Systematic bias in the calculation of spectral density from a three-dimensional spatial grid

Rodion Stepanov*
Institute of Continuous Media Mechanics, Korolyov Street 1, 614013 Perm, Russia and Department of Applied Mathematics and Mechanics, Perm National Research Polytechnic University, Komsomolskii Avenue 29, 614990 Perm, Russia

Franck Plunian
Université Grenoble Alpes, ISTerre, F-38000 Grenoble, France and CNRS, ISTerre, F-38000 Grenoble, France

Mouloud Kessar and Guillaume Balarac
Université Grenoble Alpes, LEGI, F-38000 Grenoble, France and CNRS, LEGI, F-38000 Grenoble, France
(Received 8 September 2014; published 21 November 2014)

The energy spectral density $E(k)$, where k is the spatial wave number, is a well-known diagnostic of homogeneous turbulence and magnetohydrodynamic turbulence. However, in most of the curves plotted by different authors, some systematic kinks can be observed at $k = 9$, 15, and 19. We claim that these kinks have no physical meaning and are in fact the signature of the method that is used to estimate $E(k)$ from a three-dimensional spatial grid. In this paper we give another method in order to get rid of the spurious kinks and to estimate $E(k)$ much more accurately.

DOI: 10.1103/PhysRevE.90.053309 PACS number(s): 47.11.Kb, 47.27.−i

I. MOTIVATION

Assuming isotropic and homogeneous hydrodynamic turbulence, Kolmogorov predicted that the kinetic energy spectral density should have a universal power scaling of $k^{-5/3}$ [1], where k is the spatial wave number. Since then, the energy spectral density has become a useful diagnostic tool for various configurations, including anisotropic and magnetohydrodynamic turbulence. The definition of the spectral density $E(k)$ is given by [2]

$$E(k) = \int_{|\mathbf{k}'|=k} \hat{E}(\mathbf{k}')d\mathbf{k}', \tag{1}$$

where $\hat{E}(\mathbf{k}')$ is the Fourier transform of the autocorrelation of a scalar field or the trace of the autocorrelation tensor of a vector field, e.g., velocity or magnetic field [3].

We look at definition (1) from the point of view of turbulence in a computational box. In practice, the numerical implementation of (1) for $\hat{E}(\mathbf{k}')$ given on a regular grid of mesh is not discussed. However, some common features can be distinguished in the results. As an example, a compilation of curves corresponding to kinetic, magnetic, and passive-scalar energy spectra obtained in hydrodynamic or magnetohydrodynamic turbulence is plotted in Fig. 1. Though these spectra have been obtained by various authors [4–13], using various methods, forcing, and degrees of resolution, we note a systematic bump at the scale $k = 9$, followed by two holes at scales $k = 15$ and 19. Bumpy spectra are familiar in the context of wave turbulence, usually interpreted as the signature of traveling modes [14], but they are found in time frequency only. Here, however, it is difficult to imagine any physical ground for the systematic $k = 9$, 15, and 19 kinks appearing in the inertial range. It is fair to say that usually these kinks are just ignored in discussions of physical or even numerical aspects of the results [15,16], even if the bump at $k = 9$ has already been interpreted as a physical effect [12]. Another hole at $k = 3$ might be found, but it is usually hidden by the forcing scales.

In Sec. II we show that, in fact, these kinks are produced by a systematic bias coming from the standard approach to estimating $E(k)$ on a spatial grid. In Sec. III we present a method to estimate $E(k)$ in order to circumvent this bias. Since such a bias is more striking in three-dimensional (3D) turbulence than in 2D turbulence, in this paper we consider only the case of 3D data sets. An alternative definition for the 2D case is, however, given in Sec. IV. In 1D models, such as eddy-damped quasinormal Markovian models [17] or shell models [18] of turbulence, this bias does not exist.

II. WHERE DOES THE BIAS COME FROM?

The standard approach to estimating the continuous quantity $E(k)$ from a set of Fourier modes given on a regular grid of mesh δk is to divide the Fourier space in shells S_n of thickness Δk. Then the spectral density E_n can be defined as [2]

$$E_n = \frac{(\delta k)^3}{\Delta k} \sum_{\mathbf{k}' \in S_n} \hat{E}(\mathbf{k}'), \tag{2}$$

with

$$S_n = \{\mathbf{k}' \in \mathbb{R}^3 : n\Delta k - \Delta k/2 < |\mathbf{k}'| \leqslant n\Delta k + \Delta k/2\}. \tag{3}$$

Usually it is natural to take $\Delta k = \delta k = 1$, leading to a unity prefactor in (2). The wave number k_n corresponding to shell S_n is usually taken to obey an arithmetic progression. Then it is defined as

$$k_n = n\Delta k. \tag{4}$$

The problem is that the number M_n of wave vectors $\mathbf{k}'$ belonging to S_n is not exactly proportional to the shell volume, as depicted in Fig. 2 for $\Delta k = \delta k$. The density of M_n even reaches local extrema at $k_n = 9$, 15, and 19, which clearly explains the kinks appearing in Fig. 1. Changing the value of

*rodion@icmm.ru

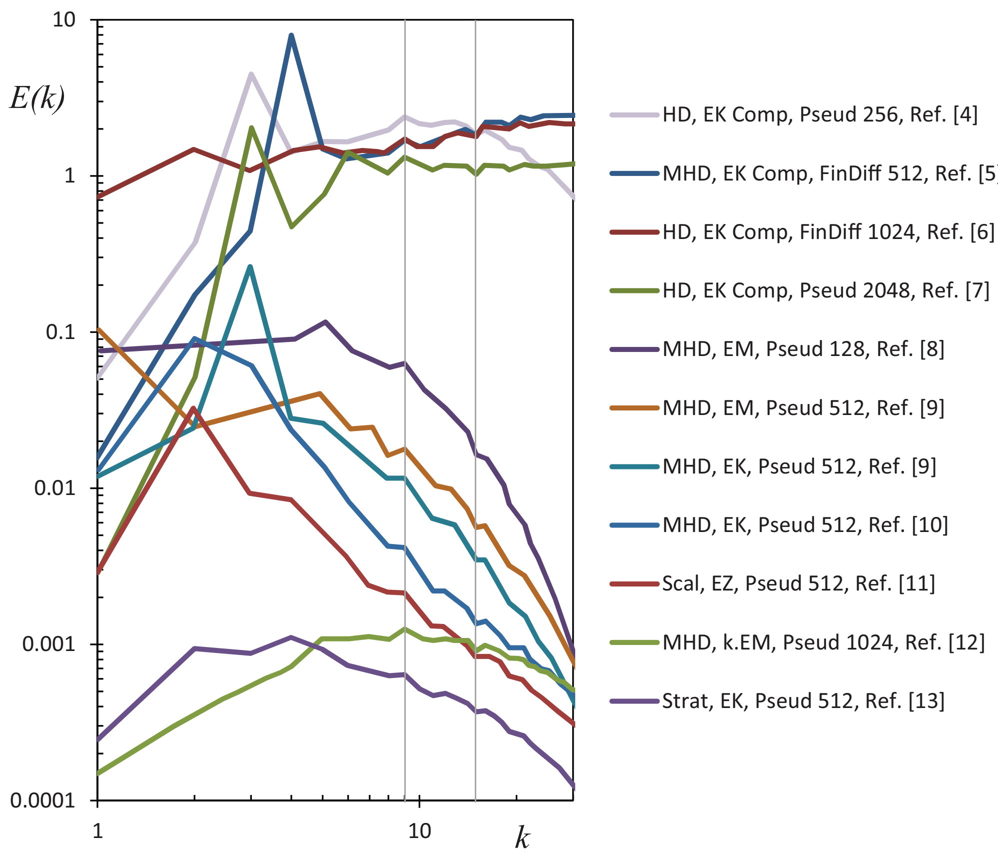

FIG. 1. (Color online) Energy spectra calculated by different authors, with different codes, different resolutions, and for different quantities. The denotations HD, MHD, and Scal stand for hydrodynamic, magnetohydrodynamic, and passive-scalar problems, respectively. The denotations EK, EM, and EZ stand for kinetic, magnetic, and passive-scalar energies, respectively. Pseud and FinDiff stand for pseudospectral and finite-difference resolution methods, respectively, and the numbers 128, 512, 1024, and 2048 correspond to the spatial resolution. The vertical grid lines $k = 9$ and 15 are highlighted as solid lines. The legend is kept in the same order as the curves from top to bottom at $k = 9$.

Δk would not help. For $\Delta k < \delta k$ the number of local extrema is getting larger, while taking $\Delta k > \delta k$ leads to a spurious power law as the result of an overaveraging procedure. In Fig. 2 we note another bump at $k = 5$, which presumably is also responsible for the peaks at $k = 5$ visible in several spectra of Fig. 1, like the one calculated by Ponty *et al.* [8].

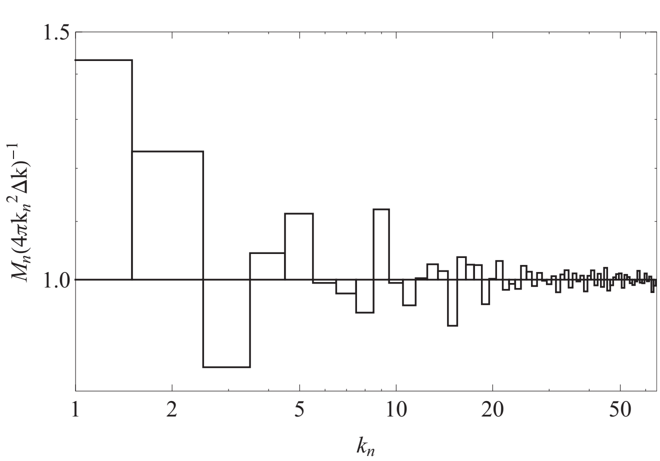

FIG. 2. Density of the number of vectors belonging to shell S_n versus k_n for $\Delta k = \delta k$.

III. HOW TO CIRCUMVENT THE BIAS

Starting from (1), we note that $E(k)$ is a surface integral, over $|\mathbf{k}'| = k$. Keeping in mind that the surface of a shell of radius $|\mathbf{k}'|$ is equal to $4\pi|\mathbf{k}'|^2$, we then introduce the following definition for the spectral density in shell S_n, now denoted E_n^*, in the form

$$E_n^* = \frac{4\pi}{M_n} \sum_{\mathbf{k}' \in S_n} \hat{E}(\mathbf{k}')|\mathbf{k}'|^2, \quad (5)$$

where again M_n is the number of vectors $\mathbf{k}'$ belonging to shell S_n.

Similarly, in order to estimate the mean wave number in shell S_n, we suggest to simply average all wave numbers belonging to S_n. This average wave number, now denoted by k_n^*, is given by

$$k_n^* = \frac{1}{M_n} \sum_{\mathbf{k}' \in S_n} |\mathbf{k}'|. \quad (6)$$

Finally, as we are looking for an energy spectral density satisfying some power law, it makes sense to use a geometric progression, instead of an arithmetic one, for k_n. Then the shells are logarithmically spaced ($n \propto \log k_n$), instead of being

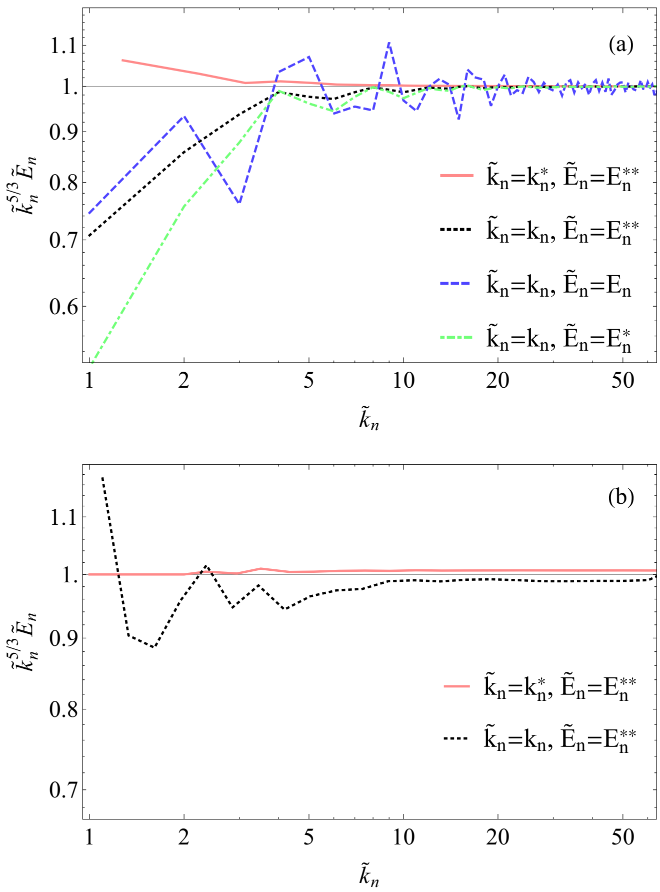

FIG. 3. (Color online) Compensated spectral density $\tilde{k}_n^{5/3}\tilde{E}_n$ versus $\tilde{k}_n$ for (a) linearly spaced shells S_n and (b) logarithmically spaced shells $S_n^{\log}$. (a) The four curves correspond to $\tilde{k}_n = k_n$ or k_n^* and $\tilde{E}_n = E_n$ or E_n^*. (b) The curves corresponds to $\tilde{E}_n = E_n^*$ and $\tilde{k}_n = k_n$ or k_n^*.

linearly spaced ($n \propto k_n$). Then we define the new shells as

$$S_n^{\log} = \{\mathbf{k}' \in \mathbb{R}^3 : \lambda^n \delta k < |\mathbf{k}'| \leqslant \lambda^{n+1}\delta k\}, \tag{7}$$

where λ is some scalar value larger than unity.

In order to test our definitions k_n^* and E_n^*, we consider a synthetic set of data with spectral coefficients $\hat{E}(\mathbf{k}') = \frac{1}{4\pi}|\mathbf{k}'|^{-11/3}$. It corresponds to the exact spectral density $E(k) = k^{-5/3}$.

In Fig. 3 we consider two cases depending on whether the shells are linearly spaced [Fig. 3(a)] or logarithmically spaced [Fig. 3(b)]. For linearly spaced shells, the curves depend on the definitions taken for the wave number and the spectral density. We immediately see that taking E_n for the spectral energy density leads to noisy results. The best result is obtained taking k_n^* and E_n^*. Now taking k_n^* and E_n^* with logarithmically spaced shells [Fig. 3(b)] leads to a result very close to the theoretical $k^{-5/3}$ curve. Though the choice of the logarithmically shell spacing λ is arbitrary, we suggest to take $\lambda = 1.21$ because it is the minimum value of λ for which we found no empty shell.

Finally, in Fig. 4 we consider data from a 256^3 direct numerical simulation (DNS) of homogeneous isotropic turbulence with a random forcing [11]. The kinetic energy spectral density $E(k)$, compensated by $k^{-5/3}$, is plotted with three

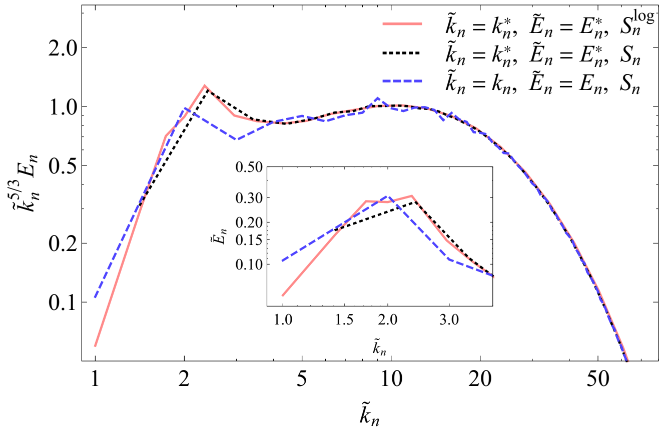

FIG. 4. (Color online) Compensated spectral density $\tilde{k}_n^{5/3}\tilde{E}_n$ versus $\tilde{k}_n$ from hydrodynamic turbulent DNS data. Two curves correspond to $\tilde{k}_n = k_n$ and $\tilde{E}_n = E_n$ or E_n^* and linearly spaced shells and the third curve corresponds to $\tilde{k}_n = k_n^*$ and $\tilde{E}_n = E_n^*$ and logarithmically spaced shells. The inset shows the spectral density at low wave numbers in the range of forcing scales.

kinds of estimates: k_n and E_n (linearly spaced shells), k_n^* and E_n^* (linearly spaced shells), and k_n^* and E_n^* (logarithmically spaced shells with $\lambda = 1.21$). As can be seen, the curves are remarkably smooth using k_n^* and E_n^*. In the inset the spectral density $E(k)$ is plotted for low values of k (without compensation). Using E_n^*, k_n^*, and logarithmically spaced shells (black curve), the almost constant plateau around $k = 2$ corresponds indeed to the forcing scales in which the energy power has been applied in the DNS.

IV. CONCLUSION

The goal of this paper was to understand why some systematic artificial kinks appear in plots of energy spectral density issued from various DNSs of 3D turbulence. We showed that they are the consequence of a non-self-similar distribution of Fourier modes in the spherical shells used to calculate the energy spectral density. We gave definitions (5) and (6) for calculating the mean energy spectral density and mean wave number in each shell. These definitions can be applied to either linearly or logarithmically spaced shells, the second one being more precise and providing a better result at low wave numbers. The same definitions can be generalized to other scalar quantities of interest, such as enstrophy, kinetic helicity in hydrodynamics, magnetic helicity, and cross helicity in magnetohydrodynamics. Finally, similar definitions can be derived for 2D problems, S_n being rings instead of shells. In this case the definition of the wave number in ring S_n is still given by (6), but the definition of spectral energy density (5) must be replaced by

$$E_n^* = \frac{2\pi}{M_n} \sum_{\mathbf{k}' \in S_n} \hat{E}(\mathbf{k}')|\mathbf{k}'|. \tag{8}$$

ACKNOWLEDGMENTS

This collaboration benefited from the International Research Group Program supported by the Perm region government. R.S. acknowledges support from Grant No.

YD-520.2013.2 from the Council of the President of the Russian Federation and Grant No. 14-01-96010 from the Russian Foundation of Basic Research. M.K., G.B., and F.P. acknowledge support from the Rhone-Alpes region through the CIBLE program. This work was granted access to the HPC resources of IDRIS under the Allocation No. 20142a0611 made by GENCI and to the supercomputer URAN of the Institute of Mathematics and Mechanics UrB RAS.

[1] A. Kolmogorov, Dokl. Akad. Nauk. SSSR **30**, 299 (1941).
[2] M. Lesieur, *Turbulence in Fluids*, 3rd ed. (Kluwer, Dordrecht, 1997).
[3] H. Tennekes and J. L. Lumley, *A First Course in Turbulence* (MIT Press, Cambridge, 1972).
[4] D. O. Gómez, P. D. Mininni, and P. Dmitruk, Adv. Space Res. **35**, 899 (2005).
[5] A. Brandenburg, Astrophys. J. **697**, 1206 (2009).
[6] W. Dobler, N. E. L. Haugen, T. A. Yousef, and A. Brandenburg, Phys. Rev. E **68**, 026304 (2003).
[7] P. D. Mininni, A. Alexakis, and A. Pouquet, Phys. Rev. E **77**, 036306 (2008).
[8] Y. Ponty, P. D. Mininni, J.-F. Pinton, H. Politano, and A. Pouquet, New J. Phys. **9**, 296 (2007).
[9] A. Alexakis, P. D. Mininni, and A. Pouquet, Phys. Rev. E **72**, 046301 (2005).
[10] D. Carati, O. Debliquy, B. Knaepen, B. Teaca, and M. Verma, J. Turbul. **7**, 1 (2006).
[11] Y. Fabre and G. Balarac, Phys. Fluids **23**, 115103 (2011).
[12] N. E. L. Haugen, A. Brandenburg, and W. Dobler, Astrophys. J. Lett. **597**, L141 (2003).
[13] W. J. T. Bos, L. Liechtenstein, and K. Schneider, Phys. Rev. E **76**, 046310 (2007).
[14] A. Figueroa, N. Schaeffer, H.-C. Nataf, and D. Schmitt, J. Fluid Mech. **716**, 445 (2013).
[15] F. K. Chow and P. Moin, J. Comput. Phys. **184**, 366 (2003).
[16] O. Desjardins, G. Blanquart, G. Balarac, and H. Pitsch, J. Comput. Phys. **227**, 7125 (2008).
[17] A. Pouquet, U. Frisch, and J. Leorat, J. Fluid Mech. **77**, 321 (1976).
[18] F. Plunian, R. Stepanov, and P. Frick, Phys. Rep. **523**, 1 (2013).