been decomposed into separable modes, the calculation of the trispectrum contribution to non-Gaussian initial conditions is an extremely efficient operation that may be performed in $\mathcal{O}(n_{\text{max}}^{4/3} \times l_{\text{max}}^3)$ operations. In this paper we have also briefly outlined how the method may be extended to higher order correlators such as the quadspectra, revealing a highly efficient algorithm in the case that the quad spectrum depends only on its wave numbers.

The estimation of non-Gaussian parameters using large-scale structure is complicated due to nonlinear evolution. In this paper we have outlined some of the issues involved. The application of the separable approximation to finding the contribution to the matter density power spectrum due to the bispectrum (as well as the matter density bispectrum contribution due to the trispectrum) has been derived. In addition, a prescription for parameter estimation in the fully nonlinear regime has been described.

While observational problems connected to surveys, such as redshift distortion and photometric errors, have not been addressed here, the generality and robustness of the methodology described in this paper suggests that a vast improvement on the scope of models investigated using large-scale structure is possible, offering a significant test of the initial conditions of the Universe. However, different large-scale structure survey strategies affect the quality of the higher order correlators that can be extracted. Given that these polyspectra can be determined efficiently and their strong scientific motivation, this should become an issue of growing importance in survey design.

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APPENDIX A: GENERAL TRISPECTRUM ESTIMATOR

In this Appendix we shall elucidate in more detail the calculations involved in arriving at the expectation value of the trispectrum estimator given by Eq. (21). This derivation is instructive for the calculation of many of the results presented in this paper.

Similarly to the case of the bispectrum, the expectation value for the estimator is found to give

$$\langle \mathcal{E} \rangle = \frac{V}{(2\pi)^3} \int \frac{d^3 \mathbf{k}_1}{(2\pi)^3} \frac{d^3 \mathbf{k}_2}{(2\pi)^3} \frac{d^3 \mathbf{k}_3}{(2\pi)^3} \frac{d^3 \mathbf{k}_4}{(2\pi)^3} \times \frac{(2\pi)_D^6(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4) T^2(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4)}{P(k_1)P(k_2)P(k_3)P(k_4)}. \quad (\text{A1})$$

Using the parametrization in terms of $(k_1, k_2, k_3, k_4, K_1, K_2)$ and expanding the Dirac delta functions using (6) and (7), we find

$$\langle \mathcal{E} \rangle = \frac{V}{(2\pi)^3} \int \frac{(k_1 k_2 k_3 k_4 K_1 K_2)^2 dk_1 dk_2 dk_3 dk_4 dK_1 dK_2}{(2\pi)^{15}} \frac{T^2(k_1, k_2, k_3, k_4, K_1, K_2)}{P(k_1)P(k_2)P(k_3)P(k_4)} (4\pi)^9 \sum_{l_1} (2l_1 + 1) \times \left(\int dx_1 x_1^2 j_{l_1}(k_1 x_1) j_0(k_2 x_1) j_{l_1}(K_1 x_1) \right) \left(\int dx_2 x_2^2 j_0(k_3 x_2) j_{l_1}(k_4 x_2) j_{l_1}(K_1 x_2) \right) \left(\int dx_3 x_3^2 j_{l_1}(k_1 x_3) j_{l_1}(k_4 x_3) j_0(K_2 x_3) \right), \quad (\text{A2})$$

where the expression on the second and third lines arises from the integration over the angular variables. Next, we use the following identity from [31,32]

$$\int_0^\infty r^2 dr j_l(kr) j_l(k'r) j_0(\rho r) = \Theta(k, k', \rho) \times \frac{\pi}{4kk'\rho} P_l\left(\frac{k^2 + k'^2 - \rho^2}{2kk'}\right), \quad (\text{A3})$$

where Θ imposes the triangle condition on wave numbers (k, k', ρ) , which is automatically satisfied for the trispectrum estimator at all points of the quadrilateral due to the Dirac delta functions, and P_l represents the l th Legendre polynomial. Finally we may further simplify using the following result from [33]:

$$\sum_{l=0}^\infty (2l+1) P_l(x) P_l(y) P_l(z) = \frac{2}{\pi \sqrt{g}}, \quad g = 1 + 2xyz - x^2 - y^2 - z^2 > 0 \\ = 0, \quad \text{otherwise.} \quad (\text{A4})$$

For the case of the trispectrum estimator we have

$$x = \frac{k_1^2 + K_1^2 - k_2^2}{2k_1 K_1}, \quad y = \frac{k_4^2 + K_1^2 - k_3^2}{2k_4 K_1}, \quad z = \frac{k_1^2 + k_4^2 - K_2^2}{2k_1 k_4}, \quad (\text{A5})$$

and the condition $g > 0$ is again satisfied for all points within the quadrilateral.

Using these expressions the expectation value of the estimator takes the following simple form:

$$\langle \mathcal{E} \rangle = \frac{V}{(2\pi)^3} \frac{1}{2\pi^4} \int_{V_T} dk_1 dk_2 dk_3 dk_4 dK_1 dK_2 \times \frac{k_2 k_3 K_2}{2\sqrt{g}} \frac{T^2(k_1, k_2, k_3, k_4, K_1, K_2)}{P(k_1)P(k_2)P(k_3)P(k_4)}. \quad (\text{A6})$$

In writing this expression we set $\delta_D(\mathbf{0}) = V/(2\pi)^3$. Therefore a suitable weight for the mode decomposition, which is a simple generalization of the discussion in [3] to include an extra diagonal, is given by $w(k_1, k_2, k_3, k_4, K_1, K_2) = k_2 k_3 K_2 / (\sqrt{g} P(k_1) P(k_2) P(k_3) P(k_4))$. We note that the factor $k_2 k_3 K_2 / (2\sqrt{g})$ may be written as

$$\frac{k_2 k_3 K_2}{2\sqrt{g}} = \frac{k_1 k_2 k_3 k_4 K_1 K_2}{\sqrt{K_1^2 K_2^2 (\sum_i k_i^2 - K_1^2 - K_2^2) - K_1^2 \kappa_{23} \kappa_{14} + K_2^2 \kappa_{12} \kappa_{34} - (k_1^2 k_3^2 - k_2^2 k_4^2) (\kappa_{12} + \kappa_{34})}} \equiv \frac{k_1 k_2 k_3 k_4 K_1 K_2}{\sqrt{g_1}}, \quad (\text{A7})$$

where we denote $\kappa_{ij} = k_i^2 - k_j^2$ and we denote the denominator $\sqrt{g_1}$ for brevity.

APPENDIX B: TRISPECTRUM CONTRIBUTION TO THE BISPECTRUM

The contribution to the galaxy bispectrum due to the primordial trispectrum is given by

$$B_g^T(k_1, k_2, k_3) = \frac{1}{(2\pi)^3} \int d^3 \mathbf{y} T(\mathbf{k}_{1,2}, \mathbf{k}_2, \mathbf{k}_3, -\mathbf{y}) F_2(\mathbf{y}, \mathbf{k}_3 - \mathbf{y}) + 2\text{perms} \\ = \frac{1}{(2\pi)^3} \int d^3 \mathbf{y} d^3 \mathbf{k}_4 T(\mathbf{k}_1, \mathbf{k}_2, \mathbf{y}, \mathbf{k}_4) F_2(\mathbf{y}, \mathbf{k}_4) \delta_D(\mathbf{k}_4 - \mathbf{k}_3 + \mathbf{y}) + 2\text{perms}, \quad (\text{B1})$$

where F_2 is given by Eq. (51) and the permutations are cyclic in (k_1, k_2, k_3) . First we consider the special case that the trispectrum depends only on the wave numbers k_1, k_2, y, k_4 such that we may write $T(k_1, k_2, y, k_4) = \sum_n \alpha_n q_r(k_1) q_s(k_2) q_t(y) q_u(k_4)$. The calculation is very similar to the power spectrum case and we find

$$B_g^T(k_1, k_2, k_3) = \sum_n \frac{\alpha_n}{4\pi^2} \frac{\sqrt{P(k_1)P(k_2)}}{(k_1 k_2)^{3/4}} \frac{q_r(k_1) q_s(k_2)}{k_3} \int_{\mathcal{V}} dy dk_4 (y k_4)^{1/4} \sqrt{P(y)P(k_4)} q_t(y) q_u(k_4) \left[\frac{5}{7} + \frac{2}{7} \left(\frac{k_4^2 + y^2 - k_3^2}{2k_4 y} \right)^2 - \left(\frac{y}{k_4} + \frac{k_4}{y} \right) \left(\frac{k_4^2 + y^2 - k_3^2}{2k_4 y} \right) \right] + 2\text{perms}, \quad (\text{B2})$$

where \mathcal{V} represents the domain for which the wave numbers (y, k_4, k_3) satisfy the triangle condition. The integral, we note again, may be written as a sum of products of one-dimensional integrals over y and k_4 .

Next we consider the more general case where the trispectrum depends also on two diagonals or equivalently the angles $\mu = \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2$ and $\nu = \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_4$. In this case we may decompose the trispectrum as

$$\frac{(k_1 k_2 y k_4)^{3/4}}{\sqrt{P(k_1)P(k_2)P(y)P(k_4)}} T(\mathbf{k}_1, \mathbf{k}_2, \mathbf{y}, \mathbf{k}_4) \\ = \sum_{n l_1 l_2} \alpha_{n l_1 l_2} q_r(k_1) q_s(k_2) q_t(y) q_u(k_4) P_{l_1}(\mu) P_{l_2}(\nu), \quad (\text{B3})$$

where $n \equiv \{r, s, t, u\}$. The calculation follows much the same lines as the special case with simplification of the formulas in this case achieved using Eq. (6), the following

identity as described in [34,35]

$$\int dx x^2 j_l(kx) j_{l'}(k'x) j_n(\rho x) \\ = \Theta(k, k', \rho) \frac{\pi}{2kk'\rho^{n+1}} \sum_L Q_{nL}(k, l, k', l') P_L \left(\frac{k^2 + k'^2 - \rho^2}{2kk'} \right) \quad (\text{B4})$$

(where the Θ function imposes the triangle condition on the three wave numbers, P_L is a Legendre polynomial, and the functions Q_{nL} may be found in [34,35]) and the identity

$$\sum_{m_1, m_2} \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & M \end{pmatrix} \begin{pmatrix} l_1 & l_2 & L' \\ m_1 & m_2 & M' \end{pmatrix} = \frac{\delta_{LL'} \delta_{MM'}}{2L + 1}. \quad (\text{B5})$$

With these considerations we find

$$\begin{aligned}
B_g^T(k_1, k_2, k_3) = & \sum_{n_1 l_1} \frac{\alpha_{n_1 l_1}}{2\pi^2} \frac{\sqrt{P(k_1)P(k_2)}}{(k_1 k_2)^{3/4}} \frac{q_r(k_1)q_s(k_2)}{k_3} P_{l_1}(\hat{\mathbf{k}}_1, \hat{\mathbf{k}}_2) P_{l_2}(\hat{\mathbf{k}}_1, \hat{\mathbf{k}}_3) \int_{\mathcal{V}} dy dk_4 (y k_4)^{1/4} \sqrt{P(y)P(k_4)} q_t(y) q_u(k_4) \\
& \times \left[\frac{17}{42} P_{l_2} \left(\frac{k_4^2 + k_3^2 - y^2}{2k_3 k_4} \right) + \frac{4\pi}{3} \sum_{l_4} \frac{(-1)^{(l_4 - l_2 + 1)/2} h_{l_2 l_4}^2}{(2l_2 + 1)} \frac{1}{y} \left(\frac{y}{k_4} + \frac{k_4}{y} \right) \sum_L Q_{1L}(k_4, l_4, k_4, l_2) P_L \left(\frac{k_4^2 + k_3^2 - y^2}{2k_3 k_4} \right) \right. \\
& \left. + \frac{16\pi}{105} \sum_{l_4} (-1)^{(l_4 - l_2 + 2)/2} \frac{h_{l_2 l_4}^2}{(2l_2 + 1) y^2} \sum_{L'} Q_{2L'}(k_4, l_4, k_4, l_2) P_{L'} \left(\frac{k_4^2 + k_3^2 - y^2}{2k_3 k_4} \right) \right] + 2\text{perms.} \quad (\text{B6})
\end{aligned}$$

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