Spectra of turbulently advected scalars that have small Schmidt number

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Exact statistical equations are derived for turbulent advection of a passive scalar having diffusivity much larger than the kinematic viscosity, i.e., small Schmidt number. The equations contain all terms needed for precise direct numerical simulation (DNS) quantification. In the appropriate limit, the equations reduce to the classical theory for which the scalar spectrum is proportional to the energy spectrum multiplied by k^{-4} , which, in turn, results in the inertial-diffusive range power law, *k*[−]17*/*3. The classical theory was derived for the case of isotropic velocity and scalar fields. The exact equations are simplified for less restrictive cases: (1) locally isotropic scalar fluctuations at dissipation scales with no restriction on symmetry of the velocity field, (2) isotropic velocity field with averaging over all wave-vector directions with no restriction on the symmetry of the scalar, motivated by that average being used for DNS, and (3) isotropic velocity field with axisymmetric scalar fluctuations, motivated by the mean-scalar-gradient-source case. The equations are applied to recently published DNSs of passive scalars for the cases of a freely decaying scalar and a mean-scalar-gradient source. New terms in the exact equations are estimated for those cases and are found to be significant; those terms cause the deviations from the classical theory found by the DNS studies. A new formula for the mean-scalar-gradient case explains the variation of the scalar spectra for the DNS of the smallest Schmidt-number cases. Expansion in Legendre polynomials reveals the effect of axisymmetry. Inertial-diffusive-range formulas for both the zero- and second-order Legendre contributions are given. Exact statistical equations reveal what must be quantified using DNS to determine what causes deviations from asymptotic relationships.

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I. INTRODUCTION

Batchelor, Howells, and Townsend (BHT) [\[1\]](#page-15-0) derived a theory for the spectrum of a scalar having a small Schmidt number (Sc) in isotropic turbulence: $Sc \equiv v/D$, where *ν* is kinematic viscosity and *D* is molecular diffusivity. If the scalar is heat, i.e., temperature, then the Prandtl number $Pr \equiv v/D$ is relevant, where *D* is thermal diffusivity. The BHT derivation was for freely decaying scalar fluctuations. For the asymptotic case of large Peclet number, Pe, and large Reynolds number, Re, and very small Sc, they obtained $E_{\phi}(k) = (\chi/3D^3)k^{-4}E(k)$, where $E_{\phi}(k)$ is the scalar's spectrum, $E(k)$ is the energy spectrum, and χ is the scalar-variance dissipation rate. A further asymptote is: if the energy spectrum has an inertial range, $E(k) \propto k^{-5/3}$, then an inertial-diffusive range can exist for which $E_{\phi}(k) \propto k^{-17/3}$. Clay [\[2\]](#page-15-0) measured temperature fluctuations in turbulent mercury for which Pr = 0.018. Howells' [\[3\]](#page-15-0) model of the scalar spectrum applies to any Sc and contains the BHT theory for $Sc \ll 1$. A solution of Howells' model resulted in finding that "the inertial-diffusive range asymptotic form, $k^{-17/3}$, cannot appear even for Pr as small as that of mercury (Pr = 0.018)" [\[4\]](#page-15-0), which agreed with a previous modeling study [\[5\]](#page-15-0) that stated "the inertial-diffusive range of temperature fluctuations in mercury ($Pr \approx 0.02$) is of very limited extent" and "a convincing measurement of an inertial-diffusive range would require $\nu/D \simeq 10^{-3}$." Verification of those statements was obtained from DNS [\[6,7\]](#page-15-0) (direct numerical simulation) which shows $E_{\phi}(k)$ osculating *k*^{−17/3} for Sc = 1/128 = 7.8 × 10^{−3} and a clear $E_{\phi}(k) \propto k^{-17/3}$ for Sc $\leq 1/512 = 2 \times 10^{-3}$. [\[6\]](#page-15-0)

DNSs of scalar fluctuations that are freely decaying [\[6\]](#page-15-0) and those produced from a mean scalar gradient [\[7\]](#page-15-0) have shown deviations from the BHT asymptotic formulas; such deviations likely result from the limited Pe attainable from existing computers. [\[6,7\]](#page-15-0) What must be calculated to quantify those deviations is determined herein. Yeung and Sreenivasan [\[6\]](#page-15-0) (hereinafter YS1) followed

the derivation method of BHT for freely decaying scalar fluctuations; Yeung and Sreenivasan [\[7\]](#page-15-0) (hereinafter YS2) did not follow the derivation method of BHT for their source; that is done here.

DNS is capable of evaluating all terms in statistical equations that are derived without approximations, i.e., exact statistical equations. Such exact equations are derived here. Other types of sources of scalar fluctuations can be calculated in the future. Therefore, a general derivation for any source is timely; it is given here. Exact equations reveal what must be quantified using DNS to determine what causes deviations from asymptotic relationships. This author considers quantifying the approach toward asymptotes more interesting than attaining the asymptote; that perspective supports alleviating the computational difficulties [\[6,7\]](#page-15-0) of very small Sc.

Bos *et al.* [\[8\]](#page-15-0) calculated two-dimensional (2D) turbulence with a uniform mean scalar gradient of magnitude *G* and deduced, in their equations [\(30\)](#page-4-0) and [\(31\)](#page-5-0), that $E_{\phi}(k) = (G^2/3D^2)k^{-4}E(k)$ and $E_{\phi}(k) \propto (G/D)^2 \varepsilon^{2/3} k^{-17/3}$ for Sc $\ll 1$. They show the $k^{-17/3}$ power law in their Fig. 5. Bos [\[9\]](#page-15-0) formulates the scalar advection in terms of an isotropic vector field for the case of a uniform mean scalar gradient and obtains results in terms of isotropic and second-order Legendre polynomials. Herr *et al.* [\[10\]](#page-15-0) use an eddy damped quasinormal Markovian (EDQNM) calculation for the case of a uniform mean scalar gradient for a range of Sc values; for $Sc = 8 \times 10^{-3}$ they show the −17*/*3 power law in their Fig. 14; they also discuss anisotropy caused by a mean scalar gradient in terms of expansion in Legendre polynomials. Both Chasnov [\[11\]](#page-16-0) and O'Gorman and Pullin [\[12\]](#page-16-0) use large eddy simulation (LES) of the velocity field to create an extensive inertial range to investigate the inertial-diffusive range of the scalar for cases of freely decaying as well as a uniform mean-scalar-gradient source. For a uniform mean scalar gradient *G*, Chasnov [\[11\]](#page-16-0) finds that the BHT formula must be modified by replacing *χ* with the factor ($\chi + 2DG^2$); that factor is also in Eq. (3.17) of O'Gorman and Pullin [\[12\]](#page-16-0), who derive it based on an asymptotic approximation in their Appendix [A.](#page-14-0) Herein, that factor is obtained effortlessly without approximation and appears below as $1 + D/D_T$ and $1 + D_T/D$; $D_T/D \equiv \chi/2DG^2$.

The derivation below retains dependence on the wave vector **k** such that it applies to the anisotropic case. The wave number *k* appears below where the equations are to be compared with the DNS results of YS1 [\[6\]](#page-15-0) and YS2 [\[7\]](#page-15-0) because they averaged over all directions of **k**. Herring [\[13\]](#page-16-0) introduced the use of Legendre-polynomial expansion to describe axisymmetry of velocity spectra. Gotoh *et. al*. [\[14\]](#page-16-0) used expansion of statistics in Legendre polynomials to investigate axisymmetric passive-scalar advection for $Pr \ge 1$. Here, their method [\[14\]](#page-16-0) is extended to the small-Sc case.

Further introduction is unnecessary because of the extensive introductions and literature references given by Yeung and Sreenivasan [\[6,7\]](#page-15-0) and Gotoh *et. al*. [\[14\]](#page-16-0). The structure of this paper is evident from the section titles.

Statistical homogeneity and temporal stationarity have not been assumed in Sec. [VI.](#page-4-0) Wherever isotropy is used for the velocity field, homogeneity is also assumed for the velocity. Where local isotropy is assumed for the scalar field, local homogeneity is also assumed for the scalar field. The axisymmetric scalar case in Sec. [VIII](#page-5-0) can have axially symmetric inhomogeneity (spatially periodic for DNS), an example of which is a mean-scalar-gradient source that is constant in direction but not in magnitude. The uniform scalar-gradient case in Secs. [IX](#page-6-0) and [XI](#page-9-0) is homogeneous.

II. DERIVATION GENERALIZED TO INCLUDE A SOURCE

The equation for the scalar fluctuation $\phi(\mathbf{x},t)$ that includes any source $s(\mathbf{x},t)$ of scalar fluctuation is [\[7\]](#page-15-0)

$$
\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = s + D \nabla^2 \phi. \tag{1}
$$

The time-derivative term *∂φ/∂t* and the source term *s* are subtracted from both sides of Eq. (1) for reasons explained in Appendix [A.](#page-14-0) In Fourier space, using incompressibility, Eq. (1) then gives

$$
i\int k_i'\widehat{u}_i(\mathbf{k}-\mathbf{k}')\widehat{\phi}(\mathbf{k}')d\mathbf{k}'-\widehat{s}(\mathbf{k})=-\frac{\partial\widehat{\phi}(\mathbf{k})}{\partial t}-Dk^2\widehat{\phi}(\mathbf{k}).
$$
\n(2)

Multiplying Eq. [\(2\)](#page-1-0) by its complex conjugate and averaging, which is denoted by angle brackets, gives

$$
\left\langle \left(i \int k'_i \widehat{u}_i(\mathbf{k} - \mathbf{k}') \widehat{\phi}(\mathbf{k}') d\mathbf{k}' - \widehat{s}(\mathbf{k}) \right) \left(-i \int k''_j \widehat{u}_j^*(\mathbf{k} - \mathbf{k}'') \widehat{\phi}^*(\mathbf{k}'') d\mathbf{k}'' - \widehat{s}^*(\mathbf{k}) \right) \right\rangle = \left\langle \left(-\frac{\partial \widehat{\phi}(\mathbf{k})}{\partial t} - Dk^2 \widehat{\phi}(\mathbf{k}) \right) \left(-\frac{\partial \widehat{\phi}^*(\mathbf{k})}{\partial t} - Dk^2 \widehat{\phi}^*(\mathbf{k}) \right) \right\rangle.
$$
 (3)

The distributive law of multiplication produces many terms from Eq. (3). We define the following simple notation (repeated subscripts imply summation over vector components) for most of the statistics that must be evaluated using DNS:

$$
\mathbf{Q}_{\phi}(\mathbf{k}) \equiv \langle \widehat{\phi}(\mathbf{k}) \widehat{\phi}^*(\mathbf{k}) \rangle, \quad \mathbf{Q}(\mathbf{k}) \equiv \frac{1}{2} \langle \widehat{u}_i(\mathbf{k}) \widehat{u}_i^*(\mathbf{k}) \rangle, \quad \chi \equiv 2D \Biggl\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_i} \Biggr\rangle, \tag{4}
$$

$$
\mathbf{T(k)} \equiv \left\langle \frac{\partial \widehat{\phi}(\mathbf{k})}{\partial t} \frac{\partial \widehat{\phi}^*(\mathbf{k})}{\partial t} \right\rangle, \tag{5}
$$

$$
\mathbf{Y}(\mathbf{k}) \equiv Dk^2 \bigg\langle \frac{\partial \widehat{\phi}(\mathbf{k})}{\partial t} \widehat{\phi}^*(\mathbf{k}) + \frac{\partial \widehat{\phi}^*(\mathbf{k})}{\partial t} \widehat{\phi}(\mathbf{k}) \bigg\rangle = Dk^2 \bigg\langle \frac{\partial (\widehat{\phi}(\mathbf{k}) \widehat{\phi}^*(\mathbf{k}))}{\partial t} \bigg\rangle, \tag{6}
$$

$$
\mathbf{X}(\mathbf{k}) \equiv \left\langle -\widehat{s}(\mathbf{k}) \left(-i \int k'_j \widehat{u}_j^*(\mathbf{k} - \mathbf{k}') \widehat{\phi}^*(\mathbf{k}') d\mathbf{k}' \right) - \widehat{s}^*(\mathbf{k}) \left(i \int k'_i \widehat{u}_i(\mathbf{k} - \mathbf{k}') \widehat{\phi}(\mathbf{k}') d\mathbf{k}' \right) \right\rangle, \tag{7}
$$

$$
S(k) \equiv \langle \widehat{s}(k)\widehat{s}^*(k) \rangle. \tag{8}
$$

$$
\mathbf{V}(\mathbf{k}) \equiv \left\langle \int \int k'_i k''_j \widehat{u}_i(\mathbf{k} - \mathbf{k}') \widehat{u}_j^*(\mathbf{k} - \mathbf{k}'') \widehat{\phi}(\mathbf{k}') \widehat{\phi}^*(\mathbf{k}'') d\mathbf{k}' d\mathbf{k}'' \right\rangle, \tag{9}
$$

$$
\mathbf{Z}(\mathbf{k}) \equiv \langle \widehat{u}_i(\mathbf{k}) \widehat{u}_j^*(\mathbf{k}) \rangle \bigg\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \bigg\rangle, \tag{10}
$$

$$
\mathbf{e}_2(\mathbf{k}) \equiv \mathbf{V}(\mathbf{k}) - \mathbf{Z}(\mathbf{k}).\tag{11}
$$

Then Eq. (3) is

$$
\mathbf{X(k)} + \mathbf{V(k)} + \mathbf{S(k)} = \mathbf{T(k)} + \mathbf{Y(k)} + D^2 k^4 \mathbf{Q}_{\phi}(\mathbf{k}).
$$
 (12)

III. DEFINITIONS OF WAVE-NUMBER SPECTRA AND COSPECTRA AND LEGENDRE-POLYNOMIAL COEFFICIENTS

Integrating the spectral and cospectral densities in Eqs. (4) – (11) over a spherical surface in **k** space defines wave-number spectra and cospectra that do not contain information about anisotropy. Scalar and energy wave-number spectra are defined by

$$
E_{\phi}(k) \equiv \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta k^2 \sin(\theta) \mathbf{Q}_{\phi}(\mathbf{k}), \quad E(k) \equiv \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta k^2 \sin(\theta) \mathbf{Q}(\mathbf{k}), \tag{13}
$$

wherein φ and θ are the azimuthal and polar angles of vector **k**. To avoid many new symbols, let

$$
T(k)
$$
, $Y(k)$, $X(k)$, $S(k)$, $V(k)$, $Z(k)$, $e_2(k)$, $\Sigma_{axi\phi}(k)$, etc., (14)

denote the wave-number spectra and cospectra obtained by integrating, as in Eq. (13), the spectral and cospectral densities in Eqs. (5) – (11) and Eq. (43) , etc. Integrating Eq. (12) over a spherical surface in **k** space, as in Eq. (13), gives

$$
X(k) + V(k) + S(k) = T(k) + Y(k) + D2k4E\phi(k).
$$
 (15)

For axisymmetry, $\mathbf{Q}_{\phi}(\mathbf{k})$ can be expressed as a function of *k* and $\mu \equiv \cos(\theta)$; hence, as $\mathbf{Q}_{\phi}(k,\mu)$ such that the integral over φ in Eq. [\(13\)](#page-2-0) gives 2π . Write $\mathbf{Q}_{\phi}(k,\mu)$ as an expansion in Legendre polynomials denoted by

$$
\mathbf{Q}_{\phi}(k,\mu) = Q_{\phi}^{\text{0th}}(k)P_0(\mu) + Q_{\phi}^{\text{1st}}(k)P_1(\mu) + Q_{\phi}^{\text{2nd}}(k)P_2(\mu) + \cdots,
$$
\n(16)

wherein the $Q_{\phi}^{\text{0th}}(k)$, $Q_{\phi}^{\text{1st}}(k)$, $Q_{\phi}^{\text{2nd}}(k)$, etc., are the coefficients of the expansion, and the Legendre polynomials are $P_0(\mu) = 1$, $P_1(\mu) = \mu$, $P_2(\mu) = (3\mu^2 - 1)/2$, etc. Substitution of Eq. (16) into Eq. [\(13\)](#page-2-0) causes only the 0th order to be nonzero. Then

$$
E_{\phi}(k) = 4\pi k^2 Q_{\phi}^{0\text{th}}(k). \tag{17}
$$

For axisymmetry, every quantity in Eq. (14) is their zero-order Legendre-polynomial coefficient multiplied by $4\pi k^2$; e.g.,

$$
T(k) = 4\pi k^2 T^{0th}(k), \quad Y(k) = 4\pi k^2 Y^{0th}(k), \dots, \quad \Sigma_{\text{axi}\phi}(k) = 4\pi k^2 \Sigma_{\text{axi}\phi}^{0th}(k), \quad \text{etc.} \tag{18}
$$

IV. ISOTROPIC RELATIONSHIPS

For isotropy, $\mathbf{Q}_{\phi}(\mathbf{k})$ and $\mathbf{Q}(\mathbf{k})$ are functions of *k* such that Eq. [\(13\)](#page-2-0) becomes

$$
E_{\phi}(k) = 4\pi k^2 \mathbf{Q}_{\phi}(k), \quad E(k) = 4\pi k^2 \mathbf{Q}(k). \tag{19}
$$

For isotropy, $\langle \hat{u}_i(\mathbf{k}) \hat{u}_j^*(\mathbf{k}) \rangle$ has a simple form that follows from the incompressibility condition $k_i\hat{u}_i(\mathbf{k}) = 0$ (i.e., the component of $\hat{u}_i(\mathbf{k})$ parallel to **k** is zero); namely,

$$
\langle \widehat{u}_i(\mathbf{k})\widehat{u}_j^*(\mathbf{k})\rangle = \left(\delta_{ij} - \frac{k_ik_j}{k^2}\right)\frac{E(k)}{4\pi k^2},\tag{20}
$$

from which $4\pi k^2 \langle \widehat{u}_i(\mathbf{k}) \widehat{u}_i^*(\mathbf{k}) \rangle = 2E(k), k_i \langle \widehat{u}_i(\mathbf{k}) \widehat{u}_j^*(\mathbf{k}) \rangle = 0$, etc.

V. BHT ASYMPTOTIC ASSUMPTIONS

Batchelor, Howells, and Townsend [\[1\]](#page-15-0) made three assumptions that are clearly described by YS1 [\[6\]](#page-15-0). The first BHT assumption is to neglect the time-derivative term in Eq. [\(2\)](#page-1-0); here, that is equivalent to $T(k) = 0$, and $Y(k) = 0$; we do not apply the first BHT assumption because we derive exact statistical equations for precise DNS analysis. The second BHT assumption is statistical independence of scalar fluctuations and velocity field; i.e., "decoupling of velocity and scalar modes" [\[6\]](#page-15-0), and that velocity contributes to **V**(**k**) at relatively high wave numbers, and that the scalar contributes to **V**(**k**) at relatively low wave numbers [\[6\]](#page-15-0). Combined with orthogonality of the Fourier components (see YS1 [\[6\]](#page-15-0)), which follows from assuming homogeneity, the second BHT assumption gives (see YS1 $[6]$)

$$
\mathbf{V}(\mathbf{k}) = \langle \widehat{u}_i(\mathbf{k}) \widehat{u}_j^*(\mathbf{k}) \rangle \left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \right\rangle + \mathbf{e}_2(\mathbf{k}) \equiv \mathbf{Z}(\mathbf{k}) + \mathbf{e}_2(\mathbf{k}). \tag{21}
$$

Here, we retain the error of assumption 2, namely, $\mathbf{e}_2(\mathbf{k})$; $\mathbf{e}_2(\mathbf{k})$ must be evaluated from Eq. [\(11\)](#page-2-0) using DNS such that our statistical equations remain exact (hence independent of the assumption of homogeneity). The third BHT assumption is isotropy of velocity and scalar fields at all scales; we do not assume isotropy.

Integrating Eq. (21) over the spherical surface in **k** space, as in Eq. [\(13\)](#page-2-0), and using notation Eq. (14) gives

$$
V(k) = Z(k) + e_2(k).
$$
 (22)

VI. LOCAL ISOTROPY OF THE SCALAR FIELD AT DISSIPATION SCALES WITH NO RESTRICTION ON THE VELOCITY FIELD

Assuming local isotropy of the scalar field at dissipation scales such that

$$
\left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \right\rangle = \frac{1}{3} \delta_{ij} \left\langle \frac{\partial \phi}{\partial x_n} \frac{\partial \phi}{\partial x_n} \right\rangle = \frac{1}{3} \delta_{ij} \frac{\chi}{2D},\tag{23}
$$

substitution of which into Eq. [\(21\)](#page-3-0) and using $\langle \hat{u}_i(\mathbf{k})\hat{u}_j^*(\mathbf{k})\rangle \delta_{ij} = \langle \hat{u}_i(\mathbf{k})\hat{u}_i^*(\mathbf{k})\rangle = 2\mathbf{Q}(\mathbf{k})$ gives

$$
\mathbf{V}(\mathbf{k}) = \mathbf{Q}(\mathbf{k}) \frac{\chi}{3D} + \mathbf{e}_{\text{iso}\phi}(\mathbf{k}) + \mathbf{e}_2(\mathbf{k}),\tag{24}
$$

where

$$
\mathbf{e}_{\text{iso}\phi}(\mathbf{k}) \equiv \langle \widehat{u}_i(\mathbf{k}) \widehat{u}_j^*(\mathbf{k}) \rangle \left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \right\rangle - \mathbf{Q}(\mathbf{k}) \frac{\chi}{3D}.
$$
 (25)

Since substituting Eq. (25) into Eq. (24) reproduces Eq. [\(21\)](#page-3-0), we see that **e**iso*^φ*(**k**) is the error of assuming local isotropy of the scalar field at dissipation scales; i.e., Eq. (23), as well as inhomogeneity, if any; **e**iso*^φ*(**k**) must be evaluated from Eq. (25) using DNS such that our statistical equation remains exact. Substitute Eq. (24) into Eq. [\(12\)](#page-2-0) and divide by D^2k^4 . Then Eq. (12), which is the same as Eq. (3) , can be written, without approximation, as

$$
\sum_{\text{iso}\phi}(\mathbf{k}) + \frac{\mathbf{S}(\mathbf{k})}{D^2 k^4} + \mathbf{Q}(\mathbf{k}) \frac{\chi}{3D^3 k^4} = \mathbf{Q}_{\phi}(\mathbf{k}),\tag{26}
$$

$$
\sum_{\text{iso}\phi}(\mathbf{k}) \equiv \frac{-\mathbf{T}(\mathbf{k}) - \mathbf{Y}(\mathbf{k}) + \mathbf{X}(\mathbf{k}) + \mathbf{e}_{\text{iso}\phi}(\mathbf{k}) + \mathbf{e}_2(\mathbf{k})}{D^2 k^4}.
$$
 (27)

The subscript iso*φ* on two quantities above is a mnemonic for this locally isotropic scalar case; the other quantities could have that subscript; that excessive notation is avoided here and similarly in the following sections as well. Note that Eqs. (26) and (27) are obtained without any assumption about the symmetry of the velocity field, e.g., without isotropy, and there is no assumption about symmetry of the scalar field except at dissipation scales. Gathering five statistics into $\sum_{i\in\phi}$ (**k**) in Eq. (27) is useful because $\sum_{\text{iso}\phi}(\mathbf{k})$ will be shown below to be the deviation from asymptotic formulas.

VII. ISOTROPIC VELOCITY FIELD WITH NO RESTRICTION ON THE SCALAR FIELD AND THE OUTCOME OF AVERAGING OVER ALL DIRECTIONS OF k

The DNS velocity fields in YS1 [\[6\]](#page-15-0) and YS2 [\[7\]](#page-15-0) are isotropic, and their average includes averaging over all directions of **k**. Substituting Eq. [\(20\)](#page-3-0) into the first term in Eq. [\(21\)](#page-3-0) gives

$$
\langle \widehat{u}_i(\mathbf{k})\widehat{u}_j^*(\mathbf{k})\rangle \left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \right\rangle = \left(\delta_{ij} - \frac{k_i k_j}{k^2}\right) \frac{E(k)}{4\pi k^2} \left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \right\rangle = \left(\frac{\chi}{2D} - \frac{k_i k_j}{k^2} \left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \right\rangle \right) \frac{E(k)}{4\pi k^2}.
$$
\n(28)

Integrating $k_i k_j / k^2$ over a spherical surface in **k** space, as in Eq. [\(13\)](#page-2-0), gives zero if $i \neq j$ and $4\pi k^2/3$ if $i = j$, i.e., $(4\pi k^2/3)\delta_{ij}$. Then,

$$
\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta k^2 \sin(\theta) \left(\frac{\chi}{2D} - \frac{k_i k_j}{k^2} \left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \right\rangle \right) \frac{E(k)}{4\pi k^2} = \frac{\chi}{3D} E(k). \tag{29}
$$

Thus, that same integration applied to Eq. (21) and using the notation in Eq. (14) gives

$$
V(k) = E(k)\frac{\chi}{3D} + e_{\text{isou}}(k) + e_2(k),
$$
\n(30)

where

$$
e_{\text{isou}}(k) \equiv Z(k) - E(k)\frac{\chi}{3D}.
$$
\n(31)

Substituting Eq. (31) into Eq. [\(30\)](#page-4-0) reproduces Eq. [\(22\)](#page-3-0); thus, we see that $e_{\text{isou}}(k)$ is the error of assuming isotropy of the velocity field combined with an average over all directions of **k**, as well as inhomogeneity, if any. To retain exact statistical equations, $e_{\text{isou}}(k)$ must be evaluated from Eq. (31).

Substituting Eq. [\(30\)](#page-4-0) into Eq. [\(15\)](#page-2-0) and dividing by D^2k^4 gives

$$
\Sigma_{\text{isou}}(k) + \frac{S(k)}{D^2 k^4} + E(k) \frac{\chi}{3D^3 k^4} = E_{\phi}(k),\tag{32}
$$

$$
\Sigma_{\text{isou}}(k) \equiv \frac{-T(k) - Y(k) + X(k) + e_{\text{isou}}(k) + e_2(k)}{D^2 k^4}.
$$
\n(33)

The statistics in Eqs. [\(26\)](#page-4-0) and [\(27\)](#page-4-0) are spectral and cospectral densities, whereas the statistics in Eqs. (32) and (33) are wave-number spectra and cospectra. That difference is very significant because Eqs. (32) and (33) rely on averaging over all directions of **k**, whereas Eqs. [\(26\)](#page-4-0) and [\(27\)](#page-4-0) do not. Thus, Eqs. [\(26\)](#page-4-0) and [\(27\)](#page-4-0) are applicable to investigation of anisotropy effects; Eqs. (32) and (33) are not. Note that Eqs. (32) and (33) require no assumption about the symmetry of the scalar field, in contrast to Eqs. (26) and (27) .

VIII. AXISYMMETRIC SCALAR FLUCTUATIONS WITH ISOTROPIC VELOCITY FIELD

Consider that the source $s(\mathbf{x},t)$ of the scalar has a single axis of symmetry, such as the direction of a spatially uniform mean scalar gradient. That gradient can be time dependent. Alternatively, the scalar fluctuations could be axisymmetric and freely decaying, etc. A unit vector in the direction of that axis is denoted **z** and $k_z \equiv \mathbf{z} \cdot \mathbf{k} = k \cos(\theta)$; θ is the angle between **z** and **k**. In this section, the average cannot be over all directions of **k**, although averaging over directions of **k** that are perpendicular to **z** can be applied. Also,

$$
\frac{k_z^2}{k^2} = \cos^2(\theta) = \mu^2, \quad \text{where} \quad \mu \equiv \cos(\theta). \tag{34}
$$

Statistics can be given as functions of arguments k, k_z , or equivalently, k, θ , or k, μ as simplifications to dependence on **k**. Below, for statistics that depend on the isotropic velocity field, but not on the scalar fluctuation, the argument is k only. With x and y the coordinate axes perpendicular to z , we have

$$
\frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_i} = \frac{\partial \phi}{\partial z} \frac{\partial \phi}{\partial z} + \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \frac{\partial \phi}{\partial y}.
$$
(35)

The ratio of parallel to perpendicular scalar-gradient variances is

$$
g_{\phi} \equiv \left\langle \frac{\partial \phi}{\partial z} \frac{\partial \phi}{\partial z} \right\rangle / \left\langle \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} \right\rangle = \left\langle \frac{\partial \phi}{\partial z} \frac{\partial \phi}{\partial z} \right\rangle / \frac{1}{2} \left\langle \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \frac{\partial \phi}{\partial y} \right\rangle.
$$
 (36)

Within Eq. [\(21\)](#page-3-0) we have the contraction of an isotropic second-rank tensor $\langle \hat{u}_i(\mathbf{k}) \hat{u}_j^*(\mathbf{k}) \rangle$ with an axisymmetric second-rank tensor *∂φ ∂xi ∂φ* $\frac{\partial \phi}{\partial x_j}$); the result is given in Appendix [B](#page-15-0) as follows:

$$
\langle \widehat{u}_i(\mathbf{k})\widehat{u}_j^*(\mathbf{k})\rangle \left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \right\rangle = \frac{\chi}{3D} \frac{E(k)}{4\pi k^2} - P_2(\mu) F \frac{\chi}{3D} \frac{E(k)}{4\pi k^2},\tag{37}
$$

wherein

$$
P_2(\mu) = \frac{3}{2}\cos^2(\theta) - \frac{1}{2} = \frac{3}{2}\left(\mu^2 - \frac{1}{3}\right)
$$
 (38)

is the second-order Legendre polynomial, and

$$
F \equiv \frac{g_{\phi} - 1}{g_{\phi} + 2}.
$$
\n(39)

The new term proportional to *F* in Eq. [\(37\)](#page-5-0) arises because of the axisymmetry of the scalar field at dissipation scales independent of the cause of that axisymmetry. Local isotropy of the scalar at dissipation scales corresponds to $g_{\phi} = 1$ [see Eq. [\(36\)](#page-5-0)], in which case, from Eq. (39) $F = 0$. Note that the two terms in Eq. [\(37\)](#page-5-0) are zero- and second-order terms of a Legendre-polynomial expression. Substitute Eq. [\(37\)](#page-5-0) into Eq. [\(21\)](#page-3-0); then the exact equation for $V(k,\mu)$ is

$$
\mathbf{V}(k,\mu) = \frac{\chi}{3D} \frac{E(k)}{4\pi k^2} - P_2(\mu) F \frac{\chi}{3D} \frac{E(k)}{4\pi k^2} + \mathbf{e}_{\text{axi}\phi}(k,\mu) + \mathbf{e}_2(k,\mu),\tag{40}
$$

where

$$
\mathbf{e}_{\text{axi}\phi}(k,\mu) \equiv \langle \widehat{u}_i(\mathbf{k})\widehat{u}_j^*(\mathbf{k})\rangle \left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \right\rangle - \left[\frac{\chi}{3D} \frac{E(k)}{4\pi k^2} - P_2(\mu) F \frac{\chi}{3D} \frac{E(k)}{4\pi k^2} \right]. \tag{41}
$$

Since substituting Eq. (41) into Eq. (40) reproduces Eq. [\(21\)](#page-3-0), we see that $\mathbf{e}_{\text{axi}\phi}(k,\mu)$ is the error of assuming local axisymmetry of the scalar field and isotropy of the velocity field; $\mathbf{e}_{\text{axi}\phi}(k,\mu)$ must be calculated from DNS to maintain exact statistical equations. Substitute Eq. (40) into Eq. [\(12\)](#page-2-0) and divide by D^2k^4 ; then the exact theory for axisymmetric scalar fluctuations at dissipation scales with an isotropic velocity field is

$$
\sum_{\text{axi}\phi}(k,\mu) + \frac{\mathbf{S}(k,\mu)}{D^2 k^4} + \frac{E(k)}{4\pi k^2} \frac{\chi}{3D^3 k^4} - \frac{E(k)}{4\pi k^2} P_2(\mu) F \frac{\chi}{3D^3 k^4} = \mathbf{Q}_{\phi}(k,\mu),\tag{42}
$$

$$
\sum_{\text{axi}\phi}(k,\mu) \equiv \frac{-\mathbf{T}(k,\mu) - \mathbf{Y}(k,\mu) + \mathbf{X}(k,\mu) + \mathbf{e}_{\text{axi}\phi}(k,\mu) + \mathbf{e}_2(k,\mu)}{D^2 k^4}.
$$
 (43)

If the scalar is locally isotropic at dissipation scales, i.e., $F = 0$, then Eqs. (42) and (43) become Eqs. [\(26\)](#page-4-0) and [\(27\)](#page-4-0), except $E(k)/4\pi k^2$ appears in Eq. (42) instead of **Q(k)** in Eq. (26) because the velocity field is assumed isotropic to obtain Eqs. (42) and (43). An average over all directions of **k**, as in Eq. [\(13\)](#page-2-0), includes an average over θ from 0 to π such that the average of $P_2(\mu)$ is 0 and also eliminates dependence on μ ; then Eqs. (42) and (43) become Eqs. [\(32\)](#page-5-0) and [\(33\)](#page-5-0).

IX. UNIFORM SCALAR-GRADIENT SOURCE WITH ISOTROPIC VELOCITY FIELD

Applying Reynolds decomposition to the equation for a scalar $\Phi = \Phi_0 + \phi$, where Φ_0 is the mean and ϕ is the scalar fluctuation, the advective term gives $\mathbf{u} \cdot \nabla \Phi = \mathbf{u} \cdot \nabla \Phi_0 + \mathbf{u} \cdot \nabla \phi$, which would appear on the left side of Eq. [\(1\)](#page-1-0). Hence, the source on the right side of Eq. (1) is $s(\mathbf{x},t) = -\mathbf{u} \cdot \nabla \Phi_0$, as in YS2 [\[7\]](#page-15-0). Let the scalar mean gradient be uniform of magnitude $G \equiv |\nabla \Phi_0|$ and in the direction of unit vector **z**, and $u_z \equiv \mathbf{z} \cdot \mathbf{u} = z_i u_i$; then $s(\mathbf{x}, t) = -Gz_i u_i$ in Eq. [\(1\)](#page-1-0), and using Eq. [\(20\)](#page-3-0), Eq. [\(8\)](#page-2-0) gives

$$
\mathbf{S}(\mathbf{k}) = \mathbf{S}(k,\mu) = G^2 z_i z_j \langle \widehat{u}_i(\mathbf{k}) \widehat{u}_j^*(\mathbf{k}) \rangle = G^2 z_i z_j \left(\delta_{ij} - \frac{k_i k_j}{k^2} \right) \frac{E(k)}{4\pi k^2}
$$

$$
= G^2 (1 - \mu^2) \frac{E(k)}{4\pi k^2} = \frac{2}{3} G^2 \frac{E(k)}{4\pi k^2} - \frac{2}{3} G^2 P_2(\mu) \frac{E(k)}{4\pi k^2}.
$$
(44)

We used $1 - \mu^2 = \frac{2}{3} - \frac{2}{3} [\frac{3}{2}(\mu^2 - \frac{1}{3})] = \frac{2}{3} - \frac{2}{3}P_2(\mu)$. From Eq. [\(38\)](#page-5-0), $P_2(\mu)$ is the second-order Legendre polynomial, and the two terms in Eq. (44) are the first two terms of a Legendre-polynomial expansion. This Eq. (44) is similar to Eq. [\(36\)](#page-5-0) of Herr *et al.* [\[10\]](#page-15-0). Whereas Eq. [\(37\)](#page-5-0) contains a term

containing $P_2(\mu)F$ caused by local axisymmetry of scalar-gradient variances, which might vanish at infinite Peclet number, Eq. [\(44\)](#page-6-0) contains the direct effect of the mean scalar gradient that is also proportional to $P_2(\mu)$, which is expected to not vanish at infinite Peclet number. The integration of Eq. [\(44\)](#page-6-0) over a spherical surface in **k** space, as in Eq. [\(13\)](#page-2-0), gives the wave-number spectrum

$$
S(k) = \frac{2}{3}G^2E(k).
$$
 (45)

Consider the study of anisotropy using expansion in Legendre polynomials as was done by Gotoh *et al.* [\[14\]](#page-16-0). Expansion in Legendre polynomials reveals the anisotropy of $\mathbf{Q}_{\phi}(k,\mu)$ and makes clear what would be discarded by averaging over all directions of **k**. Averaging over directions of **k** perpendicular to the mean scalar gradient can be applied. Below, only zero- and second-order Legendre polynomials appear; however, if $\sum_{axi\phi}(k,\mu)$ is not neglected, then that term can generate nonzero Legendre-polynomial terms in $\mathbf{Q}_{\phi}(k,\mu)$ of even order fourth and greater, as well as modify the zero- and second-order Legendre-polynomial terms in $\mathbf{Q}_{\phi}(k,\mu)$. Herr *et. al.* [\[10\]](#page-15-0) state that "the total root mean square fluctuation is conserved by the angular redistribution." A uniform scalar-gradient source causes the scalar fluctuations to be axisymmetric; also, the DNS velocity field is isotropic. Then Eqs. [\(42\)](#page-6-0) and [\(43\)](#page-6-0) apply with $S(k,\mu)$ as in Eq. [\(44\)](#page-6-0). Substituting Eq. (44) into Eq. [\(42\)](#page-6-0) and neglecting $\sum_{axi\phi}(k,\mu)$ and multiplying by $4\pi k^2$, Eq. (42) becomes

$$
E(k)\left(\frac{\chi}{3D^3k^4} + \frac{2}{3}\frac{G^2}{D^2k^4}\right) - E(k)P_2(\mu)\left(F\frac{\chi}{3D^3k^4} + \frac{2}{3}\frac{G^2}{D^2k^4}\right) = 4\pi k^2 \mathbf{Q}_{\phi}(k,\mu). \tag{46}
$$

Factoring from Eq. (46) the BHT formula, i.e., $E_{\phi}(k) = (\chi/3D^3)k^{-4}E(k)$, and using the definition of D_T/D in Eq. [\(62\)](#page-10-0), then Eq. (46) becomes

$$
4\pi k^2 \mathbf{Q}_{\phi}(k,\mu) = (\chi/3D^3)k^{-4}E(k)\left[\left(1 + \frac{D}{D_T}\right) - P_2(\mu)\left(F + \frac{D}{D_T}\right) \right] \tag{47}
$$

$$
=4\pi k^2 Q_{\phi}^{0^{\text{th}}}(k) + P_2(\mu)4\pi k^2 Q_{\phi}^{2^{\text{nd}}}(k). \tag{48}
$$

In Eq. (48) we have defined the zero- and second-order coefficients of the expansion of $4\pi k^2 \mathbf{Q}_\phi(k,\mu)$ in Legendre polynomials as follows:

$$
4\pi k^2 Q_{\phi}^{0^{\text{th}}}(k) = E_{\phi}(k) = (\chi/3D^3)k^{-4}E(k)\bigg(1 + \frac{D}{D_T}\bigg),\tag{49}
$$

$$
4\pi k^2 Q_{\phi}^{2^{nd}}(k) = -(\chi/3D^3)k^{-4}E(k)\bigg(F + \frac{D}{D_T}\bigg). \tag{50}
$$

Of course, $Q_{\phi}^{0^{\text{th}}}(k)$ and $Q_{\phi}^{2^{\text{nd}}}(k)$ are not functions of μ . Consider the case of local isotropy of scalar gradients (i.e., $F \rightarrow 0$) and the mean-squared scalar gradient much greater than G^2 (i.e., *D*/*D_T* → 0), then $E_{\phi}(k) = 4\pi k^2 Q_{\phi}^{0^{th}}(k)$ → $(\chi/3D^3)k^{-4}E(k)$ and $4\pi k^2 Q_{\phi}^{2^{nd}}(k)$ → 0. That is, the BHT formula is obtained provided that $\sum_{axi\phi}(k,\mu)$ is negligible. The ratio of $-Q_\phi^{2^{nd}}(k)$ to $Q_\phi^{0^{th}}(k)$ is

$$
a \equiv \frac{-Q_{\phi}^{\text{2nd}}(k)}{Q_{\phi}^{\text{0th}}(k)} = \frac{F + \frac{D}{D_T}}{1 + \frac{D}{D_T}},
$$
\n(51)

which does not depend on *k*, provided that $\sum_{axi\phi}(k,\mu)$ is negligible. The term $\sum_{axi\phi}(k,\mu)$ can cause *a* to depend on *k* as well as cause higher-order Legendre polynomial terms in $4\pi k^2 \mathbf{Q}_\phi(k,\mu)$; that is similar to the effect of those EDQNM terms in Herr *et al.* [\[10\]](#page-15-0) that *"*redistribute the scalar in the angular direction in **k** space."

Inertial-diffusive range formulas are obtained by substituting the inertial-range formula $E(k)$ = $C_K \epsilon^{2/3} k^{-5/3}$ into Eq. [\(47\)](#page-7-0) or equivalently into Eqs. [\(49\)](#page-7-0) and [\(50\)](#page-7-0). We obtain

$$
4\pi k^2 Q_{\phi}^{0^{\text{th}}}(k) = E_{\phi}(k) = \frac{C_K}{3} \chi \epsilon^{2/3} D^{-3} k^{-17/3} \bigg(1 + \frac{D}{D_T} \bigg),\tag{52}
$$

$$
4\pi k^2 Q_{\phi}^{\mathbb{P}^{\text{d}}}(k) = -\frac{C_K}{3} \chi \epsilon^{2/3} D^{-3} k^{-17/3} \bigg(F + \frac{D}{D_T} \bigg). \tag{53}
$$

The dependence of Eqs. (52) and (53) on *F* and D/D_T shows that R_λ can be large enough to give an inertial range, but if Sc is small enough, then Pe can be sufficiently small that the assumed asymptotic conditions $F \to 0$ and $D/D_T \to 0$ are not fulfilled.

X. FREELY DECAYING SCALAR FLUCTUATIONS

For a freely decaying scalar, this section considers the locally isotropic scalar and thus Eqs. [\(26\)](#page-4-0) and [\(27\)](#page-4-0). For freely decaying scalar fluctuations, $s(\mathbf{x},t) = 0$ such that $\mathbf{X}(\mathbf{k}) = 0$, and $\mathbf{S}(\mathbf{k}) = 0$ such that Eqs. (26) and (27) become

$$
\sum_{\text{iso}\phi}(\mathbf{k}) + \mathbf{Q}(\mathbf{k}) \frac{\chi}{3D^3 k^4} = \mathbf{Q}_{\phi}(\mathbf{k}),\tag{54}
$$

$$
\sum_{\text{iso}\phi}(\mathbf{k}) = \frac{-\mathbf{T}(\mathbf{k}) - \mathbf{Y}(\mathbf{k}) + \mathbf{e}_{\text{iso}\phi}(\mathbf{k}) + \mathbf{e}_2(\mathbf{k})}{D^2 k^4}.
$$
 (55)

Spectral and cospectral densities appear in Eq. (54) and (55) rather than wave-number spectra and cospectra because we do not assume isotropy of the scalar at all wave vectors. If $\sum_{i\in\phi}$ (**k**) is neglected, and Eq. (54) is integrated over a spherical surface in **k** space, as in Eq. [\(13\)](#page-2-0), then Eq. (54) becomes the BHT theory; i.e., $E_{\phi}(k) = (\chi/3D^3)k^{-4}E(k)$.

A. Comparison with DNS of freely decaying scalar fluctuations with averaging over all directions of k

The freely decaying case has been investigated using DNS by YS1 [\[6\]](#page-15-0), where the velocity field is isotropic and the scalar fluctuations became more isotropic as time increased. They integrate over a spherical surface in **k** space, as in Eq. [\(13\)](#page-2-0); if the scalar field is anisotropic, then only the zero-order Legendre-polynomial term remains. Performing that integration on Eqs. (54) and (55) gives the wave-number spectral result

$$
\Sigma_{\text{iso}\phi}(k) + E(k)\frac{\chi}{3D^3k^4} = E_{\phi}(k),\tag{56}
$$

$$
\Sigma_{\text{iso}\phi}(k) = \frac{-T(k) - Y(k) + e_{\text{iso}\phi}(k) + e_2(k)}{D^2 k^4}.
$$
\n(57)

They state the inertial range formula $E(k) = C_K \epsilon^{2/3} k^{-5/3}$, and $C_K = 1.62$. Substituting $E(k) =$ $C_K \epsilon^{2/3} k^{-5/3}$ in Eq. (56) results in the BHT inertial-diffusive range formula

$$
E_{\phi}(k) = \frac{C_K}{3} \chi \epsilon^{2/3} D^{-3} k^{-17/3} + \Sigma_{\text{iso}\phi}(k),
$$
 (58)

which agrees with Eq. (1.1) of YS1 [\[6\]](#page-15-0) if $\Sigma_{\text{iso}\phi}(k)$ is neglected.

Of the terms in Eq. (57), YS1 [\[6\]](#page-15-0) graph $T(k)$; $T(k)$ is seen to be negligible for Sc = 1/512 and Sc = 1*/*2048 in their Figs. 4(b) and 5. The freely decaying DNS is statistically steady for the velocity but not for the scalar. If the average does not include a time average, then $Y(k) = Dk^2 \partial E_{\phi}(k)/\partial t \neq 0$ (if the average does include a time average, see Sec. [VII](#page-4-0) of Hill $[15]$). From Eqs. (56) and (57) we want to determine if $Y(k)/D^2k^4$ is small relative to $E_{\phi}(k)$; the ratio of those two quantities is

$$
[Y(k)/D^2k^4]/E_{\phi}(k) = [\partial E_{\phi}(k)/\partial t]/Dk^2E_{\phi}(k) = \frac{1}{Dk^2}\frac{\partial \ln[E_{\phi}(k)]}{\partial t}.
$$
 (59)

YS1 [\[6\]](#page-15-0) find that after a transient period, the scalar variance decays approximately exponentially. Let the exponential decay be proportional to $\exp(-t/\tau)$; Fig. [1\(a\)](#page-12-0) of YS1 can be used to give $\tau = 1.7T_E$ for Sc = $1/512$ and $\tau = 0.90T_E$ for Sc = $1/2048$, where T_E is their large-eddy turnover time. With $\exp(-t/\tau)$ as an estimate for the decay of $E_{\phi}(k)$, we have $\partial \ln \left[E_{\phi}(k) \right] / \partial t = -1/\tau$ such that Eq. [\(59\)](#page-8-0) is $-1/Dk^2\tau$. The estimate by BHT is that $1/Dk^2 \ll \tau$, so that $1/Dk^2\tau$ is very small. Although we expect that the time scale of $E_{\phi}(k)$ decreases relative to the time scale of the scalar variance with increasing *k*, $1/Dk^2$ also decreases with increasing *k*. Hence, from Eq. [\(59\)](#page-8-0), $Y(k)/D^2k^4$ is small relative to $E_{\phi}(k)$ in Eqs. [\(56\)](#page-8-0) and [\(57\)](#page-8-0); quantification of $Y(k)$ by DNS is desirable. The comparison of the right side of equation (4.5) in YS1 [\[6\]](#page-15-0) with the spectral density of the advective term $V(k)$ (triangles and diamonds in their Figs. 4 and 5) suggests that $e_2(k)/D^2k^4$ is small relative to $E_\phi(k)$. The isotropy of their DNS and their average over all directions of **k** causes *e*iso*^φ*(*k*) to be negligible. Therefore, all terms in Eq. [\(57\)](#page-8-0) are expected to be much smaller than the other terms in Eq. [\(56\)](#page-8-0); thus, $\Sigma_{\text{iso}\phi}(k)$ is a relatively small term in Eq. [\(56\)](#page-8-0).

In their Fig. 7, YS1 $[6]$ show the ratio of the two right-most terms in Eq. [\(56\)](#page-8-0), namely, $E_{\phi}(k)/[E(k)\chi/(3D^3k^4)]$. The deviations from unity in that figure are caused by $\Sigma_{\text{iso}\phi}(k)$ in Eq. [\(57\)](#page-8-0); that cannot be otherwise (unless there is a computational error) because Eqs. [\(56\)](#page-8-0) and [\(57\)](#page-8-0) are obtained without approximation. In the inertial range, near $k\eta = 0.05$, their Fig. 7(b) shows about 50% and 20% deviation from the BHT formula for $Sc = 1/512$ and $1/2048$, respectively. With reference to their Fig. 3(d), they state an approximately 20% deviation relative to the BHT inertial-diffusive range formula $(C_K/3)\chi \epsilon^{2/3}D^{-3}k^{-17/3}$ in Eq. [\(58\)](#page-8-0) for Sc = 1/2048; that deviation is caused by $\Sigma_{\text{iso}\phi}(k)$. Their Fig. 3(d) shows little deviation from the $-17/3$ power law at $k\eta = 0.05$ for Sc = 1/512 and 1/2048, which suggests that $\Sigma_{\text{iso}\phi}(k)$ has a nearly $-17/3$ power law in an inertial-diffusive range. Quantification of $\Sigma_{\text{iso}\phi}(k)$ and its constituent terms is needed to understand their observed deviations from BHT theory.

Chasnov [\[11\]](#page-16-0) calculates an LES-velocity-field simulation to obtain extensive inertial-diffusive ranges. Note that his values of Sc are not known; but he states that they are much less than unity. Consider his Fig. 3(b) that shows the scalar spectrum for the freely decaying case. At wave numbers corresponding to the inertial range in YS1 [\[6\]](#page-15-0), his scalar spectra are above the BHT inertial-diffusive range formula by amounts that are very similar to those in Fig. 3 of YS1 for their smaller $Sc =$ 1*/*512 and 1*/*2048. Furthermore, Chasnov's Fig. 3(b) shows that the scalar spectra are close to the BHT inertial-diffusive range formula for $k/k_{C-O} \gtrsim 40$, where $k_{C-O} \equiv (\varepsilon/D^3)^{1/4} = \text{Sc}^{3/4}/\eta$ and $\eta \equiv (v^3/\varepsilon)^{1/4}$. For Sc = 1/512, $k/k_{C-O} = 40$ is $k\eta = 0.37$, and for Sc = 1/2048, $k\eta = 0.13$. At those two wave numbers for those smallest Sc values, we see in Fig. 7 of YS1 [\[6\]](#page-15-0) that their scalar spectra are also close to the BHT inertial-diffusive range formula. That is so despite the fact that $k\eta = 0.37$ and 0.13 are in the energy spectrum's dissipation range for the DNS of YS1.

XI. MEAN-SCALAR-GRADIENT CASE WITH AVERAGING OVER ALL DIRECTIONS OF k

The mean scalar gradient causes the scalar fluctuations to be axisymmetric such that the required equations are Eqs. [\(42\)](#page-6-0) and [\(43\)](#page-6-0). Now consider the DNS of the mean-uniform-scalar-gradient case by YS2 [\[7\]](#page-15-0), who used the integral over a spherical surface in **k** space, as in Eq. [\(13\)](#page-2-0). That integration causes the terms containing $P_2(\mu)$ in Eqs. [\(42\)](#page-6-0) and [\(44\)](#page-6-0) to be zero; e.g., $S(k,\mu)$ becomes Eq. [\(45\)](#page-7-0). Also, only the zero-order Legendre-polynomial term is nonzero for all quantities, as in Eqs. [\(17\)](#page-3-0) and [\(18\)](#page-3-0). Thus, all statistics become wave-number statistics having argument k , not k, μ . After multiplying by $4\pi k^2$ and using Eqs. [\(17\)](#page-3-0) and [\(18\)](#page-3-0), Eqs. [\(42\)](#page-6-0) and [\(43\)](#page-6-0) become

$$
\Sigma_{\text{axi}\phi}(k) + E(k) \left(\frac{2G^2}{3D^2 k^4} + \frac{\chi}{3D^3 k^4} \right) = E_{\phi}(k),\tag{60}
$$

$$
\Sigma_{\text{axi}\phi}(k) = \frac{-T(k) - Y(k) + X(k) + e_{\text{axi}\phi}(k) + e_2(k)}{D^2 k^4}.
$$
\n(61)

R_λ	140	140	240	240	240	390
Sc	1/128	1/512	1/128	1/512	1/2048	1/2048
Pe	11	2.8	32	7.9	2.0	4.9
D_T/D	3	0.4	7.4	1.38	0.17	0.66
g_{ϕ}	0.91	0.66	1.03	0.79	0.63	0.61
\overline{F}	-0.031	-0.13	0.01	-0.075	-0.14	-0.15
a	0.23	0.68	0.13	0.70	0.87	0.54

TABLE I. Values obtained from Table III of YS2 [\[7\]](#page-15-0); note that Pe = ReSc, and Re = $R_{\lambda}^2/15$. *F* and *a* are calculated from D_T/D and g_{ϕ} .

With neglect of $\Sigma_{axi\phi}(k)$, Eq. [\(60\)](#page-9-0) retains the proportionality $E_{\phi}(k) \propto k^{-4} E(k)$ of the BHT theory. If $G = 0$ and $\Sigma_{axi\phi}(k)$ is neglected, then Eq. [\(60\)](#page-9-0) is the BHT theory; i.e., $E_{\phi}(k) = (\chi/3D^3)k^{-4}E(k)$.

A. Comparison with DNS having a uniform scalar-gradient source with averaging over all directions of k

The uniform mean-scalar-gradient case was calculated using DNS by YS2 [\[7\]](#page-15-0), who had an isotropic velocity field. Although Eq. [\(23\)](#page-4-0) is reasonable for very large Pe, for the anisotropic (axisymmetric) case of production by a mean scalar gradient, YS2 show in their Table III that $Pe = R_{\lambda}^2$ Sc/15 is not large for the smaller Sc cases and that the ratios of scalar-gradient variances Eq. [\(36\)](#page-5-0) (i.e., g_{ϕ} in their Table III) are not near equality for those smaller Sc cases. That is, local isotropy of the scalar field at dissipation scales and therefore Eq. [\(23\)](#page-4-0) are not accurate for those DNS cases of smaller Sc.

They [\[7\]](#page-15-0) averaged over all directions of **k** such that Eqs. [\(60\)](#page-9-0) and [\(61\)](#page-9-0) apply. In their Fig. 8, YS2 show that $T(k)$ is negligible for $Sc = 1/2048$; see also their Figs. 9(c) and 9(d) for their other Sc cases. The uniform scalar-gradient-source DNS of YS2 is statistically steady. Hence, if the average does not include a time average, then $Y(k) = Dk^2 \partial E_{\phi}(k)/\partial t = 0$. (If the average does include a time average, see Sec. [VII](#page-4-0) of Hill [\[15\]](#page-16-0)). From Eqs. [\(60\)](#page-9-0) and [\(61\)](#page-9-0) we want to compare $Y(k)/D^2k^4$ with $E_{\phi}(k)$; the ratio, $\{[Y(k)/D^2k^4]/E_{\phi}(k)\} \div 2$, i.e., $[\partial E_{\phi}(k)/\partial t]/[2Dk^2E_{\phi}(k)]$, is plotted in Fig. 13 of YS2 [\[7\]](#page-15-0); that ratio is seen to be very close to zero. Therefore, $Y(k)/D^2k^4$ is either zero or very small relative to $E_{\phi}(k)$. In Fig. 8 of YS2, the spectrum of the advective term is about $1/8$ of the gradient-production spectrum; see also their Fig. 9(b) versus Figs. 9(a) and 9(c) for their smaller Sc. Hence, the assertion that the gradient-production-advective cospectrum $X(k)/D^2k^4$ is small relative to $E_{\phi}(k)$ is less certain; DNS quantification is needed. For the same reasons given in Sec. IX A, $e_{axi\phi}(k)/D^2k^4$ and $e_2(k)/D^2k^4$ are expected to be small relative to $E_{\phi}(k)$. This concludes discussion of all terms in $\Sigma_{axi\phi}(k)$ in Eq. [\(61\)](#page-9-0).

Despite the average over all directions of **k** in YS2 [\[7\]](#page-15-0), we can determine from their data the anisotropy parameters F and a as follows. Recall that F defined in Eq. [\(39\)](#page-6-0), which appears in, e.g., Eqs. [\(42\)](#page-6-0) and [\(46\)](#page-7-0), parametrizes the axisymmetry of the scalar field at dissipation scales independent of the cause of that axisymmetry. Recall that *a* defined in Eq. [\(51\)](#page-7-0) is the ratio of the second- and zero-order coefficients of the expansion of $4\pi k^2 \mathbf{Q}_{\phi}(k,\mu)$ in Legendre polynomials. The ratio of eddy diffusivity to molecular diffusivity, denoted D_T/D , is needed here because its value is given in Table III of YS2

$$
\frac{D_T}{D} \equiv \frac{\chi}{2DG^2} = \left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_i} \right\rangle / G^2.
$$
 (62)

The values of *a* in Table I obtained from Eq. [\(51\)](#page-7-0) are not significantly much less than unity. Thus, by their average over all directions of **k**, YS2 [\[7\]](#page-15-0) deleted from their analysis the significant term $Q_{\phi}^{2^{nd}}(k)$ and any higher-order Legendre polynomial terms.

TABLE II. Values of the three terms in Eq. (63) are in rows 3–5 as obtained from Fig. 16 of YS2 [\[7\]](#page-15-0) at the inertial-range wave number $k\eta = 0.05$. Values of the three terms in Eq. (64) are in rows 6–8, as obtained from Fig. 15 of YS2 [\[7\]](#page-15-0) at Chasnov's [\[11\]](#page-16-0) suggested wave numbers $k\eta = 0.74$ for Sc = 1/512 and $k\eta = 0.26$ for $Sc = 1/2048$.

R_{λ}	140	240	240	390
Sc	1/512	1/512	1/2048	1/2048
$E_{\phi}(k)(D/G)^2(3/2\varepsilon^{2/3})k^{17/3}$	3.45	6.04	2.31	3.54
$(1 + \frac{D_T}{D})C_K$	2.27	3.86	1.90	2.69
$\Sigma_{\text{axi}\phi}(k)/E_{\phi}(k)$	0.34	0.36	0.18	0.24
$E_{\phi}(k)/k^{-4}E(k)$	0.440	4.76	0.159	1.47
$\frac{2}{3}(G/D)^2(1+\frac{D_T}{D})$	0.454	5.00	0.154	1.38
$\Sigma_{\text{axi}\phi}(k)/E_{\phi}(k)$	-0.032	-0.050	0.031	0.061

Next, examine the inertial-diffusive range shown in Fig. 16 of YS2 [\[7\]](#page-15-0). In an inertial range where $E(k) = C_K \varepsilon^{2/3} k^{-5/3}$, using Eq. [\(62\)](#page-10-0), Eq. [\(60\)](#page-9-0) can be written as

$$
E_{\phi}(k)(D/G)^2(3/2\varepsilon^{2/3})k^{17/3} = \left(1 + \frac{D_T}{D}\right)C_K + \Sigma_{\text{axi}\phi}(k)(D/G)^2(3/2\varepsilon^{2/3})k^{17/3}.\tag{63}
$$

This is an exact equation for the wave-number spectrum for the inertial range and the case of a uniform mean-scalar-gradient source. For their lowest $R_{\lambda} = 140$, the smallest value of $k\eta$ in the inertial range of the energy spectrum shown in Fig. [1](#page-12-0) of YS2 is $k\eta = 0.03$; for $k\eta \gtrsim 0.06$, the energy spectrum has its spectral bump, i.e., "bottleneck effect," and dissipation range. Thus, to quantify terms in Eq. (63), only the narrow range of wave numbers $0.03 < k\eta < 0.06$ is the relevant inertial range. Figure 16 of YS2 is a plot of the left-hand side (LHS) of Eq. (63) with a dashed line at $C_K = 1.62$ (the ordinate of Fig. 16 of YS2 is mislabeled). Only their curves for their smallest Sc of 1/512 and 1/2048 show nearly constant values of LHS $\equiv E_{\phi}(k)(D/G)^2(3/2\varepsilon^{2/3})k^{17/3}$ in the relevant range $0.03 < k\eta < 0.06$. The LHS of Eq. (63) is obtained from their Fig. 16 at $k\eta = 0.05$; $(1 + \frac{D_T}{D})C_K$ is obtained using the values of D_T/D from Table [I;](#page-10-0) the right-most term in Eq. (63) is obtained from the difference of those two quantities. The result is given in rows $3-5$ in Table II for the relevant $Sc = 1/512$ and $1/2048$. The ratio of the term at the far right in Eq. (63) to *E*_φ(*k*)(*D*/*G*)²(3/2*ε*^{2/3})*k*^{17/3} gives $\Sigma_{axi\phi}(k)/E_{\phi}(k)$ in row 5.

Rows 3–5 in Table II show, as found by YS2 [\[7\]](#page-15-0), that the original BHT formula, LHS = C_K = 1.62, does not apply to this uniform-mean-gradient-source case. The term $(1 + \frac{D_T}{D})C_K$ accounts for most of the value of LHS. However, values of $\Sigma_{axi\phi}(k)/E_{\phi}(k)$ in row 5 in Table II show that the right-most terms in Eqs. [\(60\)](#page-9-0) and (63) are not negligible such that the assumed asymptotic state in which $\Sigma_{axi\phi}(k)$ becomes negligible is not attained in the inertial range of YS2.

Consider the LES velocity-field simulation by Chasnov [\[11\]](#page-16-0) for an estimate of how closely BHT inertial-diffusive asymptotic formulas are approached. For the mean-scalar-gradient case, he calculates the wave-number spectrum, i.e., the zero-order Legendre-polynomial term, such that the second- and higher-order terms are not known. Referring to the wave-number spectra in his Fig. 5, Chasnov states that the BHT inertial-diffusive result "in the far subrange (k/k_C -*O* \gtrsim 80) is well predicted," where $k_{C-O} \equiv (\varepsilon/D^3)^{1/4} = Sc^{3/4}/\eta$ and $\eta \equiv (\nu^3/\varepsilon)^{1/4}$. A value of Sc is not available from his LES, but if Sc = 1/512, then $k/k_{C-O} = 80$ corresponds to $k\eta = 80$ Sc^{3/4} = 0.74; if Sc = 1/2048, then $k/k_{C-O} = 80$ corresponds to $k\eta = 80$ Sc^{3/4} = 0.26. Now, Eq. [\(60\)](#page-9-0) can be written as

$$
\frac{E_{\phi}(k)}{k^{-4}E(k)} = \frac{2G^2}{3D^2} \left(1 + \frac{D_T}{D} \right) + \frac{\Sigma_{\text{axi}\phi}(k)}{k^{-4}E(k)}.
$$
\n(64)

FIG. 1. Left-hand side of Eq. (65) is plotted. $\Lambda = E(k) \frac{2G^2}{3D^2} (1 + \frac{D_T}{D})$. Diamonds and filled circles denote Sc = $1/512$ and Sc = $1/2048$, respectively. From left to right the three graphs correspond to $R_{\lambda} = 140, 240$, and 390, respectively.

Since YS2 [\[7\]](#page-15-0) used $G = 1$, we have $G/D = 1/D = v^{-1}$ Sc, and *v* is in their Table I. The ordinate of Fig. 15 of YS2 is $E_{\phi}(k)/k^{-4}E(k)$ which we read at Chasnov's [\[11\]](#page-16-0) suggested wave numbers *kη* = 0*.*74 for Sc = 1*/*512 and *kη* = 0*.*26 for Sc = 1*/*2048. The first term on the right-hand side of Eq. [\(64\)](#page-11-0) is known from D_T/D in Table [I](#page-10-0) and the known values of G/D . The difference of those two terms in Eq. [\(64\)](#page-11-0) gives the right-most term in Eq. [\(64\)](#page-11-0). Finally, the right-most term in Eq. [\(64\)](#page-11-0) divided by the left-most term is $\Sigma_{axi\phi}(k)/E_{\phi}(k)$. The result is given in rows 6–8 in Table II for the relevant $Sc = 1/512$ and $1/2048$. Rows 6–8 in Table II show that Eqs. [\(64\)](#page-11-0) and [\(60\)](#page-9-0) nearly balance without the terms containing $\Sigma_{axi\phi}(k)$ when the data of YS2 [\[7\]](#page-15-0) are evaluated at Chasnov's [\[11\]](#page-16-0) wave numbers. As $\Sigma_{axi\phi}(k)$ becomes insignificant, the generalized BHT asymptote is approached. Chasnov determined his wave numbers from the inertial range of his LES, whereas $k\eta = 0.74$ and *kη* = 0*.*26 are in the dissipation range of the energy spectrum of the YS2 DNS (a possible name is *"*dissipation-diffusive range" at those wave numbers). Despite that distinction, Chasnov's wave numbers apparently are the transition to the asymptotic condition that $\Sigma_{axi\phi}(k)$ becomes negligible for the DNS of YS2.

Write Eq. (64) as

$$
\frac{k^4 E_{\phi}(k)}{E(k)\frac{2G^2}{3D^2} \left(1 + \frac{D_T}{D}\right)} = 1 + \frac{\Sigma_{\text{axi}\phi}(k)}{k^{-4} E(k)\frac{2G^2}{3D^2} \left(1 + \frac{D_T}{D}\right)}.\tag{65}
$$

Figure 1 shows the same data with the same symbols as appear in Fig. 15 of YS2 [\[7\]](#page-15-0) for Sc = 1*/*512 and 1/2048, except that here their Fig. 15 data [i.e., $k^4 E_\phi(k)/E(k)$] are divided by $\frac{2G^2}{3D^2}(1 + \frac{D_T}{D})$; that is, the left-hand side of Eq. [\(64\)](#page-11-0) is plotted in Fig. 1 with a dashed line at unity indicating $\Sigma_{\text{axi}\phi}(k) = 0.$

Chasnov [\[11\]](#page-16-0) calls the range $3 \le k/k_{C-O} \le 80$ the near inertial-diffusive subrange (he uses *"*conductive" instead of *"*diffusive"). He finds that this near subrange does not scale with the Corrsin-Obukov parameters ε , χ , and $k_{C−O}$ for the mean-scalar-gradient case (as distinct from the freely decaying case), and he states *"*the precise causes of these deviations will require careful future analysis." From the present perspective, the reason is that another dimensionless parameter exists, namely, D_T/D . Other than numerical error, all aspects of the spectra in that near inertial-diffusive subrange must be quantitatively predicted by exact statistical equations.

XII. CONCLUSION

Exact statistical equations are derived for precise DNS quantification. The equations are applied to the freely decaying [\[6\]](#page-15-0) DNS and mean-scalar-gradient [\[7\]](#page-15-0) DNS for which the terms in $\Sigma_{\text{iso}\phi}(k)$ and $\Sigma_{axi\phi}(k)$, respectively, are found to be not negligible. In their Fig. 7, YS1 [\[6\]](#page-15-0) show the ratio of the two right-most terms in Eq. [\(56\)](#page-8-0), namely, $E_{\phi}(k)/[E(k)\chi/(3D^3k^4)]$. The deviations from

unity in that figure are caused by $\Sigma_{\text{iso}\phi}(k)$ in Eq. [\(57](#page-8-0)); that cannot be otherwise (unless there is a computational error) because Eqs. [\(56\)](#page-8-0) and [\(57\)](#page-8-0) are obtained without approximation. In the inertial range, at *kη* = 0*.*05, their Fig. 7(b) shows about 50% and 20% deviation from the BHT formula for $Sc = 1/512$ and $1/2048$, respectively. With reference to their Fig. 3(d), they state a roughly 20% deviation relative to the BHT inertial-diffusive range formula [\(58\)](#page-8-0) for $Sc = 1/2048$; that deviation is caused by $\Sigma_{\text{iso}\phi}(k)$. Quantification of $\Sigma_{\text{iso}\phi}(k)$ and its constituent terms is needed to understand their observed deviations from BHT theory [\[1\]](#page-15-0). As found by YS2 [\[7\]](#page-15-0), Table [II](#page-11-0) shows that the original BHT formula, LHS $= C_K = 1.62$, does not apply to this uniform-mean-gradient-source case. The term $(1 + \frac{D_T}{D})C_K$ accounts for most of the value of LHS. However, values of $\Sigma_{axi\phi}(k)/E_{\phi}(k)$ in row 5 in Table [II](#page-11-0) show that the right-most term in Eq. (63) is not negligible such that the assumed asymptotic state in which $\Sigma_{axi\phi}(k)$ becomes negligible is not attained in the data.

In Sec. [VI,](#page-4-0) the assumption of isotropy by BHT is replaced by local isotropy of the scalar in the dissipation range. Although that is not accurate for the mean-scalar-gradient DNS of YS2 [\[7\]](#page-15-0), it is obviated for a DNS with averaging over all directions of **k**. BHT neglected the time-derivative term as their first assumption. The approximate validity of that assumption is supported by the DNS of YS1 [\[6\]](#page-15-0) and YS2 [\[7\]](#page-15-0) and by the above discussion. The classical theory of BHT is obtained in the appropriate limit. New formulas for the mean-scalar-gradient case, Eqs. [\(63\)](#page-11-0) and [\(64\)](#page-11-0), are quantified in Table [II](#page-11-0) and Fig. [1](#page-12-0) for the data of YS2 for their smaller Sc cases. The theory for a uniform mean scalar gradient with an isotropic velocity field is derived in Sec. [IX,](#page-6-0) and for averaging over all directions of **k** in Sec. [XI,](#page-9-0) and is evaluated for the DNS of YS2 in Sec. [XI A.](#page-10-0) The result is that averaging over all directions of **k** retains only the zero order in the Legendre-polynomial expansion, i.e., Eq. [\(49\)](#page-7-0). The second-order Legendre term is shown to be significant by the values of *a* in Table [I](#page-10-0) for the DNS of YS2.

For the case of a mean-scalar-gradient source, the wave number that Chasnov [\[11\]](#page-16-0) identifies as beginning the asymptotic BHT inertial-diffusive range is within the dissipation-diffusive range of the DNS of YS2 [\[7\]](#page-15-0). For their DNS, that wave number is also the transition to the asymptotic condition that $\Sigma_{\text{axi}\phi}(k)$ becomes negligible.

There is more to be learned from DNS of small-Schmidt-number scalar advection by evaluating all statistics in the above exact equations. The exact statistical equations retain dependence on **k** such that they can be applied to study anisotropy. The mean-scalar-gradient DNS of YS2 [\[7\]](#page-15-0) is axisymmetric, and the scalar fluctuations are not nearly locally isotropic for their smaller Sc cases. To study that axisymmetry, an average over directions of **k** must be restricted to the plane perpendicular to the mean scalar gradient. The axisymmetry can be investigated using the expansion in Legendre polynomials, as was done by Gotoh *et al.* [\[14\]](#page-16-0) Application of that expansion gives Eqs. [\(46\)](#page-7-0)– [\(50\)](#page-7-0). Terms in equations that contain the factor $P_2(\mu)$ are the second-order Legendre-polynomial contribution. A new inertial-diffusive-range formula for the second-order Legendre contribution is given in Eq. [\(50\)](#page-7-0). Higher-order, even-order Legendre polynomial terms can appear if $\sum(\mathbf{k})$ is not neglected.

Whereas Eq. [\(37\)](#page-5-0) contains a term containing *F* caused by local axisymmetry of scalar-gradient variances, which we conjecture might vanish at infinite Peclet number, Eq. [\(44\)](#page-6-0) contains the direct effect of the mean scalar gradient, which we expect to not vanish at infinite Peclet number. The limited Peclet numbers attainable for the small-Sc case using DNS with present computers causes the second-order Legendre-polynomial coefficient to be significant relative to that of the zero order. That is seen by comparing *a* in Table [I](#page-10-0) with Fig. 6 (left side) of Gotoh *et al.* [\[14\]](#page-16-0) wherein the second order is about 10^{-2} of the zero order for their case Sc = 1.

Noise in DNS evaluations limits the number of Legendre-polynomial terms that can be accurately quantified. Based on results in this paper, this author opines that only the zero- and second-order coefficients of a Legendre polynomial expansion suffice if higher orders are affected by noise. Then, any given statistic is that statistic minus the zero- and second-order terms plus a remainder function. That remainder function is the sum of all higher-order Legendre terms, and is a function of angle. The maximum of the absolute value of that remainder function is similar to the Legendre coefficients in the sense that such maximum of Legendre polynomials is unity.

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APPENDIX A: ALTERNATIVE TO EQ. [\(2\)](#page-1-0)

Expressions for $\sum(\mathbf{k})$ and its corresponding wave-number spectra are defined in Eqs. [\(27\)](#page-4-0), [\(33\)](#page-5-0), [\(43\)](#page-6-0), [\(55\)](#page-8-0), and [\(61\)](#page-9-0). By use of Eq. [\(2\)](#page-1-0) we have attempted to cause the cospectra and error terms in expressions for $\sum(\mathbf{k})$ to be small relative to $E_{\phi}(k)$ in the limit of very large Pe and very small Sc. The terms in Eq. [\(2\)](#page-1-0) can be subtracted from both sides of Eq. [\(2\)](#page-1-0) to produce eight different versions of Eq. [\(2\)](#page-1-0); Eqs. (A1) and [\(2\)](#page-1-0) are two of the eight. Those eight versions produce eight different expressions for $\sum(\mathbf{k})$ in terms of different statistics. All of those eight expressions for $\sum(\mathbf{k})$ result in the same numerical value of $\sum(\bf{k})$ because they all appear in the same exact equations. However, even for very large Pe and very small Sc, some of those expressions for $\sum(\mathbf{k})$ contain terms that are large in magnitude, but of opposite sign, such that they subtract to produce a value of $\sum(\mathbf{k})$ that is smaller in absolute value than those large terms.

The advective and diffusive terms should not be on the same side of Eq. [\(2\)](#page-1-0) because their coherency is nearly −1 for the freely decaying case (Fig. 6 of YS1 [\[6\]](#page-15-0)). In Eq. [\(2\)](#page-1-0), $\hat{s}(\mathbf{k})$ and $Dk^2\hat{\phi}(\mathbf{k})$ are on opposite sides of that equation because, if they were on the same side of that equation, then their cospectrum would be a large term in $\sum(\mathbf{k})$ for the DNS data of YS2 [\[7\]](#page-15-0).

For example, consider if we had not subtracted the time-derivative term from both sides of Eq. [\(2\)](#page-1-0) and we began the derivation with

$$
\frac{\partial \widehat{\phi}(\mathbf{k})}{\partial t} + i \int k'_i \widehat{u}_i(\mathbf{k} - \mathbf{k}') \widehat{\phi}(\mathbf{k}') d\mathbf{k}' - \widehat{s}(\mathbf{k}) = -Dk^2 \widehat{\phi}(\mathbf{k}). \tag{A1}
$$

New cospectra would then appear, which are defined by

$$
\mathbf{U}(\mathbf{k}) \equiv \left\langle \frac{\partial \widehat{\phi}(\mathbf{k})}{\partial t} \left(-i \int k''_j \widehat{u}^*_j (\mathbf{k} - \mathbf{k}'') \widehat{\phi}^* (\mathbf{k}'') d\mathbf{k}'' \right) + \frac{\partial \widehat{\phi}^*(\mathbf{k})}{\partial t} \left(i \int k'_i \widehat{u}_i (\mathbf{k} - \mathbf{k}') \widehat{\phi}(\mathbf{k}') d\mathbf{k}' \right) \right\rangle. \tag{A2}
$$

$$
\mathbf{W}(\mathbf{k}) \equiv \left\langle \frac{\partial \widehat{\phi}(\mathbf{k})}{\partial t} [-\widehat{s}^*(\mathbf{k})] + \frac{\partial \widehat{\phi}^*(\mathbf{k})}{\partial t} [-\widehat{s}(\mathbf{k})] \right\rangle. \tag{A3}
$$

Then, the term $\mathbf{T}(\mathbf{k}) + \mathbf{Y}(\mathbf{k})$ would be absent from the right side of Eq. [\(12\)](#page-2-0) and $\mathbf{T}(\mathbf{k}) + \mathbf{U}(\mathbf{k}) + \mathbf{W}(\mathbf{k})$ would appear on the left side of Eq. (12) such that instead of Eq. (12) , we would have

$$
\mathbf{T(k)} + \mathbf{U(k)} + \mathbf{W(k)} + \mathbf{X(k)} + \mathbf{V(k)} + \mathbf{S(k)} = D^2 k^4 \mathbf{Q}_{\phi}(\mathbf{k}).
$$
 (A4)

We then obtain

$$
\sum(\mathbf{k}) \equiv \frac{\mathbf{T}(\mathbf{k}) + \mathbf{U}(\mathbf{k}) + \mathbf{W}(\mathbf{k}) + \mathbf{X}(\mathbf{k}) + \mathbf{e}_2(\mathbf{k})}{D^2 k^4}.
$$
 (A5)

The expressions for Eqs. (27) and $(A5)$ are equal because they both appear in the same exact statistical equation obtained without approximation. Comparing Eqs. (27) and $(A5)$, we see that

$$
\mathbf{U}(\mathbf{k}) + \mathbf{W}(\mathbf{k}) = -2\mathbf{T}(\mathbf{k}) - \mathbf{Y}(\mathbf{k}).\tag{A6}
$$

We have no evidence from YS1 [\[6\]](#page-15-0) or YS2 [\[7\]](#page-15-0) to expect that **U**(**k**) and **W**(**k**) are small relative to $D^2k^4\mathbf{Q}_{\phi}(\mathbf{k})$ in Eq. (A4). However, strong evidence that the right side of Eq. (A6) is small relative to $D^2k^4\mathbf{Q}_\phi(\mathbf{k})$ is given above. Hence, the left side of Eq. (A6) is small relative to $D^2k^4\mathbf{Q}_\phi(\mathbf{k})$; the reason might be that **U**(**k**) and **W**(**k**) are of opposite sign and nearly equal but relatively large in magnitude.

The above reasons are why the time-derivative term *∂φ/∂t* and the source term *s* are subtracted from both sides of Eq. (1) to produce Eq. (2) .

APPENDIX B: DERIVATION OF EQS. [\(37\)](#page-5-0)–[\(39\)](#page-6-0)

The notation g_{ϕ} is defined in Sec. [VIII.](#page-5-0) Define

$$
C \equiv \left\langle \frac{\partial \phi}{\partial z} \frac{\partial \phi}{\partial z} \right\rangle - \frac{1}{2} \left\langle \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \frac{\partial \phi}{\partial y} \right\rangle
$$
 (B1)

$$
= F \frac{\chi}{2D}.
$$
 (B2)

Wherein $F \equiv (g_{\phi} - 1)/(g_{\phi} + 2)$ as in Eq. [\(39\)](#page-6-0). The axisymmetric formula is

$$
\left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \right\rangle = z_i z_j C + \frac{\delta_{ij}}{3} \left(\frac{\chi}{2D} - C \right).
$$
 (B3)

Formula (B3) is easily verified by performing its trace and inner products with unit vector products $z_i z_j$ and $x_i x_j$.

Within Eq. (21) we have the contraction of the second-rank tensors in Eqs. (20) and $(B3)$; that is $[recall that k_z^2/k^2 = cos^2(\theta) = \mu^2 \text{ and } P_2(\mu) = \frac{3}{2}(\mu^2 - \frac{1}{3})],$

$$
\langle \widehat{u_i}(\mathbf{k})\widehat{u}_j^*(\mathbf{k})\rangle \left\langle \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_j} \right\rangle = \left[\left(\delta_{ij} - \frac{k_ik_j}{k^2} \right) \frac{E(k)}{4\pi k^2} \right] \left[z_i z_j C + \frac{\delta_{ij}}{3} \left(\frac{\chi}{2D} - C \right) \right]
$$
(B4)

$$
= \left[C + \frac{\chi}{2D} - C - \frac{k_z k_z}{k^2}C - \frac{1}{3}\left(\frac{\chi}{2D} - C\right)\right] \frac{E(k)}{4\pi k^2}
$$
 (B5)

$$
= \left[\frac{\chi}{3D} - \frac{3}{2}\left(\mu^2 - \frac{1}{3}\right)\frac{2}{3}C\right] \frac{E(k)}{4\pi k^2}
$$
(B6)

$$
= \frac{\chi}{3D} \frac{E(k)}{4\pi k^2} - P_2(\mu) F \frac{\chi}{3D} \frac{E(k)}{4\pi k^2}.
$$
 (B7)

Note that $C = 0$ substituted in Eq. (B3) gives the isotropic formula; from Eq. (B2), that corresponds to $g_{\phi} = 1$ and $F = 0$. Now, Eq. (87) is Eq. [\(37\)](#page-5-0).

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