A Passive scalar field convected by turbulence

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Classical statistical mechanics is applied to the study of a passive scalar field convected by isotropic turbulence. A complete set of independent real parameters and dynamic equations are worked out to describe the dynamic state of the passive scalar field. The corresponding Liouville equation is solved by a perturbation method based upon a Langevin–Fokker–Planck model. The closure problem is treated by a variational approach reported in earlier papers. Two integral equations are obtained for two unknown functions: the scalar variance spectrum $F(k)$ and the effective damping coefficient $\Omega(k)$. The appearance of the energy spectrum of the velocity field in the two integral equations represents the coupling of the scalar field with the velocity field. As an application of the theory, the two integral equations are solved to derive the inertial-convective-range spectrum, obtaining $F(k) = 0.61\,\chi\epsilon^{-1/3}\,k^{-5/3}$. Here χ is the dissipation rate of the scalar variance and ϵ is the dissipation rate of the energy of the velocity field. This theoretical value of the scalar Kolmogorov constant, 0.61, is in good agreement with experiments.

I. INTRODUCTION

Considerable theoretical and experimental research has been devoted to the study of a scalar field convected by turbulence.[1–20] At first sight it seems that it should be straightforward to extend our knowledge from the turbulent velocity field to the addition of a scalar to the velocity field; yet both theoretically and experimentally this problem has proved to be very difficult, even for the most simple case. The difficulty is of a twofold nature. Firstly it is due to our poor knowledge of the turbulent velocity field. Secondly it is related to the fundamental problem of how the turbulent vector velocity field and the convected scalar field are coupled to each other.

Let T be the convected scalar, which may be temperature or concentration; its fluctuating part is θ, and $T = \langle T \rangle + \theta$. The mean part $\langle T \rangle$ is assumed to be homogeneous and stationary. Then the governing equation for θ is[1–3]

$$\partial_t \theta + \mathbf{u}\cdot\partial_{\mathbf{x}}\theta = \mu\,\partial_{\mathbf{x}}^2\theta. \tag{1}$$

Here $\mathbf{u} = \mathbf{u}(\mathbf{x})$ is the turbulent velocity field, μ is the molecular diffusivity of the scalar, ∂_t means partial differentiation with respect to time t, $\partial_{\mathbf{x}}$ and $\partial_{\mathbf{x}}^2$ are, respectively, the gradient and Laplace operators. Generally Eq. (1) is both dynamically and statistically nonlinear. If the scalar θ is passive, i.e., its amplitude is small enough not to affect the velocity field, the turbulent velocity field can be considered to be independent of the passive scalar and assumed to be given. In this simple case, Eq. (1) is dynamically linear, but statistically nonlinear. An evolution equation of any lower-order correlation of the scalar-velocity field must contain some higher-order correlation of mixed type due to the term $\mathbf{u}\cdot\partial_{\mathbf{x}}\theta$ in (1). Hence, similar to the Navier–Stokes equation, Eq. (1) is equivalent to an infinite hierarchy of equations for correlations; any finite subset of the infinite hierarchy of equations is not closed, and possesses more unknowns than are determined by the subset. In order to solve this closure problem, i.e., to find proper approximate methods to convert the infinite hierarchy of equations into a closed subset, it is necessary to properly treat the coupling between the scalar and the velocity, and to express higher-order correlations of mixed type in terms of proper lower-order correlations.

By a dimensional argument or some phenomenological model, Obukov,[4] Corrsin,[5] and Batchelor[6] predicted the large-wavenumber behavior of the spectrum $F(k)$ of a passive scalar field convected by isotropic turbulence. For the inertial-convective range, they obtain

$$F(k) = B_3\chi\epsilon^{-1/3}\,k^{-5/3}, \tag{2}$$

a counterpart of the Kolmogorov inertial-range spectrum of the velocity field. Here B_3 is the (three-dimensional) scalar Kolmogorov constant, χ is the dissipation rate of the scalar variance $\langle\theta^2\rangle$, and ϵ is the dissipation rate of energy of the velocity field. Equation (2) has been confirmed by experiments,[7–13] and experimental values of B_3 range from 0.5 to 0.8. There are few theoretical calculations of B_3. Kraichnan[14] used the Lagrangian history direct-interaction approximation to solve the closure problem of Eq. (1) and obtained $B_3 = 0.208$. Gibson's phenomenological theory[15] predicted B_3 in the range 1.0 to 1.7. Lundgren's theory[16] predicts that $B_3 = 0.49$.

In this paper the variational approach to the closure problem of turbulence, reported in earlier papers,[21–23] is to be applied to the study of a passive scalar field convected by isotropic turbulence. First of all a complete set of independent real parameters and its dynamic equation are worked out to describe the passive scalar field. An approximate solution of the corresponding Liouville equation is obtained by a perturbation method based on a Langevin–Fokker–Planck (LFP) model; then higher-order correlations of the scalar-velocity field are expressed in terms of their lower-order correlations. The cost of so doing is to introduce a new unknown function $\Omega(k)$, which is determined by requiring it to optimize the LFP model. Two integral equations are obtained for two unknown functions: the scalar variance spectrum and the $\Omega(k)$, thus solving the closure problem of Eq. (1). As an application the two integral equations are solved to derive

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the inertial-convective-range spectrum (2). Finally the scalar Kolmogorov constant B_3 is numerically evaluated, $B_3 = 0.61$, which is in good agreement with experiments.

II. INDEPENDENT REAL PARAMETERS AND DYNAMIC EQUATION

The turbulent scalar-velocity field is assumed to be incompressible, isotropic, and confined within a cubic box with side L and periodic boundary conditions. Therefore we have

$$\theta(\mathbf{x}) = H \sum_{\mathbf{k}} \theta(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{x}), \tag{3a}$$

$$\mathbf{u}(\mathbf{x}) = H \sum_{\mathbf{k}} \mathbf{u}(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{x}). \tag{3b}$$

Here $H = (2\pi/L)^3$, $\Sigma_{\mathbf{k}}$ means summation over discrete wave vector $\mathbf{k}$, and the $\theta(\mathbf{k})$ and $\mathbf{u}(\mathbf{k})$ are discrete Fourier transforms of the scalar and the velocity, respectively. Substituting (3) into (1), we have

$$(d_t + \mu k^2)\theta(\mathbf{k}) = -iH \sum_{\mathbf{p}} \mathbf{k}\cdot\mathbf{u}(\mathbf{r})\theta(\mathbf{p}), \tag{4}$$

with $\mathbf{r} = \mathbf{k} - \mathbf{p}$. Here $\mathbf{p}$ and $\mathbf{r}$ are also discrete wave vectors; d_t means differentiation with respect to time t. Since the scalar $\theta(\mathbf{x})$ is a real quantity,

$$\theta^{(1)}(-\mathbf{k}) = \theta^{(1)}(\mathbf{k}) \text{ and } \theta^{(2)}(-\mathbf{k}) = -\theta^{(2)}(\mathbf{k}). \tag{5}$$

Here $\theta^{(1)}(\mathbf{k})$ and $\theta^{(2)}(\mathbf{k})$ are the real and imaginary parts of $\theta(\mathbf{k})$, respectively. Let $\mathbf{u}^{(1)}(\mathbf{k})$ and $\mathbf{u}^{(2)}(\mathbf{k})$ be the real and imaginary parts of $\mathbf{u}(\mathbf{k})$ respectively; after some manipulation, (4) becomes

$$(d_t + \mu k^2)\theta^{(a)}(\mathbf{k}) = H \sum_{\mathbf{p}} D^{abc}\mathbf{k}\cdot\mathbf{u}^{(b)}(\mathbf{r})\theta^{(c)}(\mathbf{p}), \tag{6}$$

with $\mathbf{r} = \mathbf{k} - \mathbf{p}$. The real-imaginary-part indexes a, b, and c take on 1 and 2. The Einstein summation convention is used for repeated b and c. The coefficients D^{abc} are defined as follows:

$$D^{abc} = \begin{cases} 0, & \text{if } a+b+c = 3 \text{ or } 5, \\ -1, & \text{if } a=2,\ b=1 \text{ and } c=1, \\ 1, & \text{otherwise}. \end{cases} \tag{7}$$

Because of (5), $\theta^{(a)}(\mathbf{k})$ are not independent, although they are real. In order to get independent real modal parameters, we combine the wave vector $\mathbf{k}$ and the real-imaginary-part index a into one single index i (do not confuse it with the imaginary unit) in the following way:

$$i = (a,\mathbf{k}), \quad -i = (a, -\mathbf{k}), \tag{8a}$$

$$i > 0 \text{ if } (k_3 > 0) \text{ or } (k_2 > 0, k_3 = 0)(k_1 > 0, k_2 = 0, k_3 = 0). \tag{8b}$$

The new modal parameters Y_i are defined as follows:

$$Y_i = e(i)\theta^{(a)}(\mathbf{k}), \tag{9}$$

where $e(i) = -1$ if $(i < 0, a = 2)$, otherwise $e(i) = 1$. Then (5) becomes

$$Y_{-i} = Y_i. \tag{10}$$

Therefore $[Y_i; i > 0]$ constitutes a complete set of independent real parameters for the scalar field and the dynamic equation (6) becomes

$$(d_t + \mu_i)Y_i = \sum_j B_{ij} Y_j. \tag{11}$$

Here $\mu_i = \mu k^2$, Σ_i means summation over j, i and j take on positive integers only, and

$$B_{ij} = HD^{abc}\,[\mathbf{k}\cdot\mathbf{u}^{(b)}(\mathbf{k}-\mathbf{p})e(i)e(j) + \mathbf{k}\cdot\mathbf{u}^{(b)}(\mathbf{k}+\mathbf{p})e(i)e(-j)]. \tag{12}$$

Einstein's summation convention is used for the index b; and

$$B_{ij} = 0 \quad \text{if } i = j. \tag{13}$$

For the study of high-wavenumber dynamics, the model of stationary homogeneous turbulence is assumed. In order to maintain the stationarity of the turbulent scalar field, some external source of the type $\mu_i' Y_i$ is introduced at low wavenumbers; then the dynamic equation (11) becomes

$$[d_t + (\mu_i - \mu_i')]\,Y_i = \sum_j B_{ij} Y_j, \tag{14}$$

Here μ_i' is different from zero only at low wavenumbers.

III. CONDITIONAL PROBABILITY DISTRIBUTION AND LIOUVILLE EQUATION

According to (12) B_{ij} is a linear functional of $\mathbf{X} = [X_i; i > 0]$, and X_i are the real modal parameters of the turbulent velocity field defined in Ref. 21. Since the scalar field is passive, the probability distribution $P(\mathbf{X})$ of the velocity field is independent of $\mathbf{Y} = [Y_i; i > 0]$ and can be determined by the method proposed in Refs. 21 and 22. Therefore Eq. (11) or (14) is a dynamically linear but statistically nonlinear stochastic equation. The $\mathbf{X}$ and $\mathbf{Y}$ are, respectively, the state vectors of the scalar field and the velocity field. The state vector of the whole scalar-velocity field is $[\mathbf{X},\mathbf{Y}]$. All possible sets of $[\mathbf{X},\mathbf{Y}]$ or all possible states of the scalar-velocity field, constitute a phase space, called scalar-velocity or X-Y phase space. The corresponding probability distribution over an ensemble of numerous realizations of the turbulent scalar-velocity field is

$$P(\mathbf{X},\mathbf{Y}) = P(\mathbf{X})P(\mathbf{Y}/\mathbf{X}). \tag{15}$$

Here $P(\mathbf{Y}/\mathbf{X})$ is the conditional probability distribution of the scalar when the state of the velocity field is given. Corresponding to the three different probability distributions $P(\mathbf{X},\mathbf{Y})$, $P(\mathbf{X})$, and $P(\mathbf{Y}/\mathbf{X})$, we have the following three different statistical or ensemble averages.

$$\langle\cdots\rangle = \int d\mathbf{X} \int d\mathbf{Y}\,(\cdots)P(\mathbf{X},\mathbf{Y}), \tag{16a}$$

$$\langle\cdots\rangle x = \int d\mathbf{X}\,(\cdots)P(\mathbf{X}), \tag{16b}$$

$$\langle\cdots\rangle y = \int d\mathbf{Y}\,(\cdots)P(\mathbf{Y}/\mathbf{X}). \tag{16c}$$

Equations (16b) and (16c) are partial ensemble averages over $\mathbf{X}$ and $\mathbf{Y}$, respectively. From (15) and (16),

$$\langle\cdots\rangle = \langle\langle\cdots\rangle_y\rangle_x. \tag{16d}$$

If $(\cdots)$ is independent of $\mathbf{Y}$,

$$\langle\cdots\rangle = \langle\cdots\rangle_x. \tag{16e}$$

From the dynamic equation (14), the Liouville equation for the conditional probability distribution $P(\mathbf{Y}/\mathbf{X})$ is

$$\partial_t P(\mathbf{Y}/\mathbf{X}) + \mathbf{L}P(\mathbf{Y}/\mathbf{X}) = 0, \tag{17}$$

where $\mathbf{L}$ is the Liouville operator and

$$\mathbf{L} = -\sum_i (\mu_i - \mu_i')\partial_{Yi} Y_i + \sum_{ij} B_{ij} Y_j \partial_{Yi}. \tag{18}$$

Here ∂_{Yi} means partial differentiation with respect to Y_i, and Σ_{ij}, means summation over i and j. Since $P(\mathbf{X})$ has been determined in Ref. 21, if we can solve Eq. (17) to determine $P(\mathbf{Y}/\mathbf{X})$, then by (16) we can calculate various statistical properties of the turbulent scalar-velocity field. In the next section the Liouville equation (17) for a stationary turbulence is solved by a perturbation method based upon a Langevin–Fokker–Planck model.

IV. LANGEVIN–FOKKER–PLANCK MODEL AND PERTURBATION SOLUTION

Similar to the Langevin–Fokker–Planck model proposed for the turbulent velocity field in Ref. 21, it is assumed that the right-hand side of the dynamic equation (14) for the scalar field can be approximated by a linear damping force $-\beta_i Y_i$ plus a random force of the type of white noise f_i:

$$\sum_j B_{ij} Y_j \approx -\beta_i Y_i + f_i. \tag{19}$$

The number of the adjustable coefficients β_i in the approximation (19) is infinity; the approximation can be made as good as possible by choosing the optimum β_i. By (19) the dynamic equation (14) becomes

$$d_t Y_i \approx -\Omega_i Y_i + f_i, \quad \Omega_i = \beta_i + (\mu_i - \mu_i'). \tag{20}$$

Its Liouville equation is the Fokker–Planck equation, and the corresponding Liouville operator is the Fokker–Planck operator

$$\mathbf{L}^{(f)} = -\sum_i \Omega_i [\partial_{Yi} Y_i + G_i \partial_{Yi}^2]. \tag{21}$$

It will be shown later that G_i is related to the mean modal strength. Hence the simplified model (9) implies that the real Liouville operator (18) can be approximated by the Fokker–Planck operator,

$$\mathbf{L} \approx \mathbf{L}^{(f)}. \tag{22}$$

By taking partial ensemble average over $\mathbf{X}$, the Liouville equation (17) becomes

$$\partial_t \langle P(\mathbf{Y}/\mathbf{X})\rangle_x = -\langle \mathbf{L}P(\mathbf{Y}/\mathbf{X})\rangle_x. \tag{23}$$

For a stationary turbulent scalar-velocity field, $\langle P(\mathbf{Y}/\mathbf{X})\rangle_x$ is independent of time; although generally it is a function of time, we have

$$\langle \mathbf{L}P(\mathbf{Y}/\mathbf{X})\rangle_x = 0. \tag{24}$$

Its particular solution is $\mathbf{L}P(\mathbf{Y}/\mathbf{X}) = 0$ or

$$[\mathbf{L}^{(f)} + (\mathbf{L} - \mathbf{L}^{(f)})]P(\mathbf{Y}/\mathbf{X}) = 0. \tag{25}$$

According to (22), $\Delta\,\mathbf{L} = \mathbf{L} - \mathbf{L}^{(f)}$ can be considered to be a small perturbation operator. Let $P(\mathbf{Y}/\mathbf{X}) = p^{(0)} + p^{(1)} + \cdots$, by the perturbation method, we have

$$\mathbf{L}^{(f)} p^{(0)} = 0, \tag{26a}$$

$$\mathbf{L}^{(f)} p^{(1)} = -\Delta\,\mathbf{L} p^{(0)} = -\mathbf{L} p^{(0)}. \tag{26b}$$

Similar to the derivation of Sec. V of Ref. 21, finally we have

$$P(\mathbf{Y}/\mathbf{X}) = \Big(1 - \sum_i (\mu_i - \mu_i')(Y_i - G_i)/(2\Omega_i G_i) + \sum_{ij} B_{ij} Y_i Y_j / [G_i(\Omega_i + \Omega_j)]\Big) p^{(0)}, \tag{27a}$$

where

$$p^{(0)} = \prod_i (2\pi G_i)^{-1/2} \exp[-Y_i/(2G_i)] \tag{27b}$$

is the Gaussian density function.

V. CORRELATIONS

By using (15), (16), (27), and the expression for $P(\mathbf{X})$ obtained in Ref. 21, it is possible to calculate various correlations of the turbulent scalar-velocity field. First of all we have

$$\langle Y_i Y_j \rangle = \langle Y_i \rangle \delta_{ij}, \tag{28}$$

where δ_{ij} is the Kronecker symbol and

$$\langle Y_i^2 \rangle = G_i[1 - (\mu_i - \mu_i')/\Omega_i]. \tag{29a}$$

In the convective range, $\mu_i = \mu_i' = 0$, we have

$$\Omega_i = \beta_i \text{ and } \langle Y_i^2 \rangle = G_i. \tag{29b}$$

Hence the physical meaning of G_1 is the mean modal strength. For isotropic turbulence $\langle Y_i^2\rangle$, G_i and Ω_i are functions of k only; and $G_i = G(k)$, $\Omega_i = \Omega(k)$. By (3a) and (9), it can be proved that

$$\langle \theta^2 \rangle = \int F(k)dk, \tag{30a}$$

and

$$F(k) = 4\pi k^2 g(k), \; g(k) = 2H\langle Y_i^2\rangle = 2HG_i. \tag{30b}$$

Here $F(k)$ is the three-dimensional scalar variance spectrum.

The triple correlation of mixed type

$$\langle B_{ij} Y_i Y_j \rangle = \int d\,\mathbf{X} \int d\,\mathbf{Y}\, B_{ij} Y_i Y_j P(\mathbf{X}) P(\mathbf{Y}/\mathbf{X}) = [\langle B_{ij} B_{ij}\rangle G_j + \langle B_{ij} B_{ji}\rangle G_i]/(\Omega_i + \Omega_j). \tag{31}$$

According to (12) B_{ij} is independent of $\mathbf{Y}$; its correlations can be calculated by (16e), and the formula for $P(\mathbf{X})$ in Ref. 21. After long manipulation, we have

$$\langle B_{ij} B_{ij} \rangle = 0.5\,H\{\mathbf{k}\cdot\mathbf{P}(\mathbf{k}-\mathbf{p})\cdot\mathbf{k} q(|\mathbf{k}-\mathbf{p}|) + \mathbf{k}\cdot\mathbf{P}(\mathbf{k}+\mathbf{p})\cdot\mathbf{k} q(|\mathbf{k}+\mathbf{p}|)\}, \tag{32a}$$

$$\langle B_{ji} B_{ji} \rangle = \langle B_{ij} B_{ij} \rangle, \tag{32b}$$

$$\langle B_{ij} B_{ji} \rangle = -\langle B_{ij} B_{ij} \rangle. \tag{32c}$$

Here $\mathbf{P}(\mathbf{k}) = \mathbf{I} - \mathbf{kk}/k^2$ is the projector operator,[21] $\mathbf{I}$ is the identity operator and $q(k) = 2H\langle X_i^2\rangle$ is the energy spectrum of the velocity field. In the derivation of (32) we have used the following property of $\mathbf{P}(\mathbf{k})$:

$$\mathbf{P}(\mathbf{k} \pm \mathbf{p})\cdot\mathbf{p} = \mp \mathbf{P}(\mathbf{k} \pm \mathbf{p})\cdot\mathbf{k}. \tag{33}$$

By Eqs. (31) and (32) we have solved one fundamental problem of the theory of a passive scalar field convected by turbulence: how to express the higher-order correlation of mixed type in terms of proper lower-order correlations. The cost is to introduce an infinite number of new unknown Ω_i, which will be determined by requiring that they have to optimize the approximation (19) or (22).

VI. VARIANCE EQUATION AND VARIANCE TRANSFER FUNCTION

Multiplying (11) by Y_i and then taking the ensemble average, using (30), we obtain the variance equation of the scalar field,

$$(d_t + 2\mu k^2)F(k) = S(k); \tag{34a}$$

$$S(k) = 16\pi H k^2 \sum_j \langle B_{ij} Y_i Y_j \rangle \tag{34b}$$

is the scalar variance transfer spectrum function. By (31) and (32), after some manipulation (34b) becomes

$$S(k) = 8\pi H k^2 \sum_{\mathbf{p}} \frac{q(|\mathbf{k}-\mathbf{p}|)\mathbf{k}\cdot\mathbf{P}(\mathbf{k}-\mathbf{p})\cdot\mathbf{k}[g(p)-g(k)]}{\Omega(k)+\Omega(p)}. \tag{34c}$$

Let the size of the cubic box containing turbulence approach infinity; after some manipulation finally we have

$$S(k) = 16\pi^2 k^4 \int_0^\infty dp\, C(k,p) p^4 \frac{g(p)-g(k)}{\Omega(k)+\Omega(p)}, \tag{34d}$$

where

$$C(k,p) = C(p,k) = \int_0^\pi d\phi \sin^3\phi \frac{q(|\mathbf{k}-\mathbf{p}|)}{|\mathbf{k}-\mathbf{p}|^2}. \tag{34e}$$

Here ϕ is the angle made by vectors $\mathbf{k}$ and $\mathbf{p}$.

Similar to the energy transfer function of the velocity field, the scalar variance transfer function is defined as

$$U(k) = \int_k^\infty dr\, S(r). \tag{35a}$$

Since the integrand in (34d) changes sign when k and p are interchanged, from (34d) and (35a) we have

$$U(k) = 16\pi^2 \int_k^\infty dr \int_0^k dp\, C(r,p)(rp)^4 \frac{g(p)-g(r)}{\Omega(r)+\Omega(p)}. \tag{35b}$$

In the convective range the variance transfer function is independent of k and is equal to the dissipation rate of scalar variance

$$\chi = 2\mu \int_0^\infty dk\, k^2 F(k). \tag{36}$$

Therefore in the convective range,

$$\chi = 16\pi^2 \int_k^\infty dr \int_0^k dp\, C(r,p)(rp)^4 \frac{g(p)-g(r)}{\Omega(r)+\Omega(p)}. \tag{37}$$

VII. VARIATIONAL APPROACH AND Ω EQUATION

The scalar variance spectrum $F(k)$ and $g(k)$ are related by (30b). The energy spectrum $q(k)$ can be determined by solving the closure problem of the Navier–Stokes equation.[21,22] Hence the variance equations (34) or (37) contain two unknown functions $g(k)$ and $\Omega(k)$. Another equation of $g(k)$ and $\Omega(k)$ is needed to solve the closure problem of the convected passive scalar field. The validity and error of the perturbation solution (27) depend upon the validity and error of the LFP model (19)–(22). The effective damping coefficient $\boldsymbol{\Omega} = [\Omega_i; i>0]$ is to be adjusted to optimize the LFP model, i.e., to minimize its error. This is similar to the optimum-parameter-estimation problem in control theory. The usual approach is the mean-square estimation method,[21,24] i.e., the optimum $\boldsymbol{\Omega}$ has to minimize the mean-square error of the approximation (19) which is

$$\mathfrak{L} = \sum_i \left\langle \left(\sum_j B_{ij} Y_j - (-\beta_i Y_i) \right)^2 \right\rangle. \tag{38}$$

By variational calculation, we have

$$\partial_{\Omega i}\, \mathfrak{L} = 0. \tag{39}$$

From (38) and (39), by using (28)–(32), after long manipulation finally we have (see Appendix)

$$g(k)\Omega(k) = 4\pi k^2 \int_0^\infty dp\, C(k,p) p^4 \Omega(p) \frac{g(k)-g(p)}{[\Omega(k)+\Omega(p)]^2}. \tag{40}$$

The Ω equation (40) and the variance equations (34) or (37) constitute a closed set of integral equations for two unknown functions $g(k)$ and $\Omega(k)$. This solves the closure problem of the convection-diffusion equation (1). As an application, in the next section the two integral equations will be solved to derive the inertial-convective-range spectrum (2) and to evaluate numerically the scalar Kolmogorov constant B_3.

VIII. INERTIAL-CONVECTIVE RANGE

The idealized model of the inertial-convective range of a turbulent scalar-velocity field is an energy source and a scalar variance source at zero wavenumber, an energy sink and a scalar variance sink at infinity wavenumber, with an energy flow and a scalar variance flow across the spectrum at the constant rates ϵ and χ, respectively. According to Ref. 21 in the inertial range,

$$q(k) = \mathrm{Ko}\, \epsilon^{2/3} k^{-11/3}/(4\pi), \quad \mathrm{Ko} = 1.2. \tag{41}$$

Substitute (41) into (34e), and we have

$$C(k,p) = \mathrm{Ko}\, \epsilon^{2/3} \varsigma(k,p)/(4\pi), \tag{42a}$$

$$\begin{aligned} \varsigma(k,p) = 0.75(kp)^{-3}\{ &\tfrac{1}{11}(k^2-p^2)^2 \\ &\times [|\mathbf{k}+\mathbf{p}|^{-11/3} - |\mathbf{k}-\mathbf{p}|^{-11/3}] \\ &- 0.4(k^2+p^2)[|\mathbf{k}+\mathbf{p}|^{-5/3} - |\mathbf{k}-\mathbf{p}|^{-5/3}] \\ &- [|\mathbf{k}+\mathbf{p}|^{1/3} - |\mathbf{k}-\mathbf{p}|^{1/3}]\}. \end{aligned} \tag{42b}$$

Let

$$g(k) = Ak^m, \quad \Omega(k) = Bk^n, \tag{43}$$

and $p = xk$; Eq. (40) then becomes

$$B^2 = \mathrm{Ko}\, \epsilon^{2/3} k^{4/3-2n} \int dx\, \varsigma(1,x) x^{4+n} \frac{(1-x^m)}{(1+x^n)^2}. \tag{44}$$

Since B is a constant, from (44)

$$n = 2/3. \tag{45}$$

Let $B = D\epsilon^{1/3}$, then

$$\Omega(k) = D\epsilon^{1/3} k^{2/3}, \tag{46}$$

and (44) becomes

$$D^2 = \mathrm{Ko} \int_0^\infty dx\, \varsigma(1,x) x^{4+n} \frac{(1-x^m)}{(1+x^n)^2}. \tag{47}$$

Let $p = xk$, $r = yk$, and by using (43) and (46), Eq. (37) becomes

$$\chi = 4\pi \operatorname{Ko} \epsilon^{1/3}(A/D)k^{11/3+m} \times \int_1^\infty dy \int_0^1 dx\, \varsigma(y,x)(xy)^4 \frac{x^m - y^m}{x^n + y^n}. \tag{48}$$

Since χ is a constant, from (48),

$$m = -\tfrac{11}{3}. \tag{49}$$

Let $A = B_3\chi\epsilon^{-1/3}/(4\pi)$, from (43) and (48); we then have

$$F(k) = 4\pi k^2 g(k) = B_3\chi\epsilon^{-1/3}k^{-5/3}, \tag{50}$$

$$\frac{D}{B_3} = \operatorname{Ko} \int_1^\infty dy \int_0^1 dx\, \varsigma(y,x)(xy)^4 \frac{x^m - y^m}{x^n + y^n}. \tag{51}$$

Equation (50) is simply the inertial-convective-range spectrum (2). We have derived it as a consequence of the dynamic equation (1) by the method of statistical mechanics.

From (41), (45), (47), (49), and (51), by numerical computation we have

$$D^2 = 0.25, \quad D/B_3 = 0.82. \tag{52}$$

Therefore

$$D = 0.5 \text{ and } B_3 = 0.61. \tag{53}$$

IX. COMPARISON WITH EXPERIMENTS

A series of experiments have been made to test the validity of the spectrum (50) and to determine the scalar Kolmogorov constant B_3.[7–13] There is some confusion about the experimental data of the scalar Kolmogorov constant due to its different definitions. The 3-D scalar Kolmogorov constant B_3 used in this paper is defined by Eq. (2) or (50), and correspond to the 3-D spectrum $F(k)$. In experiments the 1-D spectrum $F_1(k)$ is measured, and a corresponding 1-D scalar Kolmogorov constant B_1 is determined;

$$F_1(k) = B_1\chi\epsilon^{-1/3}k^{-5/3}. \tag{54}$$

Some authors[12] prefer to use 0.5χ as the dissipation rate, and introduce a new 1-D scalar Kolmogorov constant B_1',

$$F_1(k) = B_1'(0.5\chi)\epsilon^{-1/3}k^{-5/3}. \tag{55}$$

The relationships between B_1, B_1', and B_3 are[2,7,12]

$$B_1' = 2B_1 \text{ and } B_3 = (5/3)B_1. \tag{56}$$

The experimental values of B_1, B_1', and B_3 are given in Table I. The experimental values of B_3 are between 0.5 and 0.8. The present theoretical prediction ($B_3 = 0.61$) is in good agreement with the experiments. This is very encouraging and is a further justification of the variational approach to the closure problem proposed in Ref. 21.

TABLE I. Experimental values of the scalar Kolmogorov constant.

Reference	B_1	B_1'	B_3
Gibson and Schwarz (1963)[7]	0.35	0.70	0.58
Gurvich and Zubkovskii (1966)[8]	0.45	0.90	0.75
Grant *et al.* (1968)[9]	0.31	0.62	0.52
Panofsky (1969)[10]	0.35	0.70	0.58
Paquin and Pond (1971)[12]	0.41	0.82	0.68
Wyngaard and Cote (1971)[11]	0.40	0.80	0.67
Champagne *et al.* (1977)[13]	0.45	0.90	0.75

X. DISCUSSION

The theoretical value of B_3, 0.208, obtained by Kraichnan[14] is too small. Gibson's phenomenological theory[15] predicts that B_3 is between 1.0 and 1.7, which is too large. Lundgren's theoretical prediction[16] $B_3 = 0.49$ is better, but still is lower than the experimental data. In Lundgren's theory some adjustable parameters are needed to specify the energy spectrum, and Corrsin's independent hypothesis is used to relate the Lagrangian and Eulerian statistics. In present theory there is no adjustable parameter and Corrsin's independent hypothesis is not needed.

Dimensional arguments can predict that the inertial-range energy spectrum and the inertial-convective-range scalar variance spectrum are proportional to $k^{-5/3}$, but cannot determine the values of the Kolmogorov constants Ko and B_3. The theory developed in Ref. 21 and in this paper can prove that the $k^{-5/3}$ spectrum is actually a consequence of the corresponding dynamic equation, the Navier–Stokes equation or the convection-diffusion equation (1), moreover it can determine the values of Ko and B_3. This situation is somehow similar to the relationship between thermodynamics and statistical mechanics.

At the present time we have no formal proof of the convergence of the perturbation method used here. A relevant problem is the possibility of the perturbation solution (27) being negative when the modal parameters Y_i are very large. As discussed in Ref. 21 this probability is very small or nearly zero.

The Liouville operator $\mathbf{L}$ (18) is called an unsolvable operator, because we don't know how to obtain the exact solution of its corresponding Liouville equation. On the contrary the Fokker–Planck operator $\mathbf{L}^{(f)}$ is a solvable operator, since we know that the exact solution of its corresponding Liouville equation, the Fokker–Planck equation, is the Gaussian density function. In the perturbation-variation method developed in Ref. 21 and this paper, the solvable operator $\mathbf{L}^{(f)}$ is used to approximate the unsolvable operator $\mathbf{L}$, and the exact solution of the solvable operator is used as a zero-order approximate solution of the unsolvable operator. The success of this method depends upon the proper choice of the solvable operator. The studies reported in Refs. 21–23 and in this paper show that choosing the Fokker–Planck operator as the solvable operator is successful, although it is not clear whether this choice is the best one.

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APPENDIX: DERIVATION OF THE Ω EQUATION (40)

Substituting (38) into (39) and using (28)–(29), we have

$$\begin{aligned} G_i\Omega_i = {} & -\sum_j [\langle B_{ij}B_{ij}\rangle G_j + \langle B_{ij}B_{ji}\rangle G_i]/(\Omega_i + \Omega_j) \\ & + \sum_j \{\Omega_i[\langle B_{ij}B_{ij}\rangle G_j + \langle B_{ij}B_{ji}\rangle G_i] \\ & + \Omega_j[\langle B_{ji}B_{ji}\rangle G_i + \langle B_{ij}B_{ji}\rangle G_j]\}/(\Omega_i + \Omega_j)^2. \end{aligned} \tag{A1}$$

For isotropic turbulence, G_i and Ω_i are functions of k only, $G_i = G(k)$ and $\Omega_i = \Omega(k)$. By means of (30b) and (32), Eq. (A1) becomes

$$g(k)\Omega(k) = 2H \sum_{\mathbf{p}} q(r)\mathbf{k}\cdot\mathbf{P}(\mathbf{r})\cdot\mathbf{k}\Omega(p) \frac{g(k) - g(p)}{[\Omega(k) + \Omega(p)]^2}, \tag{A2}$$

with $\mathbf{r} = \mathbf{k} - \mathbf{p}$. Let the size of the cubic box containing turbulence approach infinity. The summation over the discrete wave vector $\mathbf{p}$ approaches a 3-D integral, and (A2) becomes

$$\begin{aligned} g(k)\Omega(k) &= 2\int\int\int d\mathbf{p} \\ &\quad \times k^2 p^2 \sin^2\phi\, q(r)\Omega(p) \frac{g(k) - g(p)}{\{r[\Omega(k) + \Omega(p)]\}^2} \\ &= 4\pi \int_0^\infty dp \int_0^\pi d\phi \\ &\quad \times k^2 p^4 \sin^3\phi\, q(r)\Omega(p) \frac{g(k) - g(p)}{\{r[\Omega(k) + \Omega(p)]\}^2}, \end{aligned} \tag{A3}$$

with $\mathbf{r} = \mathbf{k} - \mathbf{p}$. Here ϕ is the angle made by vectors $\mathbf{k}$ and $\mathbf{p}$. By means of $r = |\mathbf{k} - \mathbf{p}|$ and Eq. (34e), from (A3) we have

$$g(k)\Omega(k) = 4\pi k^2 \int_0^\infty dp\, C(k,p)p^4\Omega(p) \frac{g(k) - g(p)}{[\Omega(k) + \Omega(p)]^2}, \tag{A4}$$

which is simply the Ω equation (40). The derivation of Eq. (3d) is similar.

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