Turbulence Fluctuations and New Universal Realizability Conditions in Modeling

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(Received 25 July 1996)

General turbulent mean statistics are shown to be characterized by a variational principle. The variational functionals, or "effective actions," have experimental consequences for turbulence fluctuations and are subject to realizability conditions of positivity and convexity. An efficient Rayleigh-Ritz algorithm is available to calculate approximate effective actions within probability density function (PDF) closures. Examples are given for Navier-Stokes and for a three-mode system of Lorenz. The new realizability conditions succeed at detecting *a priori* the poor predictions of PDF closures even when the classical second-order moment realizability conditions are satisfied. [S0031-9007(97)02680-X]

PACS numbers: 47.27.Sd, 05.40.+j, 47.11.+j, 47.27.−i

It does not seem to be a well-recognized fact that general turbulence mean statistics—such as mean velocity or pressure profiles—are characterized by a variational principle. However, in nonequilibrium statistical mechanics it was pointed out long ago by Onsager [1,2] that mean histories satisfy a "principle of least action." The so-called Onsager-Machlup action determines the probability of fluctuations away from the most probable state. Close to thermal equilibrium there is a standard fluctuation-dissipation relation, so that the action has the physical interpretation of a "dissipation function." Onsager's variational principle reduces then to a principle of least dissipation.

Recently it has been pointed out by one of us [3,4] that a similar *effective action* $\Gamma[z]$ exists in turbulent flow for *any* random variable $Z(t)$. This action function (i) is nonnegative, $\Gamma[z] \geq 0$, (ii) has the ensemble mean $\overline{z}(t)$ as its unique minimum $\Gamma[\overline{z}] = 0$, and (iii) is convex, $\lambda\Gamma[z_1] + (1-\lambda)\Gamma[z_2] \geq \Gamma[\lambda z_1 + (1-\lambda)z_2]$, $0 < \lambda < 1$. These are realizability conditions [5] which arise from positivity of the underlying statistical distributions. As a consequence, the mean value $\overline{z}(t)$ is characterized by a "principle of least effective action." Just as is Onsager's action, this functional is related to fluctuations. In particular, in statistically stationary turbulence, the time-extensive limit of the effective action, $V[z] \equiv \lim_{T\to\infty} \frac{1}{T}\Gamma[\{z(t) = z\colon 0 < t < T\}]$, the so-called *effective potential,* determines the probability of fluctuations in the empirical time average $\overline{Z}_T \equiv \frac{1}{T}\int_0^T dt\, Z(t)$ away from the (time-independent) ensemble-mean value $\overline{z}$. More precisely, the probability for any value z of the time average $\overline{Z}_T$ to occur is given by

$$\mathrm{Prob}(\{\overline{Z}_T \approx z\}) \sim \exp(-T\, V[z])\,. \tag{1}$$

This agrees with the standard ergodic hypothesis, according to which, as $T \to \infty$, the empirical time average must converge to the ensemble mean, $\overline{Z}_T \to \overline{z}$, with probability one in every flow realization. Equation (1) refines that hypothesis, by giving an exponentially small estimate of the probability at a large (but finite) T to observe fluctuations away from the ensemble mean.

The realizability conditions on the effective action or effective potential hold even when there are no classical second-moment realizability conditions on the means themselves. Thus, energy spectra or Reynolds stresses (second moments) must be positive, but mean velocity profiles (first moments) or energy transfer (third moments) do not satisfy simple realizability conditions [5]. The new realizability conditions thus have great potential significance in modeling if they can be efficiently calculated within turbulence closures. In [3,4] we have shown that there is a simple Rayleigh-Ritz algorithm within probability density function (PDF) closures—such as mapping closures [6–8] or generalized Langevin models [9,10]—by which the corresponding approximate values of the effective action or effective potential may be readily calculated.

As a simple example, we consider first a three-mode system of Lorenz [11], in which the equations of motion are

$$\dot{x}_i = A_i x_j x_k - \nu_i x_i + f_i\,, \tag{2}$$

with i, j, k a cyclic permutation of $1, 2, 3$, with $A_1 + A_2 + A_3 = 0$ imposed on interaction coefficients A_i for energy conservation, with ν_i positive damping coefficients, and $f_i(t)$ white-noise random forces with covariance $2\kappa_i$. This dynamics has been used often as a first test of closure ideas [12–14]. We consider a simple mapping closure proposed by Bayly for the three-mode system [15], which models the realizations by a quadratic map $X_i = \beta_i N_i + \beta_4 N_j' N_k'$ of independent standard Gaussian variables N_i, N_i', $i = 1, 2, 3$. The resulting closure equations for the second moments $M_i = \langle x_i^2\rangle$, $i = 1, 2, 3$ and the third moment $T = \langle x_1 x_2 x_3\rangle$ are

$$\dot{M}_i = 2A_i T - 2\nu_i M_i + 2\kappa_i \tag{3}$$

for $i = 1, 2, 3$ and

$$\dot{T} = A_1 M_2 M_3 + A_2 M_1 M_3 + A_3 M_1 M_2 - (\nu_1 + \nu_2 + \nu_3) T \,. \quad (4)$$

These are just the *quasinormal (QN) equations* for the three-mode system, obtained by neglecting the fourth-order cumulants [16]. It was already noted by Kraichnan [12] that, unlike for Navier-Stokes, the QN closure for the three-mode system predicts all positive energies. In fact, for $A_1 = 2$, $A_2 = A_3 = -1$, $\kappa_1 = 1$, $\kappa_2 = \kappa_3 = 0.001$, $\nu_1 = 0.001$, $\nu_2 = \nu_3 = 1$ it gives steady-state values

$$M_1^{(\mathrm{QN})} \approx 1.49875, \qquad M_2^{(\mathrm{QN})} = M_3^{(\mathrm{QN})} \approx 0.50025\,, \quad T^{(\mathrm{QN})} \approx -0.49925\,. \quad (5)$$

All of the second moments are positive, as required by realizability. However, direct numerical simulation (DNS) of the three-mode dynamics itself gives

$$M_1^{(\mathrm{DNS})} = 4.46 \pm 0.03\,, \quad M_2^{(\mathrm{DNS})} = M_3^{(\mathrm{QN})} = 0.49876 \pm 0.00002\,, \quad T^{(\mathrm{DNS})} = -0.49776 \pm 0.00002\,. \quad (6)$$

While the QN predictions for M_2, M_3, and T are within $\frac{1}{3}\%$ of the DNS values, M_1 is underpredicted by 66% in the QN approximation. As is well known, satisfaction of realizability cannot guarantee that a prediction is correct. However, failure of realizability certainly implies that the predictions are in error. In Figs. 1–3 we graph the approximate effective potentials of the energy variables $E_i = \frac{1}{2}x_i^2$, $i = 1, 2$ and triple product $\Pi = x_1 x_2 x_3$ in the QN closure as calculated by the Rayleigh-Ritz algorithm for the above PDF model. The numerical method is outlined below and described in detail in [4,17]. It is apparent that V_{E_2} and V_Π satisfy realizability but that V_{E_1}—which is negative and concave—does not. Thus, one may infer *a priori* that the QN prediction for the mean of E_1 is not converged. In this case, the failure of realizability of the predicted V_{E_1} succeeds at detecting the poor prediction for the mean value, even though the classical second-moment condition $M_1 \geq 0$ is satisfied. In the same plots in Figs. 2 and 3 we have graphed also the effective potentials V_{E_2} and V_Π obtained from DNS. They do not agree with the QN potentials as closely as do the corresponding means: the accurate prediction of fluctuations is a much more stringent demand on the closure. However, we note that the predictions of Bayly's PDF closure [15] are at least qualitatively correct for V_{E_2} and V_Π and give correctly the order of magnitude of the averaging time needed to eliminate fluctuations in those variables. Of course, the prediction of V_{E_1} is not even qualitatively correct.

The Rayleigh-Ritz algorithm used in obtaining the approximate potentials from the PDF closure involves a fixed point problem very similar to (and, in fact, generalizing) the fixed point condition determining the predicted steady-state moments themselves. The system of equations that must be solved in general is

$$\frac{\partial V_0}{\partial \mathbf{M}}(\mathbf{M}, \mathbf{h})\alpha_0 + \left(\frac{\partial \mathbf{V}}{\partial \mathbf{M}}\right)^{\top}(\mathbf{M}, \mathbf{h}) \cdot \boldsymbol{\alpha} = V_0(\mathbf{M}, \mathbf{h})\boldsymbol{\alpha}\,, \quad (7)$$

$$\mathbf{V}(\mathbf{M}, \mathbf{h}) = V_0(\mathbf{M}, \mathbf{h})\mathbf{M}\,, \quad (8)$$

$$\alpha_0 + \boldsymbol{\alpha} \cdot \mathbf{M} = 1\,. \quad (9)$$

The vector $\mathbf{M} = (M_1, \ldots, M_k)$ contains the moments of the closure, e.g., in the case above, $k = 4$ (and $M_4 = T$). It is less easy to describe the role of the $\boldsymbol{\alpha}$ variables, but they are closely related to infinitesimal disturbances of the $\mathbf{M}$'s which would appear in a linear stability analysis of the fixed-point moments. (They evolve like covectors of the disturbances.) $\mathbf{h}$ is the vector of "perturbation fields," one associated with each variable Z_i for which the potential is to be determined. In our

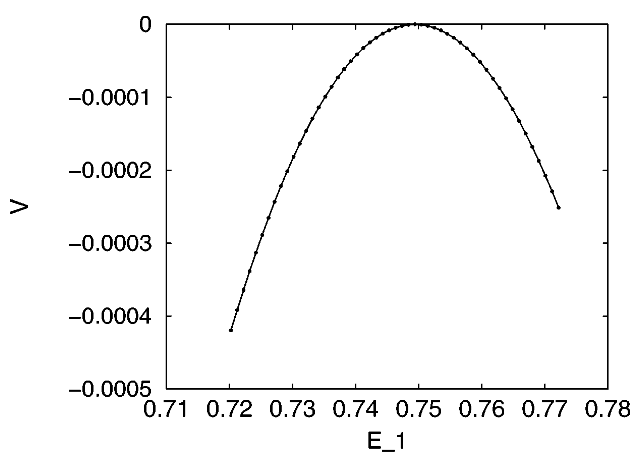

FIG. 1. Effective potential for energy in mode 1 in quasinormal closure.

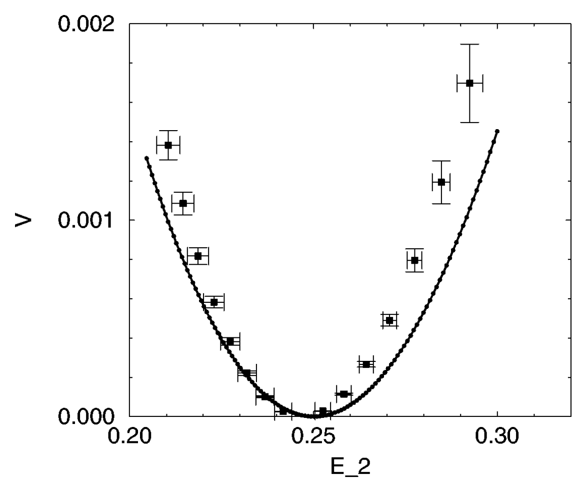

FIG. 2. Effective potential for energy in mode 2 in quasinormal closure (DNS with error bars).

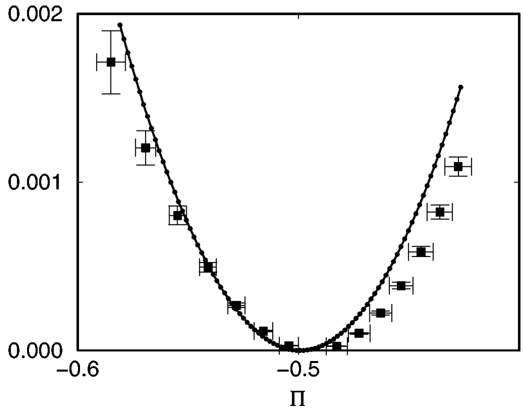

FIG. 3. Effective potential for triple moment in quasinormal closure (DNS with error bars).

previous calculation $\mathbf{h} = (h_{E_1}, h_{E_2}, h_\Pi)$. When $\mathbf{h} = \mathbf{0}$ the vector $\mathbf{V}(\mathbf{M},\mathbf{h})$ coincides with the dynamical vector $\mathbf{V}(\mathbf{M})$ which appears in the closure equation: $\dot{\mathbf{M}} = \mathbf{V}(\mathbf{M})$ [cf. Eqs. (3) and (4) above]. The perturbations for $\mathbf{h} \neq \mathbf{0}$ are determined by the method discussed in [4]. The 0 component $V_0(\mathbf{M},\mathbf{h})$ is associated with the zeroth moment $M_0 \equiv 1$ and it may be written explicitly here as $V_0(\mathbf{M},\mathbf{h}) = \frac{1}{2}h_{E_1}M_1 + \frac{1}{2}h_{E_2}M_2 + h_\Pi M_4$. It is easy to check that, when $\mathbf{h} = \mathbf{0}$, the stationary moments $\mathbf{M}_*$ along with $\alpha_{*0} = 1, \boldsymbol{\alpha}_* = \mathbf{0}$ solve the system Eqs. (7)–(9). Once the solutions $\alpha_{*0}(\mathbf{h}), \boldsymbol{\alpha}_*(\mathbf{h}), \mathbf{M}_*(\mathbf{h})$ are known for $\mathbf{h} \neq \mathbf{0}$, the effective potential V_{Z_i} is constructed as a function of h_i via $V_{Z_i}[h_i] = -\boldsymbol{\alpha}_*(h_i) \cdot \mathbf{V}[\mathbf{M}_*(h_i)]$. To obtain the potential as a function of z_i, the expected value $\mathbf{Z}_*(\mathbf{h}) = \mathbf{z}$ must be inverted to give h_i as a function of z_i. For full details of the algorithm, see [4,17].

Our results point toward significant new directions in turbulence modeling. The new realizability conditions apply individually to *all* predicted means. We see above that they can successfully discriminate between poor predictions for one set of variables and good predictions for another. Calculating each point on the graph of an effective potential curve within a closure requires just the same amount of computation as that to calculate the predicted mean. It is therefore very easy to apply the above realizability conditions as a check to detect poor predictions in advance, without expensive testing by experiment or simulation. This gives a strong incentive to the development of PDF closures, such as those in Refs. [6–10]. In conjunction with our variational method they can give some *a priori* information in turbulence modeling. This is a unique advantage, almost never obtained in other statistical closure methods.

It remains to be seen how well the Rayleigh-Ritz algorithm works to calculate effective potentials and effective actions for Navier-Stokes turbulence when used in conjunction with physically motivated PDF closures. It is thus worthwhile to give one example of the method for a statistically time-dependent Navier-Stokes flow. The simplest such situation is freely decaying homogeneous and isotropic turbulence with random initial data. We consider a model energy spectrum

$$E(k,t) = \begin{cases} Ak^m & k \leq k_L(t), \\ \alpha\varepsilon^{2/3}(t)k^{-5/3} & k_L(t) \leq k \leq k_d(t), \\ 0 & k \geq k_d(t), \end{cases} \tag{10}$$

which has been adopted before in this problem [18,19]. As long as $0 < m < 4$ it is commonly believed that there is a permanence of the low-wave-number spectrum. This motivates one to adopt the above self-preserving form, in which the shape of the spectrum is unchanged in time except through its dependence on the parameters $\varepsilon(t)$, $k_L(t)$, and $k_d(t)$. At high Reynolds number there is only one independent such parameter, since the relation $k_L(t) = [\frac{\alpha}{A}\varepsilon(t)]^{\frac{3}{3m+5}}$ is required by continuity and, when $k_L(t) \ll k_d(t)$, $k_d(t) = (\frac{4}{3\alpha\nu})^{3/4}\varepsilon^{1/4}(t)$ also holds [19]. The remaining time dependence is determined by considering the evolution of the mean energy $E(t) = \frac{1}{2}\langle v^2(t)\rangle$. For the above form of the spectrum it is not hard to show [19] that the dissipation $\varepsilon(t) = \frac{\nu}{2}\sum_{ij}\langle(\partial_i v_j + \partial_j v_i)^2\rangle$ is given as

$$\varepsilon(t) = \Lambda_m E^p(t), \tag{11}$$

with $\Lambda_m^{-1} = \alpha^{3/2}(\frac{1}{m+1} + \frac{3}{2})^{\frac{3m+5}{2m+2}} A^{\frac{1}{m+1}}$ and $p = \frac{3m+5}{2m+2}$. Thus, employing the Navier-Stokes equation via its energy balance, one obtains the closed equation

$$\dot{E}(t) = -\Lambda_m E^p(t). \tag{12}$$

Its solution gives a prediction for the energy-decay law, as $E_*(t) = E_0[(t - t_0^*)/\Delta t]^{-n}$, $n = (2m+2)/(m+3)$; see [19].

It is interesting to make a check on the various hypotheses involved in these predictions by means of the effective action $\Gamma[E]$ for the energy history $E(t)$. As a simple PDF model for the above closure, one may adopt a Gaussian random velocity field with the assumed self-similar spectrum Eq. (10). The Rayleigh-Ritz approximation of the effective action within the Gaussian *Ansatz* can be analytically evaluated [20], with the result

$$\Gamma^{(\mathrm{Gauss})}[E] = \frac{3}{2(p-2)\Lambda_m}\int_0^\infty dt \times \frac{[\dot{E}(t) + \Lambda_m K^p(t)][\dot{K}(t) + \Lambda_m K^p(t)]}{K^{p+1}(t)}, \tag{13}$$

where $K(t)$ is a variational parameter satisfying

$$\Lambda_m K^p(t) + \dot{E}(t) = (p-2) \times \Lambda_m[E(t) - K(t)]K^{p-1}(t). \tag{14}$$

It is easy to check that, if the predicted closure mean energy $E_*(t)$ satisfying $\dot{E}_*(t) = -\Lambda_m E_*^p(t)$ is substituted, then $\Gamma^{(\mathrm{Gauss})}[E_*] = 0$. Further insight is obtained by considering small perturbations $E(t) = E_*(t) + \delta E(t)$ from the predicted mean. By a straightforward calculation it follows that

$$\Gamma^{(\mathrm{Gauss})}[E] = \frac{3}{8(p-1)\Lambda_m} \int_0^\infty dt \times \frac{[\delta \dot{E}(t) + \Lambda_m p E_*^{p-1}(t) \delta E(t)]^2}{E_*^{p+1}(t)} + O(\delta E^3). \quad (15)$$

This is the same law of fluctuations as would be realized with the Langevin equation

$$\delta \dot{E}(t) + \Lambda_m p E_*^{p-1}(t) \delta E(t) = \sqrt{2R_*(t)}\, \eta(t) \quad (16)$$

obtained by linearization of the energy-decay equation around its solution $E_*(t)$ and by addition of a white-noise random force $\eta(t)$, with its coefficient given by

$$R_*(t) = \frac{2(p-1)}{3} \varepsilon_*(t) E_*(t). \quad (17)$$

Thus, the smaller fluctuations from the ensemble-mean value are predicted to decay according to a linearized law, similar to the Onsager regression hypothesis for equilibrium fluctuations. Likewise, the expression Eq. (17) is a *fluctuation-dissipation relation* analogous to that in equilibrium. A concrete consequence, testable by experiment, is the following prediction for the two-time correlation:

$$\langle \delta E(t) \delta E(t') \rangle = \left(\frac{t - t_0^*}{\Delta t}\right)^{-(n+1)} \left(\frac{t' - t_0^*}{\Delta t}\right)^{-(n+1)} \left\{ (\delta E_0)^2 + \frac{2}{3} E_0^2 \left[\left(\frac{t_{\min} - t_0^*}{\Delta t} \right)^2 - 1 \right] \right\}, \quad \text{with } t_{\min} = \min\{t, t'\}.$$

Note that the coefficient $(p-1)$ in front of the action is >0 as long as $m > -3$. In fact, $m > -1$ is required to give a finite energy. Thus, for all permissable values of m, the approximate action $\Gamma^{(\mathrm{Gauss})}[E]$ satisfies realizability. One should be cautioned again that satisfaction of realizability is only a consistency check and cannot guarantee correctness of predictions. Failure of realizability, as observed in the three-mode model, is more practically useful, although in a purely negative way.

The previous examples and our variational method are discussed in greater detail in forthcoming papers [17,20]. Here, we simply wished to illustrate briefly the use of the action principle. Future work will study the success of the new realizability conditions in detecting poor closure predictions for more realistic Navier-Stokes flows, of greater interest to practical engineering. It should be clear that very general PDF *Ansätze* may be employed in our method, either by guessing a functional form of the PDF or by hypothesizing "surrogate" random variables to model the actual flow realizations. Any guess of the turbulence statistics—such as the "synthetic turbulence" models of [21]—may be input to yield predictions for realistic problems. We therefore expect our method to be a flexible framework within which to develop novel turbulence closures. Insights from simulation, experiment, and recent theoretical developments can be readily incorporated. The advantage of the variational formulation is that it provides built-in checks of statistical closures which may detect a sizable fraction of faulty predictions in advance. By doing so cheaply, it can provide great savings in turbulence modeling for practical engineering purposes.

We thank R. H. Kraichnan for his interest in and encouragement of this work. Numerical computations were carried out at the Center for Computational Science at Boston University and the Department of Mathematics at the University of Arizona.

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