Linear stochastic models of nonlinear dynamical systems

Gregory L. Eyink
Department of Mathematics, University of Arizona, Tucson, Arizona 85721
(Received 3 June 1998)

We investigate in this work the validity of linear stochastic models for nonlinear dynamical systems. We exploit as our basic tool a previously proposed Rayleigh-Ritz approximation for the *effective action* of nonlinear dynamical systems started from random initial conditions. The present paper discusses only the case where the probability density function *Ansatz* employed in the variational calculation is ''Markovian,'' i.e., is determined completely by the *present* values of the moment averages. In this case we show that the Rayleigh-Ritz effective action of the complete set of moment functions that are employed in the closure has a quadratic part which is always formally an Onsager-Machlup action. Thus, subject to satisfaction of the requisite realizability conditions on the noise covariance, a linear Langevin model will exist which reproduces exactly the joint two-time correlations of the moment functions. We compare our method with the closely related formalism of principal oscillation patterns (POP), which, in the approach of Penland, is a method to derive such a linear Langevin model empirically from time-series data for the moment functions. The predictive capability of the POP analysis, compared with the Rayleigh-Ritz result, is limited to the regime of small fluctuations around the most probable future pattern. Finally, we shall discuss a *thermodynamics of statistical moments* which should hold for all dynamical systems with stable invariant probability measures and which follows within the Rayleigh-Ritz formalism. [S1063-651X(98)13111-2]

PACS number(s): 05.40.+j, 05.45.+b, 92.60.Wc, 05.70.Ln

I. INTRODUCTION

We consider nonlinear dynamical systems governed by (possibly nonautonomous) differential equations:

$$\dot{\mathbf{x}}=\hat{\mathbf{U}}(\mathbf{x},t). \tag{1.1}$$

We may take $\mathbf{x}=(x_1,\ldots,x_p)^\top$ to have any number of components, possibly infinitely many, formally including infinite-dimensional dynamical systems governed by partial differential equations, etc. In many contexts the dynamics of a selected set of variables $\hat{\boldsymbol{\psi}}(\mathbf{x})=(\hat{\psi}_1(\mathbf{x}),\ldots,\hat{\psi}_n(\mathbf{x}))^\top$ is of interest. Of course, by the chain rule

$$\partial_t\hat{\boldsymbol{\psi}}=(\hat{\mathbf{U}}\cdot\nabla_{\mathbf{x}})\hat{\boldsymbol{\psi}}:=\hat{\mathbf{V}}. \tag{1.2}$$

When the dynamics is nonlinear, the right-hand side $\hat{\mathbf{V}}$ of Eq. (1.2) cannot generally be expressed in terms of the functions $\hat{\boldsymbol{\psi}}$ themselves. For example, when $\hat{\mathbf{U}}(\mathbf{x})$ and $\hat{\boldsymbol{\psi}}(\mathbf{x})$ are polynomial functions of $\mathbf{x}$, the right-hand side consists of higher-degree polynomials. This is a manifestation of the *closure problem* of nonlinear dynamical systems.

If one considers the initial-value problem with random initial data, a common strategem to obtain mean values $\mathbf{m}(t):=\langle\hat{\boldsymbol{\psi}}\rangle_t$ is to make a *moment closure* approximation $\langle(\hat{\mathbf{U}}\cdot\nabla_{\mathbf{x}})\hat{\boldsymbol{\psi}}\rangle_t\approx\mathbf{V}(\mathbf{m},t)$ for some function $\mathbf{V}$ of the selected moments, so that a closed equation

$$\dot{\mathbf{m}}(t)=\mathbf{V}(\mathbf{m},t) \tag{1.3}$$

is obtained. Likewise, if one is interested in *fluctuations* of the variables $\hat{\boldsymbol{\psi}}(t)$, then one can make an approximation that

$$\dot{\hat{\boldsymbol{\psi}}}(t)\approx\mathbf{V}(\hat{\boldsymbol{\psi}},t)+\hat{\mathbf{q}}(t), \tag{1.4}$$

where $\hat{\mathbf{q}}(t)$ is a *random force* of known statistics, which is supposed to represent the effects of neglected variables beyond the subset $\hat{\boldsymbol{\psi}}$ retained. Such a model—if it is valid—will clearly give important information about predictability of the variables $\hat{\boldsymbol{\psi}}(t)$. For example, conditional probabilities $P(\boldsymbol{\psi},t|\boldsymbol{\psi}_0,t_0)$ are implied, which express precisely the limits on predicting the moment variables at a future time t given their values at the present time t_0. One is thus interested to know the possibilities and limitations of such a stochastic modelization.

In previous work [1,2] we have studied fluctuations of nonlinear dynamics by an *action principle*. Such an approach to fluctuation theory goes back to the work of Onsager and Machlup [3]. They showed that a *linear Langevin dynamics*

$$\dot{\hat{\boldsymbol{\psi}}}(t)=\mathbf{A}(t)\hat{\boldsymbol{\psi}}+\hat{\mathbf{q}}(t), \tag{1.5}$$

in which $\hat{\mathbf{q}}(t)$ is a Gaussian random force with zero mean and covariance

$$\langle\hat{\mathbf{q}}(t)\hat{\mathbf{q}}^\top(t')\rangle=2\mathbf{Q}(t)\delta(t-t'), \tag{1.6}$$

can always be completely and equivalently reformulated in terms of an action functional $\Gamma[\boldsymbol{\psi}]$:

$$\Gamma[\boldsymbol{\psi}]=\frac{1}{4}\int_{t_0}^{\infty}dt(\dot{\boldsymbol{\psi}}-\mathbf{A}\boldsymbol{\psi})^\top\mathbf{Q}^{-1}(\dot{\boldsymbol{\psi}}-\mathbf{A}\boldsymbol{\psi}). \tag{1.7}$$

The interpretation of this functional is as a ''fluctuation potential'' for time histories. That is, the probability that a particular fluctuation value $\boldsymbol{\psi}(t)$ occurs for the random variable $\hat{\boldsymbol{\psi}}(t)$ is given in terms of the Onsager-Machlup action by the exponential formula

$$\text{Prob}(\hat{\boldsymbol{\psi}}(t)\approx\boldsymbol{\psi}(t):-\infty<t<+\infty)\sim e^{-\Gamma[\boldsymbol{\psi}]}. \tag{1.8}$$

This gives the most direct probabilistic significance of the Onsager-Machlup action. The fact that the action is a quadratic functional of $\boldsymbol{\psi}$ is consistent with the fact that the solution of the linear Langevin equation is a normal random variable, with a Gaussian probability distribution.

Although the Onsager-Machlup theory as originally developed was restricted to linear Langevin dynamics, the action method is completely general: For any statistical dynamical system and for any selected subset of random variables $\hat{\boldsymbol{\psi}}$, an *effective action* $\Gamma[\boldsymbol{\psi}]$ can be introduced which plays the same role as the Onsager-Machlup action does for linear Langevin dynamics. It also has an interpretation as a fluctuation potential for the empirical average over N independent samples [4], i.e.,

$$\text{Prob}\left(\frac{1}{N}\sum_{n=1}^{N}\hat{\boldsymbol{\psi}}^{(n)}(t)\approx\boldsymbol{\psi}(t):-\infty<t<+\infty\right)\sim\exp(-N\Gamma[\boldsymbol{\psi}]). \tag{1.9}$$

[The additional factor of N in the exponent in Eq. (1.9) is discussed more below. See Eqs. (2.44)–(2.46).] The effective action is also a generating functional for all (irreducible) multitime correlations of the variables $\hat{\boldsymbol{\psi}}(t)$, of arbitrary order, and thus completely characterizes the distribution of those variables. To be precise, if the effective action is expanded into a functional power series in $\delta\boldsymbol{\psi}(t):=\boldsymbol{\psi}(t)-\langle\hat{\boldsymbol{\psi}}(t)\rangle$, as

$$\Gamma[\boldsymbol{\psi}]=\sum_{k=2}\frac{1}{k!}\int dt_1\cdots\int dt_k\Gamma^{(k)}_{i_1\cdots i_k}(t_1,\ldots,t_k)\times\delta\psi_{i_1}(t_1)\cdots\delta\psi_{i_k}(t_k), \tag{1.10}$$

then the coefficients are just the irreducible multitime correlators [5]. The correlators with $k\geqslant 3$ would all be zero for a Gaussian process. We shall not review these subjects further here, since they have been thoroughly discussed elsewhere [1,2].

In our earlier works, we developed a Rayleigh-Ritz approximation method by which the effective actions $\Gamma[\mathbf{z}]$ of *any* set of random variables $\hat{\mathbf{Z}}$ may be calculated within a moment-closure scheme based upon an *Ansatz* for a probability density function (PDF). In particular, an approximate effective action may be obtained for $\hat{\boldsymbol{\psi}}$, the moment variables retained in the closure. We shall show here that such a Rayleigh-Ritz approximate effective action $\Gamma_*[\boldsymbol{\psi}]$ of the moment variables themselves is not only a formal generalization of the Onsager-Machlup action, but is actually much more closely related. In fact, we shall show that the leading quadratic term in the Taylor expansion (1.10) of $\Gamma_*[\boldsymbol{\psi}]$ is always precisely of the Onsager-Machlup form, when the PDF *Ansatz* employed in the Rayleigh-Ritz calculation is ''Markovian.'' By the latter specification we denote PDF *Ansätze* which are completely determined by the *present* values which they assign to averages of the moment functions. Our result means that, for such a ''Markovian'' PDF *Ansatz*, there is *always* formally a linear Langevin dynamics such as Eq. (1.5) which gives predictions for the two-time correlations $\langle\delta\hat{\boldsymbol{\psi}}(t)\delta\hat{\boldsymbol{\psi}}^{\top}(t')\rangle$ that are the same as those given by the Rayleigh-Ritz effective action. In general, however, for higher-order correlations, the linear Langevin model and the Rayleigh-Ritz effective action will not yield the same predictions.

It is our purpose here to present the derivation of the linear Langevin model via the effective action method and to discuss its physical interpretation and limits of applicability. The effective action provides a framework to derive not only the linear theory but also the higher-order statistics (higher order in terms of the size of the fluctuations or the order of the correlator). It thus provides a means to assess the size of the corrections to the linear description. On the other hand, the linear Langevin model gives always the leading-order contribution to the effective action and, therefore, many of the important features of the full Rayleigh-Ritz approximation are essentially entirely determined by the linear equation. We shall in addition give a more intuitive derivation of the Langevin model within moment-closure methodology, but not using a systematic or formal scheme. While such a derivation provides no possibility to assess limitations of the linear description, nevertheless it provides insight into the physical assumptions involved. We shall also compare our method with the principal oscillation pattern (POP) analysis, which is a well-known method to extract linear stochastic models empirically from time-series data [6]. Finally, we shall conclude with some general discussion on the thermodynamics of moment-averages for dynamical systems with stable statistics. In particular, we discuss the law of entropy increase and fluctuation-dissipation relations at the linear level.

II. RAYLEIGH-RITZ EFFECTIVE ACTION OF MOMENT VARIABLES

A. Reprise of the Rayleigh-Ritz method

The Rayleigh-Ritz approximation of the effective action is based upon a variational formulation of the moment-closure scheme. This is just a variational formulation of the method of weighted residuals [7] to solve $\partial_t\mathcal{P}=-\nabla_{\mathbf{x}}\cdot(\hat{\mathbf{U}}\mathcal{P}):=\hat{\mathcal{L}}\mathcal{P}$, the Liouville equation for the phase-space distribution $\mathcal{P}$. The basic ingredients of a moment closure are (i) a set of *moment functions* $\hat{\boldsymbol{\psi}}(\mathbf{x},t)=(\hat{\psi}_1(\mathbf{x},t),\ldots,\hat{\psi}_n(\mathbf{x},t))$ and (ii) a PDF *Ansatz* $\mathcal{P}(\mathbf{x};\mathbf{m},t)$, conveniently parametrized by the mean values $m_i=\langle\hat{\psi}_i\rangle$, $i=1,\ldots,n$, which it assigns to those functions. The variable t is included to denote an *explicit* time dependence, i.e., any time dependence other than the implicit one through parameters $\boldsymbol{\alpha}(t),\mathbf{m}(t)$. The $\boldsymbol{\alpha}$-type parameters appear in the variational formulation of the closure, in which one incorporates all of the moment functions into a single linear combination,

$$\mathcal{A}(\mathbf{x};\boldsymbol{\alpha},t)=\sum_{i=0}^{n}\alpha_i\hat{\psi}_i(\mathbf{x},t). \tag{2.1}$$

Note that the constant function $\hat{\psi}_0(\mathbf{x},t)\equiv 1$ must be included in the sum in order to satisfy the final-time condition $\mathcal{A}(\infty)\equiv 1$. The PDF *Ansatz* $\mathcal{P}(\mathbf{x};\mathbf{m},t)$ is subject to an initial condition that it match the considered initial distribution $\mathcal{P}_0$ for the problem, $\mathcal{P}(\mathbf{x};\mathbf{m},t_0)=\mathcal{P}_0$, in the weighted-residual sense that the averages of the n moment functions $\hat{\boldsymbol{\psi}}(t)$ must match. Then, it is not hard to show that the *moment-closure equation*

$$\dot{\mathbf{m}}(t)=\mathbf{V}(\mathbf{m}(t),t), \tag{2.2}$$

where $\mathbf{V}(\mathbf{m},t) := \langle(\partial_t+\hat{\mathcal{L}}^\dagger)\hat{\boldsymbol{\psi}}(t)\rangle_{\mathbf{m},t}$, is the result of varying the *action functional*

$$\Gamma[\mathcal{A},\mathcal{P}]=\int_{t_0}^{\infty}dt[\langle\mathcal{A}(t),\dot{\mathcal{P}}(t)\rangle-\langle\mathcal{A}(t),\hat{\mathcal{L}}\mathcal{P}(t)\rangle] \tag{2.3}$$

over the above *Ansätze* for $\mathcal{A}(t),\mathcal{P}(t)$, with variational parameters $\alpha_0(t),\boldsymbol{\alpha}(t),\mathbf{m}(t)$. The Euler-Lagrange equations for $\mathbf{m}(t)$ are just Eq. (2.2) while the equations for $\alpha_0(t),\boldsymbol{\alpha}(t)$ have the unique solution $\alpha_0(t)\equiv 1,\boldsymbol{\alpha}(t)\equiv\mathbf{0}$ subject to the final conditions.

The Rayleigh-Ritz approximation to the effective action $\Gamma_*[\mathbf{z}]$ of a set of random variables $\hat{\mathbf{Z}}$ is obtained, in general, as the stationary point $\Gamma_*[\mathbf{z}]=\Phi_{\text{st.pt.}\mathcal{A},\mathcal{P}}\Gamma[\mathcal{A},\mathcal{P}]$ varied over $\mathcal{A}(t),\mathcal{P}(t)$ of the above forms, subject to the additional constraints of unit overlap

$$\langle\mathcal{A}(t),\mathcal{P}(t)\rangle=1 \tag{2.4}$$

and fixed expectation

$$\langle\mathcal{A}(t),\hat{\mathbf{Z}}(t)\mathcal{P}(t)\rangle=\mathbf{z}(t) \tag{2.5}$$

for each given history $\mathbf{z}(t)$, for all times t after the initial time t_0. [Recall that $\hat{\mathbf{Z}}(t)$ is an observable in the ''Schrödinger picture'' and that the only time dependence is explicit.]

We show here that the Rayleigh-Ritz approximation $\Gamma_*[\boldsymbol{\psi}]$ to the effective action of the moment variables themselves has, in general, a quadratic part which is just an Onsager-Machlup action, when closure is achieved within the framework outlined above. Other closure schemes are conceivable within the Rayleigh-Ritz formalism and may even better represent the physics in certain situations. A ''Markovian'' approximation has been made above, in assuming that the PDF *Ansatz* $\mathcal{P}(\cdot;\mathbf{m},t)$ is parametrized by only the *present value* $\mathbf{m}(t)$ of the n moment averages. This is by no means necessary. More generally, one may assume that $\mathcal{P}[\cdot;\mathbf{m},t]$ is a functional of the entire *past mean history* $\{\mathbf{m}(s):s<t\}$ of the n moment functions. In that case, the closure equation becomes

$$\dot{\mathbf{m}}(t)=\mathbf{V}[t;\mathbf{m}], \tag{2.6}$$

in which $\mathbf{V}[t;\mathbf{m}]$ is now also a functional over the past mean history. It is not hard to show that an *exact* equation always exists of the form (2.6) for a suitable choice of the functional $\mathbf{V}[t;\mathbf{m}]$. (For example, see [8], Appendix A1.) Thus, a closure incorporating such history effects is likely to be more faithful to the physics, in general. Our work here does not discuss this more general case, but confines itself to the ''Markovian'' *Ansatz*. Although this is restrictive, it is nevertheless the case that most practical closures considered in the literature are of this type. It is also possible, even within this more restrictive ''Markovian'' framework, to include some history effects. This may be done, for example, by constructing a closure using not only the n moment functions $\hat{\boldsymbol{\psi}}(t)$, but also the corresponding n *velocity functions* [this definition generalizes that in Eq. (1.2) to the case with explicit time dependence]

$$\hat{\mathbf{V}}(t):=(\partial_t+\hat{\mathcal{L}}^\dagger)\hat{\boldsymbol{\psi}}(t). \tag{2.7}$$

In this case, the closure equations become, instead of Eq. (2.2),

$$\begin{aligned}\dot{\mathbf{m}}(t)&=\mathbf{V}(t),\\ \dot{\mathbf{V}}(t)&=\mathbf{G}(\mathbf{m}(t),\mathbf{V}(t),t),\end{aligned} \tag{2.8}$$

where $\mathbf{G}(\mathbf{m},\mathbf{V},t):=\langle(\partial_t+\hat{\mathcal{L}}^\dagger)\hat{\mathbf{V}}(t)\rangle_{\mathbf{m},\mathbf{V},t}$ is the average *acceleration* of the moment functions within a PDF *Ansatz* depending jointly upon $\mathbf{m},\mathbf{V}$. Such schemes may be continued indefinitely to higher orders, e.g., the next stage would be to include a dependence jointly upon $\mathbf{m},\mathbf{V},\mathbf{G}$ in the PDF *Ansatz*. All of the results of this work carry over to such closures in terms of higher-order time derivatives, if one simply considers the enlarged set of moment functions $\hat{\boldsymbol{\Psi}}=(\hat{\boldsymbol{\psi}},\hat{\mathbf{V}}),(\hat{\boldsymbol{\psi}},\hat{\mathbf{V}},\hat{\mathbf{G}})$, etc. A linear Langevin model will always formally exist within such closure schemes which will exactly reproduce the predictions of the Rayleigh-Ritz effective action for the two-time statistics of the moment variables $\hat{\boldsymbol{\Psi}}$ considered.

B. Rayleigh-Ritz effective action: Exact expressions

It is the main purpose of this paper to demonstrate the latter essential fact. We will begin by developing some exact expressions for $\Gamma_*[\boldsymbol{\psi}]$. Substituting the given forms of $\mathcal{A}(t),\mathcal{P}(t)$ into the action (2.3), one obtains

$$\Gamma=\sum_{i=1}^{n}\int_{t_0}^{\infty}dt\,\alpha_i(t)[\dot{m}_i(t)-V_i(\mathbf{m}(t),t)]. \tag{2.9}$$

The overlap constraint (2.4) may be incorporated by eliminating the coefficient $\alpha_0(t)$, giving

$$\mathcal{A}(t)=1+\sum_{j=1}^{n}\alpha_j(t)[\hat{\psi}_j(t)-m_j(t)]. \tag{2.10}$$

With that choice, the fixed expectation constraint (2.5) becomes

$$\psi_i(t)=m_i(t)+\sum_{j=1}^{n}\alpha_j(t)C_{ij}(t), \tag{2.11}$$

where $\mathbf{C}(t):=\langle\hat{\boldsymbol{\psi}}(t)\hat{\boldsymbol{\psi}}^\top(t)\rangle_t-\mathbf{m}(t)\mathbf{m}^\top(t)$ defines the covariance matrix of the moment functions. Equation (2.11) is easy to invert, with the result that $\boldsymbol{\alpha}(t)=\mathbf{C}^{-1}(t)[\boldsymbol{\psi}(t)-\mathbf{m}(t)]$. It is convenient to denote the inverse of the covariance matrix by $\boldsymbol{\Gamma}(t):=\mathbf{C}^{-1}(t)$. Substituting the above results for $\boldsymbol{\alpha}(t)$, the action becomes

$$\Gamma_*[\boldsymbol{\psi};\mathbf{m}]=\int_{t_0}^{\infty}dt[\dot{\mathbf{m}}(t)-\mathbf{V}(\mathbf{m}(t),t)]^\top\boldsymbol{\Gamma}(t)[\boldsymbol{\psi}(t)-\mathbf{m}(t)]. \tag{2.12}$$

In this expression, all of the constraints have been properly incorporated, and the only remaining variational parameters are the $\mathbf{m}(t)$ variables. A set of variational equations must be developed to determine these, derived from the stationarity condition of the action.

Before carrying out this variation, however, it is useful to introduce some auxiliary quantities. Define, within the PDF *Ansatz* employed, a single-time cumulant-generating function

$$F(\mathbf{h}|\mathbf{m}(t),t):=\ln\langle\exp(\mathbf{h}\cdot\hat{\boldsymbol{\psi}}(t))\rangle_t \tag{2.13}$$

for the moment functions $\hat{\boldsymbol{\psi}}(t)$, where $\mathbf{m}(t)$ is the mean of the moment function within the PDF *Ansatz*. That is, the partial derivatives

$$C^{(p)}_{i_1\cdots i_p}(t)=\frac{\partial^p F}{\partial h_{i_1}\cdots\partial h_{i_p}}(\mathbf{h}|\mathbf{m}(t),t)|_{\mathbf{h}=\mathbf{0}} \tag{2.14}$$

are just the pth-order cumulants of the $\hat{\boldsymbol{\psi}}(t)$ within the *Ansatz*. The Legendre transform

$$H(\boldsymbol{\mu}|\mathbf{m}(t),t):=\sup_{\mathbf{h}}[\boldsymbol{\mu}\cdot\mathbf{h}-F(\mathbf{h}|\mathbf{m}(t),t)], \tag{2.15}$$

a *generalized entropy*, is the generating function of irreducible correlation functions. That is,

$$\Gamma^{(p)}_{i_1\cdots i_p}(t)=\frac{\partial^p H}{\partial \mu_{i_1}\cdots\partial \mu_{i_p}}(\boldsymbol{\mu}|\mathbf{m}(t),t)|_{\boldsymbol{\mu}=\mathbf{m}(t)}. \tag{2.16}$$

In particular, the relations hold that

$$\begin{aligned}\Gamma^{(1)}_i(t)&=h_i(\mathbf{m}(t),t),\\ \Gamma^{(2)}_{ij}(t)&=C^{-1}_{ij}(t)=\frac{\partial h_i}{\partial\mu_j}(\mathbf{m}(t),t).\end{aligned} \tag{2.17}$$

The latter relation will prove crucial in what follows.

It may be worthwhile to explain the intuitive significance of these single-time quantities before continuing with the development of the formulas for the action. They are all part of a general *thermodynamics of moments*. Thus, the entropy H is a form of Boltzmann's entropy, with his original sign convention, i.e., positive and convex. It is related to fluctuation probabilities of the empirical ensemble averages $\overline{\boldsymbol{\psi}}_N(t):=1/N\sum_{n=1}^N\hat{\boldsymbol{\psi}}^{(n)}(t)$ at time t by

$$\mathcal{P}(\overline{\boldsymbol{\psi}}_N(t)\approx\boldsymbol{\mu}|\mathbf{m}(t),t)\sim e^{-N\cdot H(\boldsymbol{\mu}|\mathbf{m}(t),t)}, \tag{2.18}$$

where the samples $\hat{\boldsymbol{\psi}}^{(n)}(t)$ are all independently chosen from the ensemble $\mathcal{P}(\cdot|\mathbf{m}(t),t)$. In other words, $H\propto-\ln\mathrm{Prob}$, which is Boltzmann's famous relation. Because we have defined probabilities with respect to the measure $\mathcal{P}(\cdot|\mathbf{m}(t),t)$, this quantity corresponds to what is in mathematics called the *relative entropy*. The latter is an entropy of probability measures analogous to Gibbs', but with respect to an arbitrary *a priori* measure $\mathcal{P}$. Thus,

$$\mathcal{H}(\mathcal{Q}|\mathcal{P}):=\int\mathcal{Q}\ln\left(\frac{\mathcal{Q}}{\mathcal{P}}\right). \tag{2.19}$$

It is not hard to show that

$$H(\boldsymbol{\mu}|\mathbf{m}(t),t)=\min_{\mathcal{Q}:\langle\boldsymbol{\psi}(t)\rangle_{\mathcal{Q}}=\boldsymbol{\mu}}\mathcal{H}(\mathcal{Q}|\mathcal{P}(\cdot|\mathbf{m}(t),t)). \tag{2.20}$$

This is a basic relation between the "thermodynamic" entropy $H(\cdot|\mathbf{m}(t),t)$ and the "statistical mechanics" measure $\mathcal{P}(\cdot|\mathbf{m}(t),t)$. It is a form of the *maximum entropy principle.* [This is indeed a maximum principle in terms of the usual entropies $S(\boldsymbol{\mu}|\mathbf{m}(t),t)=-H(\boldsymbol{\mu}|\mathbf{m}(t),t)$ and $\mathcal{S}(\mathcal{Q}|\mathcal{P})=-\mathcal{H}(\mathcal{Q}|\mathcal{P})$.] A good mathematical reference is [9]. As we shall see later, $H_*(t):=H(\mathbf{m}(t)|\mathbf{m}_*(t),t)$ should satisfy the second law of thermodynamics, $dH_*(t)/dt<0$, when $\mathbf{m}_*(t)$ is the predicted mean history of the moment functions and $\mathbf{m}(t)$ is any other solution of the closure equations sufficiently near $\mathbf{m}_*(t)$. The derivatives of H also have thermodynamic significance. For example, the first derivatives $\mathbf{h}(\boldsymbol{\mu}|\mathbf{m}_*(t),t):=\partial H/\partial\boldsymbol{\mu}(\boldsymbol{\mu}|\mathbf{m}_*(t),t)$ are the *thermodynamic forces* which give the departure of the moments $\boldsymbol{\mu}$ from the predicted means $\mathbf{m}_*(t)$. Note, therefore, that $\mathbf{h}(\boldsymbol{\mu}|\mathbf{m}_*(t),t)=\boldsymbol{0}$ if and only if $\boldsymbol{\mu}=\mathbf{m}_*(t)$. On the other hand, the Legendre transform

$$F(\mathbf{h}|\mathbf{m}(t),t):=\sup_{\boldsymbol{\mu}}[\boldsymbol{\mu}\cdot\mathbf{h}-H(\boldsymbol{\mu}|\mathbf{m}(t),t)], \tag{2.21}$$

is a *generalized free energy*. It was defined already in Eq. (2.13) above via the logarithm of the "partition function" $Z(\mathbf{h}|\mathbf{m}(t),t):=\langle\exp(\mathbf{h}\cdot\hat{\boldsymbol{\psi}}(t))\rangle_{\mathbf{m}(t),t}$.

With this background, let us return to our analysis of the Rayleigh-Ritz effective action. Equation (2.17) yields immediately a useful expression, complementary to Eq. (2.12):

$$\Gamma_*[\boldsymbol{\psi};\mathbf{m}]=\int_{t_0}^{\infty}dt\left[\frac{d}{dt}\mathbf{h}(\mathbf{m}(t),t)-\frac{\partial\mathbf{h}}{\partial t}(\mathbf{m}(t),t)-\mathbf{W}(\mathbf{m}(t),t)\right]^\top[\boldsymbol{\psi}(t)-\mathbf{m}(t)], \tag{2.22}$$

where we have defined the new vector by matrix multiplication:

$$\mathbf{W}(\mathbf{m}(t),t):=\boldsymbol{\Gamma}(\mathbf{m}(t),t)\mathbf{V}(\mathbf{m}(t),t). \tag{2.23}$$

Indeed, it follows from the chain rule and Eq. (2.17) that

$$\frac{d}{dt}\mathbf{h}(t)=\boldsymbol{\Gamma}(t)\dot{\mathbf{m}}(t)+\frac{\partial\mathbf{h}}{\partial t}(t). \tag{2.24}$$

Because of symmetry of $\boldsymbol{\Gamma}$, it follows that $(\boldsymbol{\Gamma}(t)\dot{\mathbf{m}}(t))^\top=\dot{\mathbf{m}}^\top(t)\boldsymbol{\Gamma}(t)$. Thus, we may use the previous relation to write

$$[\dot{\mathbf{m}}(t)-\mathbf{V}(t)]^\top\boldsymbol{\Gamma}(t)=\left[\frac{d}{dt}\mathbf{h}(t)-\frac{\partial\mathbf{h}}{\partial t}(t)-\mathbf{W}(t)\right]^\top. \tag{2.25}$$

When substituted into Eq. (2.12), the result is Eq. (2.22). This is a more convenient form for variation. Indeed, setting $\delta\Gamma/\delta m_k(t)=0$ gives

$$\sum_j \Gamma_{jk}[\dot{\psi}_j-\dot{m}_j]+\sum_j \left(\frac{\partial\Gamma_{jk}}{\partial t}+\frac{\partial W_j}{\partial m_k}\right)(\psi_j-m_j) + \sum_j [\dot{m}_j-V_j]\Gamma_{jk}=0, \tag{2.26}$$

where the relations (2.17) and (2.25) have again been employed. Simplifying, we obtain finally

$$(\dot{\boldsymbol{\psi}}-\mathbf{V})^\top\boldsymbol{\Gamma}+(\boldsymbol{\psi}-\mathbf{m})^\top\left(\frac{\partial\boldsymbol{\Gamma}}{\partial t}+\frac{\partial\mathbf{W}}{\partial\mathbf{m}}\right)=\mathbf{0}. \tag{2.27}$$

This is the *variational equation* to determine $\mathbf{m}(t)$ for a given $\boldsymbol{\psi}(t)$. When it is employed to eliminate $\mathbf{m}(t)$ in Eq. (2.12) or Eq. (2.22), the result is $\Gamma_*[\boldsymbol{\psi}]$, the final Rayleigh-Ritz approximation to the effective action of the moment variables $\hat{\boldsymbol{\psi}}(t)$ in the closure.

One more transformation of the action is useful. We may write Eq. (2.12) as the sum of two terms:

$$\Gamma_*[\boldsymbol{\psi}]=-\int_{t_0}^{\infty}dt[\dot{\boldsymbol{\psi}}-\dot{\mathbf{m}}]^\top\boldsymbol{\Gamma}[\boldsymbol{\psi}-\mathbf{m}] + \int_{t_0}^{\infty}dt[\dot{\boldsymbol{\psi}}-\mathbf{V}]^\top\boldsymbol{\Gamma}[\boldsymbol{\psi}-\mathbf{m}]. \tag{2.28}$$

In the first term we integrate once by parts, while in the second we use Eq. (2.27). This yields

$$\Gamma_*[\boldsymbol{\psi}]=\frac{1}{2}\int_{t_0}^{\infty}dt(\boldsymbol{\psi}-\mathbf{m})^\top\left[\frac{d}{dt}\boldsymbol{\Gamma}-2\frac{\partial\boldsymbol{\Gamma}}{\partial t}-\frac{\partial\mathbf{W}}{\partial\mathbf{m}}-\left(\frac{\partial\mathbf{W}}{\partial\mathbf{m}}\right)^\top\right] \times(\boldsymbol{\psi}-\mathbf{m}). \tag{2.29}$$

Up until this point, no approximation has been made except Rayleigh-Ritz. Equation (2.29) is the most convenient form to calculate the quadratic part of the Rayleigh-Ritz action.

C. Quadratic-order action and linear Langevin model

We shall now calculate the quadratic part of the full Rayleigh-Ritz effective action $\Gamma_*[\boldsymbol{\psi}]$. An important quantity which appears is the *linear stability operator* about a solution $\mathbf{m}(t)$ of the moment-closure equations $\dot{\mathbf{m}}=\mathbf{V}(\mathbf{m},t)$, that is,

$$\mathbf{A}(t):=\frac{\partial\mathbf{V}}{\partial\mathbf{m}}(\mathbf{m}(t),t). \tag{2.30}$$

The subscript * shall be used hereafter to indicate that the substitution of the particular solution $\mathbf{m}_*(t)$ for given initial data $\mathbf{m}_{0*}$ has been made: thus, $\mathbf{A}_*(t):=\partial\mathbf{V}/\partial\mathbf{m}(\mathbf{m}_*(t),t)$. It is easy to relate $\partial\mathbf{W}/\partial\mathbf{m}$ to the linear stability operator. In fact, from the definition of $\mathbf{W}$ in Eq. (2.23) it follows that

$$\frac{\partial W_i}{\partial m_j}=\Gamma^{(3)}_{ijk}V_k+\Gamma_{ik}A_{kj}, \tag{2.31}$$

where $\Gamma^{(3)}_{ijk}(t)=\partial\Gamma_{ij}/\partial m_k(\mathbf{m}(t),t)$ denotes the single-time third-order irreducible correlation function within the PDF *Ansatz*. Using this function again,

$$\frac{d}{dt}\Gamma_{ij}=\frac{\partial\Gamma_{ij}}{\partial t}+\sum_k \Gamma^{(3)}_{ijk}\dot{m}_k=(\partial_t+\dot{\mathbf{m}}\cdot\nabla_{\mathbf{m}})\Gamma_{ij}. \tag{2.32}$$

Then, by means of Eqs. (2.31) and (2.32), we can see that

$$\frac{d}{dt}\boldsymbol{\Gamma}-2\frac{\partial\boldsymbol{\Gamma}}{\partial t}-\frac{\partial\mathbf{W}}{\partial\mathbf{m}}-\left(\frac{\partial\mathbf{W}}{\partial\mathbf{m}}\right)^\top =-\frac{\partial\boldsymbol{\Gamma}}{\partial t}+(\dot{\mathbf{m}}-2\mathbf{V})\cdot\nabla_{\mathbf{m}}\boldsymbol{\Gamma}-\boldsymbol{\Gamma}A-(\boldsymbol{\Gamma}\mathbf{A})^\top. \tag{2.33}$$

Furthermore, using $\dot{\mathbf{m}}_*=V(\mathbf{m}_*,t)$, it follows that

$$-\frac{\partial\boldsymbol{\Gamma}_*}{\partial t}+(\dot{\mathbf{m}}_*-2\mathbf{V}_*)\cdot\nabla_{\mathbf{m}}\boldsymbol{\Gamma}_*=-\frac{\partial\boldsymbol{\Gamma}_*}{\partial t}-(\mathbf{V}_*\cdot\nabla_{\mathbf{m}})\boldsymbol{\Gamma}_* =-\frac{d}{dt}\boldsymbol{\Gamma}_*. \tag{2.34}$$

The effective action to quadratic order in deviations $\delta\boldsymbol{\psi}(t):=\boldsymbol{\psi}(t)-\mathbf{m}_*(t)$ from the solution $\mathbf{m}_*(t)$ of the moment equation is then found to be

$$\Gamma^{(2)}_*[\delta\boldsymbol{\psi}]=\frac{1}{2}\int_{t_0}^{\infty}dt(\delta\boldsymbol{\psi}-\delta\mathbf{m})^\top\left[-\frac{d}{dt}\boldsymbol{\Gamma}_*-\boldsymbol{\Gamma}_*\mathbf{A}_* -(\boldsymbol{\Gamma}_*\mathbf{A}_*)^\top\right](\delta\boldsymbol{\psi}-\delta\mathbf{m}). \tag{2.35}$$

In this expression, the quantity $\delta\mathbf{m}(t):=\mathbf{m}(t)-\mathbf{m}_*(t)$ is to be determined in terms of $\delta\boldsymbol{\psi}(t)$ from the variational equation (2.27) linearized about the solution $\boldsymbol{\psi}_*(t)=\mathbf{m}_*(t)$. It is convenient to rewrite Eq. (2.27) as

$$\dot{\boldsymbol{\psi}}-\mathbf{V}(\boldsymbol{\psi},t)+[\mathbf{V}(\boldsymbol{\psi},t)-\mathbf{V}(\mathbf{m},t)] +\mathbf{C}\left[\frac{\partial\boldsymbol{\Gamma}}{\partial t}+\left(\frac{\partial\mathbf{W}}{\partial\mathbf{m}}\right)^\top\right](\boldsymbol{\psi}-\mathbf{m})=\mathbf{0}. \tag{2.36}$$

Using again Eqs. (2.31) and (2.32), it is then straightforward to linearize this equation, yielding the variational equation for $\delta\mathbf{m}(t)$:

$$(\delta\dot{\boldsymbol{\psi}}-\mathbf{A}_*\delta\boldsymbol{\psi})-2\mathbf{Q}_*\boldsymbol{\Gamma}_*(\delta\boldsymbol{\psi}-\delta\mathbf{m})=\mathbf{0}, \tag{2.37}$$

where the definition has been introduced

$$2\mathbf{Q}_*:=-\mathbf{C}_*[\dot{\boldsymbol{\Gamma}}_*+\boldsymbol{\Gamma}_*\mathbf{A}_*+\mathbf{A}_*^\top\boldsymbol{\Gamma}_*]\mathbf{C}_* =\dot{\mathbf{C}}_*-\mathbf{A}_*\mathbf{C}_*-\mathbf{C}_*\mathbf{A}_*^\top. \tag{2.38}$$

Note that $\mathbf{L}_*:=-\mathbf{A}_*\mathbf{C}_*$ is the *Onsager matrix*, in terms of which the linearized closure equation may be written in force-flux form: $\delta\dot{\boldsymbol{\psi}}=-\mathbf{L}_*\delta\mathbf{h}$. Then Eq. (2.38) may be restated as

$$\mathbf{Q}_* = \frac{1}{2}\dot{\mathbf{C}}_* + \mathbf{L}_*^s, \tag{2.39}$$

with $\mathbf{L}_*^s := (\mathbf{L}_* + \mathbf{L}_*^\top)/2$ denoting the symmetric part of the matrix $\mathbf{L}_*$.

One may now obtain a final form for $\Gamma_*^{(2)}[\delta\boldsymbol{\psi}]$ by eliminating $\delta\mathbf{m}(t)$ from Eq. (2.35) by means of Eq. (2.37) and by using the definition (2.38) of $\mathbf{Q}_*$. One obtains

$$\Gamma_*^{(2)}[\delta\boldsymbol{\psi}] = \frac{1}{4}\int_{t_0}^{\infty} dt(\delta\dot{\boldsymbol{\psi}} - \mathbf{A}_*\delta\boldsymbol{\psi})^\top \mathbf{Q}_*^{-1}(\delta\dot{\boldsymbol{\psi}} - \mathbf{A}_*\delta\boldsymbol{\psi}). \tag{2.40}$$

This is the final result. One observes that it has the form of an *Onsager-Machlup action*. That is, the Rayleigh-Ritz result for $\Gamma_*^{(2)}[\delta\boldsymbol{\psi}]$ is formally equivalent to the effective action that would be obtained for the solution of a linear Langevin model $\delta\boldsymbol{\psi}_+(t)$ of the fluctuation variable $\delta\hat{\boldsymbol{\psi}}(t)$. To be precise, the model stochastic equation is

$$\delta\dot{\boldsymbol{\psi}}_+ = \mathbf{A}_*(t)\delta\boldsymbol{\psi}_+ + \mathbf{q}(t), \tag{2.41}$$

where $\mathbf{q}(t)$ is a random force, white noise in time, with zero mean and covariance

$$\langle \mathbf{q}(t)\mathbf{q}^\top(t')\rangle = 2\mathbf{Q}_*(t)\delta(t-t'). \tag{2.42}$$

Note, in this context, that Eq. (2.39) is the time-dependent generalization of the *fluctuation-dissipation relation* (of the first type), connecting the noise covariance matrix $\mathbf{Q}_*$ and the symmetric (dissipative) part $\mathbf{L}_*^s$ of the Onsager matrix. For details, see Sec. VI.

To understand the significance of the linear Langevin model, we must recall some basic facts about the effective action itself. As noted earlier, the effective action is a generating functional for irreducible multitime correlation functions. That is, the kth-order irreducible correlator is given by

$$\Gamma^{(k)}_{i_1\cdots i_k}(t_1,\ldots,t_k) = \frac{\delta^k\Gamma}{\delta\psi_{i_1}(t_1)\cdots\delta\psi_{i_k}(t_k)}[\mathbf{m}_*]. \tag{2.43}$$

In particular, these coincide with functional Taylor coefficients in the series expansion (1.10). Furthermore, the irreducible correlators of order up to k determine all of the *cumulants*—or connected correlators— $C^{(k)}_{i_1\cdots i_k}(t_1,\ldots,t_k)$ up to the same order k. [For example, for $k=2$,

$$C_{i_1i_2}(t_1,t_2) = (\Gamma^{-1})_{i_1i_2}(t_1,t_2);$$

for $k=3$,

$$C_{i_1i_2i_3}(t_1,t_2,t_3) = \sum_{j_1j_2j_3}\int ds_1\int ds_2\int ds_3 C_{i_1j_1}(t_1,s_1) \times C_{i_2j_2}(t_2,s_2)C_{i_3j_3}(t_3,s_3) \times \Gamma_{j_1j_2j_3}(s_1,s_2,s_3);$$

etc. See [5].] From these two facts we see that knowledge of the Taylor series of $\Gamma_*[\psi]$ up to terms of degree k is equivalent to knowledge of the Rayleigh-Ritz predictions for all multitime correlators up to order k. In particular, knowledge of the quadratic term in the effective action, $\Gamma_*^{(2)}[\delta\boldsymbol{\psi}]$, is equivalent to knowledge of all two-time correlators as predicted by Rayleigh-Ritz. Because knowledge of the linear model is equivalent to knowledge of that quadratic ''Onsager-Machlup'' part, the key conclusion that we draw is that *the linear Langevin model is the unique such model to reproduce exactly all the two-time correlators predicted by Rayleigh-Ritz*. However, for correlators of higher than second order, the two will in general disagree.

A simple observation which underlines this last point is the following: the solution $\delta\boldsymbol{\psi}_+(t)$ of the linear Langevin model is always a *Gaussian* random function, while the *true* fluctuation variable $\delta\hat{\boldsymbol{\psi}}(t)$ is in general *non-Gaussian*. Thus, although higher-order cumulants than second are zero for the Langevin solution $\delta\boldsymbol{\psi}_+(t)$, they are generally nonzero for the true fluctuation variable $\delta\hat{\boldsymbol{\psi}}(t)$. Of course, it is clear that for any random process $\delta\hat{\boldsymbol{\psi}}(t)$ there is a Gaussian random process $\delta\boldsymbol{\psi}_+(t)$ which has the same mean and variance (when those exist). In fact, there is only one such Gaussian process, in the sense that its distribution on the path space of histories is uniquely determined. This result is sometimes called the Khinchin-Cramér theorem. One way to construct such a Gaussian process is via the central limit theorem.

The connection of the linear Langevin model to the central limit theorem is quite deep. In fact, the precise empirical significance of the linear Langevin model is that its predictions should be valid for the normalized sum variable:

$$\delta\hat{\boldsymbol{\psi}}_N(t) := \frac{1}{\sqrt{N}}\sum_{n=1}^{N}\delta\hat{\boldsymbol{\psi}}^{(n)}(t), \tag{2.44}$$

in the limit $N\to\infty$, where the sum is over N independent, identically distributed samples. To prove this fact, recall that the effective action is a fluctuation potential for the empirical average over N independent samples, in the sense of Eq. (1.9). Now we consider the probability of a small fluctuation value differing from the ensemble mean by terms of order $O(1/\sqrt{N})$. That is, we consider fluctuations

$$\boldsymbol{\psi}(t) = \mathbf{m}_*(t) + \frac{\delta\boldsymbol{\psi}(t)}{\sqrt{N}}, \tag{2.45}$$

for $\delta\boldsymbol{\psi}(t) = O(1)$. Substituting Eq. (2.45) into Eq. (1.9) and employing the functional Taylor expansion (1.10) of $\Gamma[\boldsymbol{\psi}]$, it is then straightforward to show that

$$\mathrm{Prob}(\delta\hat{\boldsymbol{\psi}}_N(t) \approx \delta\boldsymbol{\psi}(t)) \sim \exp\left[-\Gamma^{(2)}[\delta\boldsymbol{\psi}] + O\left(\frac{1}{\sqrt{N}}\right)\right]. \tag{2.46}$$

In the limit as $N\to\infty$ we arrive at the stated result. It is clear that the distribution of $\delta\hat{\boldsymbol{\psi}}_N(t)$ is Gaussian in the limit. [In fact, we have just repeated above one of the standard proofs in the literature of the central limit theorem.] Furthermore, $\Gamma^{(2)}[\boldsymbol{\psi}]$ acts as the Onsager-Machlup action of the limiting Gaussian variable, hence described also by the equivalent linear Langevin model.

It is extremely important to emphasize that the existence of such a linear Langevin model has only been formally established, and only for the Rayleigh-Ritz approximation

$\Gamma_*[\psi]$. In general, the central limit theorem only guarantees that a Gaussian process should exist with the same mean and covariance and not necessarily a process obtained from a stochastic differential equation or, for that matter, even a Markov process. It is thus a very striking prediction of the Rayleigh-Ritz method with a ''Markovian'' *Ansatz*—and far from obviously true—that the two-time correlations should be reproducible by such a linear Langevin model. Indeed, this prediction can fail in a very striking way: the noise covariance $\mathbf{Q}_*(t)$ given formally by Eq. (2.38) may turn out not to be non-negative! Of course, non-negativity is a fundamental requirement for any true covariance function. If it fails, then the ''linear Langevin model'' exists only in some formal sense and there is no actual stochastic process which realizes the model. Put another way, the Rayleigh-Ritz approximation $\Gamma_*[\psi]$ might fail to satisfy the *realizability properties* requisite for any true effective action. The relevant realizability properties (positivity, unicity of minimizer, convexity) have been discussed at length elsewhere [1,10]. It is easy to see that these properties of $\Gamma_*[\psi]$ will hold, at least for $\psi(t)$ close to the mean history $\mathbf{m}_*(t)$, if and only if $\Gamma_*^{(2)}[\delta\psi]\geqslant 0$, with strict inequality for all $\delta\psi(t)\neq 0$. Furthermore, examination of the Onsager-Machlup action (2.40) shows that realizability of $\Gamma_*^{(2)}[\delta\psi]$ holds if and only if the formal noise covariance $\mathbf{Q}_*(t)$ appearing in the Langevin model is positive.

III. A SIMPLE EXAMPLE

It is interesting to compare the linear Langevin model with the full nonlinear Rayleigh-Ritz approximation. In general, this should allow one to assess the limitations of the Langevin model for any given problem, in particular, to assess quantitatively how large are the corrections to its predicted Gaussian statistics. To illustrate the comparison of the Langevin dynamics and full Rayleigh-Ritz approximation, we will discuss here very briefly a three-mode model already considered in [10,11]. This is a simple ''one-step cascade'' model of dissipative turbulent dynamics, originally introduced by Lorenz in 1960 [12]. The dynamics are just the Euler equations of a top, but stochastically driven and linearly damped. The three modes are $\mathbf{x}=(x_1,x_2,x_3)$, of which the first is the driven, unstable mode, and the second two are stable, damped modes. More specifically, the equations of motion are given by

$$\dot{x}_i=A_i x_j x_k-\nu_i x_i+f_i, \tag{3.1}$$

with i,j,k a cyclic permutation of 1,2,3. Note that $A_1+A_2+A_3=0$ for conservation of energy by the nonlinear terms, the damping constants are $\nu_i>0$, $i=1,2,3$, and the random driving forces are zero mean with covariance

$$\langle f_i(t)f_j(t')\rangle=2\kappa_i\delta(t-t'), \tag{3.2}$$

all $\kappa_i>0$, $i=1,2,3$. A ''χ^2'' PDF *Ansatz* was proposed for this system by Bayly, which leads to the quasinormal closure equations. For full details of the model and closure, we refer to [10,11]. Here we will simply remind the reader that the basic moments in the quasinormal closure are the three modal energies $\hat{E}_i=(1/2)x_i^2$, $i=1,2,3$ and the triple moment $\hat{T}=x_1x_2x_3$, which gives the energy transfer out of the unstable driven mode and into the stable, damped modes. In the notations of this paper, the closure dynamics is given by $\dot{\mathbf{m}}=\mathbf{V}(\mathbf{m})$ with

$$\mathbf{m}=\begin{pmatrix} E_1\\ E_2\\ E_3\\ T\end{pmatrix} \quad \text{and} \quad \mathbf{V}(\mathbf{m})=\begin{pmatrix} A_1T-2\nu_1E_1+\kappa_1\\ A_2T-2\nu_2E_2+\kappa_2\\ A_3T-2\nu_3E_3+\kappa_3\\ 4(A_1E_2E_3+A_2E_1E_3+A_3E_1E_2)-(\nu_1+\nu_2+\nu_3)T\end{pmatrix}. \tag{3.3}$$

Although very simple, this model and closure will illustrate several key features of our method. In addition to the key comparison of the full Rayleigh-Ritz approximation and the linear Langevin model, it will allow us to discuss some important issues concerning realizability.

The parameters of the linear Langevin model arising from the χ^2 closure for the three-mode system are easy to determine. The general form of the model is given in Eqs. (2.41) and (2.42). The dynamical matrix $\mathbf{A}$ (here time-independent, since we consider only the statistical steady state) is given by the linearization of the closure equation, $\mathbf{A}=\partial\mathbf{V}/\partial\mathbf{m}$, or

$$\mathbf{A}=\begin{pmatrix} -2\nu_1 & 0 & 0 & A_1\\ 0 & -2\nu_2 & 0 & A_2\\ 0 & 0 & -2\nu_3 & A_3\\ 4(A_2E_3+A_3E_2) & 4(A_1E_3+A_3E_1) & 4(A_1E_2+A_2E_1) & -(\nu_1+\nu_2+\nu_3)\end{pmatrix}. \tag{3.4}$$

To obtain the matrix $\mathbf{A}_*$ appearing in the Langevin model for a specific situation, the corresponding moments $\mathbf{m}_*$ satisfying the fixed-point condition $\mathbf{V}(\mathbf{m}_*)=\mathbf{0}$ must be substituted. The noise covariance $\mathbf{Q}$ can be calculated as the symmetric part of the Onsager matrix $\mathbf{L}$, and the latter is derivable from $\mathbf{L}=-\mathbf{AC}$, once the matrix covariance $\mathbf{C}$ of the moment functions ψ is known. The latter is provided by the PDF *Ansatz*, in this case Bayly's χ^2 *Ansatz*. A simple calculation in that case gives

$$\mathbf{C}=\begin{pmatrix} 2E_1^2+\frac{3}{2}T^{4/3} & \frac{1}{2}T^{4/3} & \frac{1}{2}T^{4/3} & 2E_1T+3T^{5/3} \\ \frac{1}{2}T^{4/3} & 2E_2^2+\frac{3}{2}T^{4/3} & \frac{1}{2}T^{4/3} & 2E_2T+3T^{5/3} \\ \frac{1}{2}T^{4/3} & \frac{1}{2}T^{4/3} & 2E_3^2+\frac{3}{2}T^{4/3} & 2E_3T+3T^{5/3} \\ 2E_1T+3T^{5/3} & 2E_2T+3T^{5/3} & 2E_3T+3T^{5/3} & 8E_1E_2E_3+4(E_1+E_2+E_3)T^{4/3}+19T^2 \end{pmatrix}. \tag{3.5}$$

Again, the matrices $\mathbf{C}_*$ and, therefore, $\mathbf{Q}_*$ are obtained by substituting the fixed-point moment values $\mathbf{m}_*$. It is worth emphasizing that $\mathbf{V}$ and $\mathbf{C}$ are the *only* statistical inputs required from the PDF ansatz at the level of the linear Langevin model. If one is not interested to carry out a full nonlinear Rayleigh-Ritz calculation, then these are the only quantities that need be provided *a priori* to construct the linear model.

For the steady-state dissipative cascade of the three-mode dynamics, it is quite easy to calculate both $\mathbf{A}_*$ and $\mathbf{Q}_*$. We have done so numerically with the same choice of parameter values of the three-mode model as in our earlier work [10,11]. The results given to four decimal places are

$$\mathbf{A}_*=\begin{pmatrix} -0.002 & 0.000 & 0.000 & 2.000 \\ 0.000 & -2.000 & 0.000 & -1.000 \\ 0.000 & 0.000 & -2.000 & -1.000 \\ -2.001 & -0.996 & -0.996 & -2.001 \end{pmatrix} \tag{3.6}$$

and

$$\mathbf{Q}_*=\begin{pmatrix} 3.385 & 0.545 & 0.545 & -6.868 \\ 0.545 & 0.246 & -0.796 & 1.815 \\ 0.545 & -0.796 & 0.246 & 1.815 \\ -6.868 & 1.815 & 1.815 & 8.428 \end{pmatrix}. \tag{3.7}$$

The matrix $\mathbf{A}_*$ can be easily checked to have all eigenvalues with negative real parts. This indicates that the closure fixed point $\mathbf{m}_*$ is linearly stable. However, it turns out that the putative noise covariance $\mathbf{Q}_*$ has eigenvalue spectrum 13.426, 1.042, 1.031, and -3.194. One of the eigenvalues is negative. Thus, there is a breakdown of realizability in the Langevin model for this dissipative cascade state.

Such a breakdown is also known to occur frequently in applications of the POP method, which we shall discuss at some length in Sec. V. For example, Penland in her fundamental work [6] obtained negative eigenvalues for $\mathbf{Q}_*$ in a POP analysis of a different quadratically nonlinear three-mode system, the chaotic Lorenz model. Her interpretation of this realizability breakdown is that it was due to nonlinearities of the Lorenz model that could not be modeled as white-noise random forces. This may be true, but it is not necessarily an indication that the linear Langevin model fails completely, for all statistics of the system. In our earlier work [10,11] we have pointed out that the χ^2 *Ansatz* for our three-mode system—despite its leading to a nonrealizable linear Langevin model—nevertheless produces very good quantitative predictions for several statistics. For example, E_2, E_3, and T are all predicted to within about 0.3% and only the value of E_1 is badly underpredicted (by a factor of 3). Thus, simply labeling the model as ''bad'' because it leads to a nonpositive noise covariance $\mathbf{Q}_*$ would be counterproductive, for good predictions would then be thrown out with the bad ones. What is needed are realizability diagnostics that are more focused and selective, which can help to pinpoint precisely which predictions are good and which are bad.

In [10,11] we have proposed that such diagnostics in the statistical steady state are provided by the *effective potentials*. For any dynamical variable $\hat{\mathbf{Z}}(t)$ of the system, the effective potential $V(\mathbf{z})$ is a fluctuation potential for the empirical time average $\overline{\mathbf{Z}}_T := 1/T\int_0^T dt\hat{\mathbf{Z}}(t)$. That is,

$$\mathrm{Prob}(\overline{\mathbf{Z}}_T\approx\mathbf{z})\sim\exp(-TV(\mathbf{z})), \tag{3.8}$$

in the limit as $T\to\infty$. Because the effective potential is a measure of likelihood of fluctuations in the very time average used empirically to define the mean statistics, it is plausible that it should be quite sensitive to the failure of the closure for individual variables. The effective potential can be obtained analytically via the time-extensive limit of the effective action

$$V(\mathbf{z}) := \lim_{T\to\infty}\frac{1}{T}\Gamma[\mathbf{z}_T], \tag{3.9}$$

in which

$$\mathbf{z}_T(t) := \begin{cases} \mathbf{z} & \text{for } 0<t<T \\ 0 & \text{otherwise.} \end{cases} \tag{3.10}$$

Thus, it is easy to adapt the Rayleigh-Ritz algorithm to calculate the effective potentials. In [10,11] we have applied the full nonlinear Rayleigh-Ritz algorithm in the three-mode system using the χ^2 *Ansatz* to calculate the effective potentials of modal energies E_1 and E_2 and of the triple moment T. It was found there that the potentials V_{E_2} and V_T are positive and convex, satisfying realizability, whereas the potential V_{E_1} was negative and convex, i.e., realizability-violating. In this case, therefore, the effective potentials were—as conjectured—successful in discriminating the good predictions from the bad.

Here we wish to calculate these same effective potentials, but using just the linear model rather than the full Rayleigh-

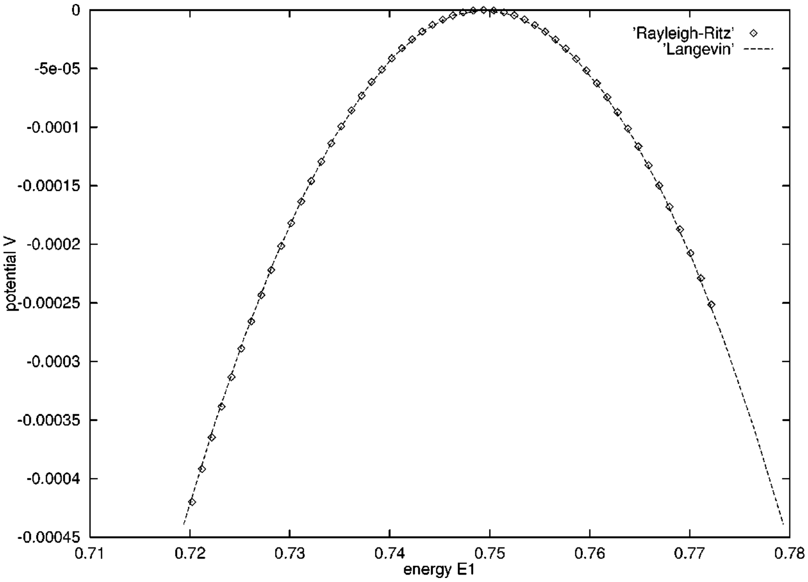

FIG. 1. Approximate effective potentials of E_1: Rayleigh-Ritz vs Langevin model. The nominal physical units are $[V]=1/(\text{time})$ and $[E_1]=(\text{length/time})^2$. However, the quantities have been nondimensionalized by time and length scales appropriate to the two unstable modes, i.e., by setting $\nu_2=\nu_3=1$ for $[\nu_i]=1/(\text{time})$ and $A_2=A_3=-1$ for $[A_i]=1/(\text{length})$.

Ritz approximation. In general, a linear Langevin dynamics such as Eq. (1.5) gives easily the joint effective potential of all variables $\hat{\boldsymbol{\psi}}$ therein, via the time-extensive limit of the Onsager-Machlup action (1.7). Thus, from Eq. (2.40) one obtains directly the quadratic term

$$V_*^{(2)}(\boldsymbol{\psi})=\frac{1}{4}\mathbf{K}_*:\delta\boldsymbol{\psi}\delta\boldsymbol{\psi}, \tag{3.11}$$

with $\delta\boldsymbol{\psi}=\boldsymbol{\psi}-\mathbf{m}_*$ and $\mathbf{K}_*:=\mathbf{A}_*^\top\mathbf{Q}_*^{-1}\mathbf{A}_*$. Here the dynamical matrix $\mathbf{A}_*$ and noise covariance $\mathbf{Q}_*$ in the Langevin model are evaluated at the steady-state values $\mathbf{m}_*$ of the moment averages. The effective potential of any single one of the moment variables can then be obtained by *minimizing* over the others:

$$V_*^{(2)}(\psi_i)=\min_{\psi_j,j\neq i}V_*^{(2)}(\boldsymbol{\psi}). \tag{3.12}$$

Since the joint effective potential (3.11) is a simple quadratic form, this minimization is easy to carry out. In fact, if $\mathbf{K}_*^{ii}$ is the minor matrix obtained from $\mathbf{K}_*$ by deleting the ith row and column and $\mathbf{k}_*^i$ is the vector obtained by deleting the element k_*^{ii} from the ith column, then

$$V_*^{(2)}(\psi_i)=\frac{1}{4}\kappa_*^{ii}\delta\psi_i^2, \tag{3.13}$$

with $\kappa_*^{ii}:=k_*^{ii}-(\mathbf{K}_*^{ii})^{-1}:\mathbf{k}_*^i\mathbf{k}_*^i$. These last formulas allow a direct computation of the effective potentials of moment variables from the parameters appearing in the Langevin model.

In Figs. 1–3 we have plotted the parabolic effective potentials V_{E_1}, V_{E_2}, and V_T obtained in this manner from the linear Langevin model corresponding to the χ^2 *Ansatz*. The plots cover exactly the same range as those in [10,11], where the potentials were calculated by the full nonlinear Rayleigh-Ritz algorithm. For comparison, we have plotted both pairs of potentials together in Figs. 1–3, the new ones using the linear Langevin model and the earlier ones from the full Rayleigh-Ritz approximation. Two points deserve to be em-

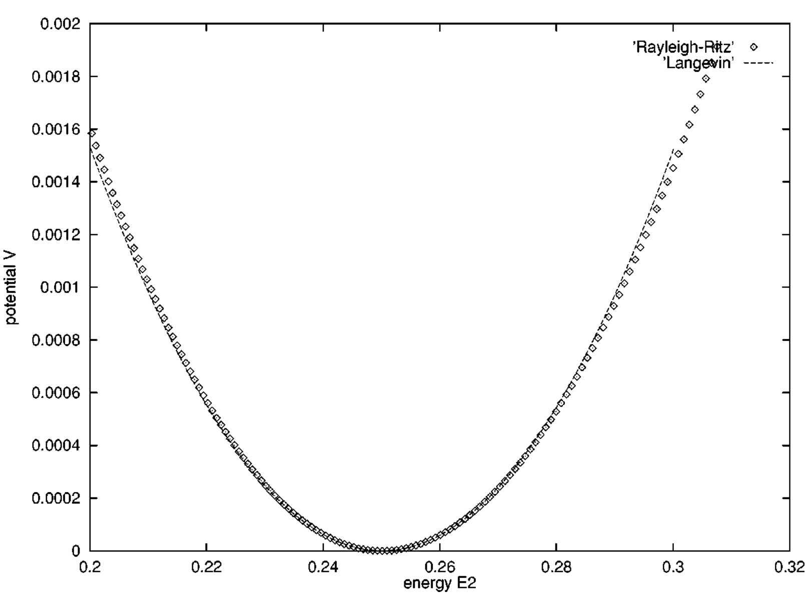

FIG. 2. Approximate effective potentials of E_2: Rayleigh-Ritz vs Langevin model Same remarks as for Fig. 1.

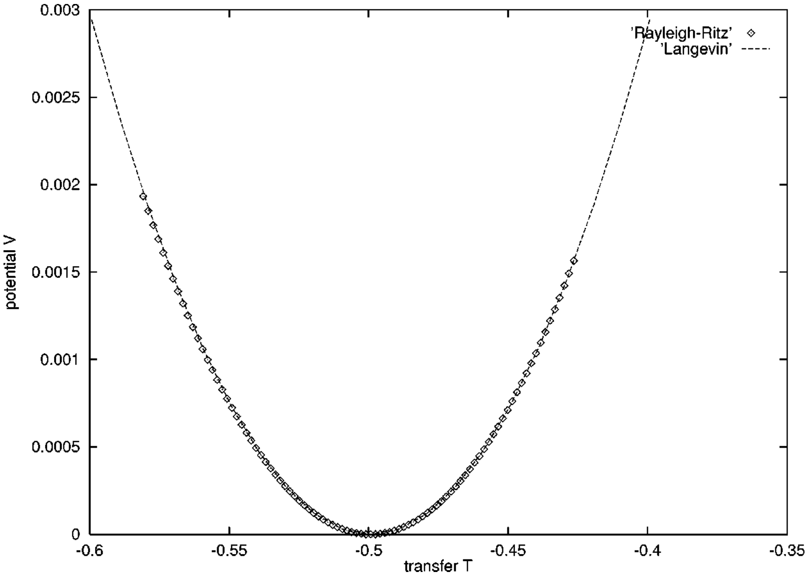

FIG. 3. Approximate effective potentials of T: Rayleigh-Ritz vs Langevin model. The nominal physical units of T are (length/time)^3, but it has been nondimensionalized through the length and time scales of the unstable modes, as described in the caption of Fig. 1.

phasized. First, the computational expense of the Langevin model calculation is considerably lower than the full Rayleigh-Ritz calculation. Each of the separate symbols on the Rayleigh-Ritz effective potential curves was obtained by solving numerically a fixed point problem, coming from a perturbed closure equation. On the other hand, the Langevin model calculation required the solution of *just one* fixed point problem, to determine the mean moment values at the bottom of the potentials. Those are all that are needed to calculate the curvatures κ_*^{ii} and hence the quadratic potential curves via Eq. (3.13). Thus, the number of fixed point symbols appearing in each of the Rayleigh-Ritz curves is a quantitative measure of the numerical superiority of the Langevin model calculation. Second, we see that the two calculation schemes lead to essentially equivalent results in this example, at least for fluctuations up to 20% of the mean value. At least in this range, essentially the same predictions for fluctuations are obtained for the linear model as for the full Rayleigh-Ritz approximation, and at greatly reduced expense.

Of course, over a wider range of fluctuations one should no longer expect that the two calculation schemes will agree. In general, the full Rayleigh-Ritz calculation should capture important non-Gaussian fluctuation effects that are missed by the simpler Langevin model. In Figs. 4 and 5 the two realizable potentials in the three-mode example are plotted over wider ranges, V_{E_2} and V_T, calculated again both by the full Rayleigh-Ritz method and by the linear Langevin model. Clearly, for fluctuations 1–2 times the means, the full Rayleigh-Ritz calculation yields nonparabolic potentials associated to non-Gaussian statistics. The range where the two calculations agree gives an *a priori* indication of the size of the fluctuations for which the linear model may be trusted. In the case of V_{E_2} we see that fluctuations $\sim$40% of the mean are well-described by the linear model, while for V_T the percentage is $\sim$60%. Of course, it is an important question not just whether the Rayleigh-Ritz calculation gives different results, but whether it *improves* upon the predictions of the linear model. In [10,11] it was already shown that the Rayleigh-Ritz effective potentials V_{E_1} and V_T give quite good quantitative results for fluctuations over the smaller

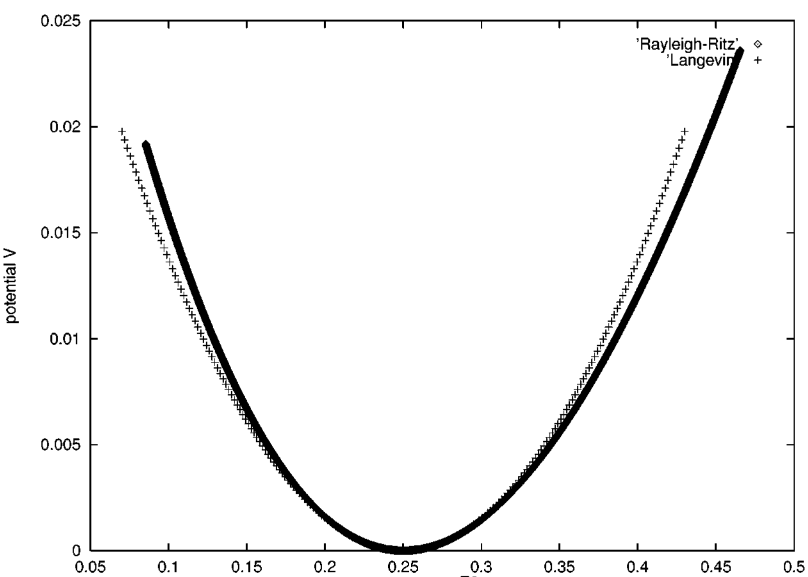

FIG. 4. Approximate effective potentials of E_2 over a wider range: Rayleigh-Ritz vs Langevin model. Same remarks as for Fig. 1.

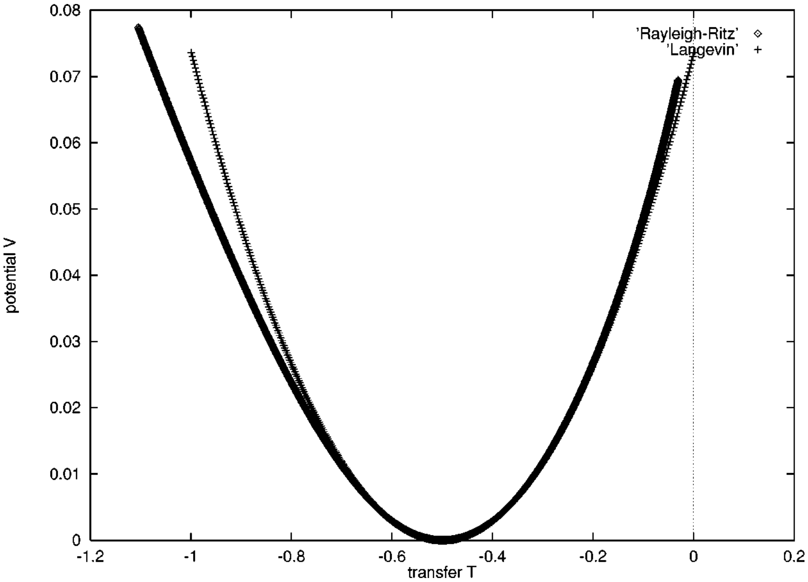

FIG. 5. Approximate effective potentials of T over a wider range: Rayleigh-Ritz vs Langevin model. Same remarks as for Fig. 3.

ranges plotted in Figs. 2 and 3. However, there the full Rayleigh-Ritz and linear Langevin models substantially agree. It is difficult to get accurate results for effective potentials in the wider ranges directly from numerical simulation of the three-mode dynamics, because of the increasing rarity of those large fluctuation events. Thus, we will not show directly an improved agreement of the full Rayleigh-Ritz calculation for the effective potentials in the wider ranges. Nevertheless, one important observation can be made. Because $x_2^2>0$ in *every* realization, there must be zero probability for events with $E_2<0$. For this reason, the true effective potential V_{E_2} must blow up, i.e., diverge to positive infinity, as the negative values of E_2 are approached. However, because the effective potential predicted by the linear Langevin model is a simple parabola, it will intersect the ordinate axis $E_2=0$ at some *finite* value of V. It will thus predict some positive probability of seeing negative values $E_2<0$ (as would be true if the fluctuations δE_2 were indeed Gaussian random variables.) However, as can be seen from Fig. 4, the full Rayleigh-Ritz result for V_{E_2} is rising faster than the parabolic potential from the linear model as $E_2\downarrow 0$. This is the correct tendency, as indicated above, and represents a qualitative improvement of the full Rayleigh-Ritz calculation. In general, one may expect that the full Rayleigh-Ritz calculation will give a more refined result, because it uses more information both from the dynamics and from the PDF *Ansatz* than the Langevin model.

Nevertheless, it is plausible to believe—again quite in general—that the quadratic part will be the term which dominates the effective potential sufficiently close to the minimum. The only way to violate this expectation is to have $\kappa_*^{ii}=0$ and $V(\psi_i)=O(\delta\psi_i^3)$. Barring such cases of accidental degeneracy, one can see that the quadratic term $V_*^{(2)}$ will well approximate the full V_* sufficiently near to the minimum. In that regime, the linear Langevin model shall account for the main tendencies of the full theory. In particular, the Rayleigh-Ritz effective potential will satisfy necessary realizability conditions in the vicinity of the mean, when the Langevin model itself is realizability. Thus, realizability of the Rayleigh-Ritz effective potential is, close to the mean history, equivalent to the realizability for a linear Langevin model. It is thus particularly important to understand the physical hypotheses underlying the validity of such a model.

IV. A PHYSICAL DERIVATION OF THE LINEAR LANGEVIN EQUATION

We shall now explain how exactly the same linear Langevin model can be obtained from a more physically transparent argument. Indeed, we shall show that the previous result for the quadratic order action can be recovered from a single physical hypothesis: It is a basic assumption of the PDF-based moment closure methodology that, to characterize a probability distribution in phase space, it is enough to know the mean values it assigns to the moment functions. In that case, the distribution is assumed to be described with sufficient accuracy by the PDF *Ansatz* which yields the same mean values for those moment functions. Let $\langle\cdot|\hat{\boldsymbol{\psi}}(s), s<t\rangle$ denote the expectation over the conditioned ensemble given the past history $\{\hat{\boldsymbol{\psi}}(s),s<t\}$ of the moment variables before time t. *Our basic assumption is that the PDF Ansatz can be employed as well as an approximation for such an ensemble conditioned on the past values.* More specifically, we shall assume that the approximation is valid that

$$\langle\hat{\mathbf{V}}(t)|\hat{\boldsymbol{\psi}}(s),s<t\rangle\approx\langle\hat{\mathbf{V}}(t)\rangle_{\hat{\boldsymbol{\psi}}(t),t}:=\mathbf{V}(\hat{\boldsymbol{\psi}}(t),t). \quad (4.1)$$

This is just a mathematical restatement of the hypothesis. Indeed, the conditioned ensemble yields the expected values $\langle\hat{\boldsymbol{\psi}}(t)|\hat{\boldsymbol{\psi}}(s),s<t\rangle=\hat{\boldsymbol{\psi}}(t)$ and $P(\cdot;\hat{\boldsymbol{\psi}}(t),t)$ is thus the choice of the PDF *Ansatz* which matches those expected values. [Note that $P(\cdot;\hat{\boldsymbol{\psi}}(t),t)$ really means $P(\cdot;\mathbf{m},t)|_{\mathbf{m}=\hat{\boldsymbol{\psi}}(t)}$, i.e., the average over phase space with respect to $P(\cdot;\mathbf{m},t)$ is always taken first, and then, subsequently, the *random* variable $\hat{\boldsymbol{\psi}}(t)$ is substituted for $\mathbf{m}$.] We shall employ this hypothesis mainly for the regime of small fluctuations, where

$$\mathbf{V}(\hat{\boldsymbol{\psi}}(t),t)=\mathbf{V}(\mathbf{m}_*(t),t)+\mathbf{A}_*(t)\delta\hat{\boldsymbol{\psi}}(t)+O(\delta\hat{\boldsymbol{\psi}}^2). \quad (4.2)$$

We have set $\delta\hat{\boldsymbol{\psi}}(t) := \hat{\boldsymbol{\psi}}(t) - \mathbf{m}_*(t)$, the fluctuation variable.

We now consider the consequences of our hypothesis for the dynamics of the fluctuations. We may write, without any approximation,

$$\partial_t \hat{\boldsymbol{\psi}}(t) = \hat{\mathbf{V}}(t) = \langle \hat{\mathbf{V}}(t) | \hat{\boldsymbol{\psi}}(s), s<t \rangle + \hat{\mathbf{q}}(t), \tag{4.3}$$

where the above equation is simply an implicit definition of the quantity $\hat{\mathbf{q}}(t)$:

$$\hat{\mathbf{q}}(t) := \hat{\mathbf{V}}(t) - \langle \hat{\mathbf{V}}(t) | \hat{\boldsymbol{\psi}}(s), s<t \rangle. \tag{4.4}$$

It follows directly from this definition that $\langle \hat{\mathbf{q}}(t) \rangle = 0$ and that

$$\langle \hat{\boldsymbol{\psi}}(s) \hat{\mathbf{q}}^\top(t) \rangle = 0 \tag{4.5}$$

for all $s<t$. If we now invoke our hypothesis in Eq. (4.3), then we see that

$$\partial_t \hat{\boldsymbol{\psi}}(t) \approx V(\hat{\boldsymbol{\psi}}(t), t) + \hat{\mathbf{q}}(t). \tag{4.6}$$

In other words, within the approximation considered, the *random* moment functions $\hat{\boldsymbol{\psi}}(t)$ satisfy the same closure equations as the mean values $\mathbf{m}(t) = \langle \hat{\boldsymbol{\psi}}(t) \rangle_t$, but with an additional stochastic noise $\hat{\mathbf{q}}(t)$ which is decorrelated from earlier values of the moment functions. This is very similar to the *regression hypothesis* made by Onsager, according to which fluctuations should decay on average according to the same macroscopic equation obeyed by the means. It is clear that it is exactly at this point in the heuristic derivation that a ''Markovian'' approximation has been made. It was emphasized by Onsager and Machlup ([3], p. 1509) that the regression hypothesis is, for a Gaussian random process, actually equivalent to the Markov property.

In the regime of small fluctuations $\delta\hat{\boldsymbol{\psi}}(t)$, we may derive a more specific formulation. There, to linear order accuracy, the equation following from the hypothesis is

$$\delta\dot{\hat{\boldsymbol{\psi}}}(t) \approx \mathbf{A}_*(t)\,\delta\hat{\boldsymbol{\psi}}(t) + \hat{\mathbf{q}}(t). \tag{4.7}$$

Because of the linear relation, it is clear that consistency requires the force $\hat{\mathbf{q}}(t)$ to be white noise in time. Indeed, Eq. (4.7) can be solved explicitly, as

$$\delta\hat{\boldsymbol{\psi}}(t) = \mathbf{G}_*(t,t_0)\,\delta\hat{\boldsymbol{\psi}}(t_0) + \int_{t_0}^t \mathbf{G}_*(t,r)\hat{\mathbf{q}}(r)\,dr, \tag{4.8}$$

where we have introduced the (retarded) matrix Green's function

$$\mathbf{G}_*(t,t_0) := T\exp\left[\int_{t_0}^t \mathbf{A}_*(r)\,dr\right]\theta(t-t_0). \tag{4.9}$$

It then follows by substituting $\delta\hat{\boldsymbol{\psi}}(s)$ from Eq. (4.8) into Eq. (4.5) that

$$\int_{t_0}^s \mathbf{G}_*(s,r)\langle \hat{\mathbf{q}}(r)\hat{\mathbf{q}}^\top(t)\rangle\,dr = 0 \tag{4.10}$$

for all s less than t. Differentiating with respect to s then gives

$$\langle \hat{\mathbf{q}}(s)\hat{\mathbf{q}}^\top(t)\rangle = 0 \tag{4.11}$$

for all $s<t$. Thus, we see that the force must be δ-correlated in time:

$$\langle \hat{\mathbf{q}}(s)\hat{\mathbf{q}}^\top(t)\rangle = 2\mathbf{Q}_*(t)\,\delta(s-t). \tag{4.12}$$

[In principle the matrix $\mathbf{Q}_*(t)$ in Eq. (4.12) could be a differential operator with a finite-degree polynomial dependence on ∂_t. We make the simplest assumption that $\mathbf{Q}_*(t)$ is an ordinary matrix function.] The noise covariance function $\mathbf{Q}_*(t)$ is uniquely determined if we assume, consistent with our hypothesis, that the fluctuation covariance $\mathbf{C}(t) := \langle \delta\hat{\boldsymbol{\psi}}(t)\,\delta\hat{\boldsymbol{\psi}}^\top(t)\rangle_t$ is the same as $\mathbf{C}_*(t)$ given by the PDF *Ansatz*. In that case, the noise covariance is uniquely obtained from the relation

$$2\mathbf{Q}_* = \dot{\mathbf{C}}_* - \mathbf{A}_*\mathbf{C}_* - \mathbf{C}_*\mathbf{A}_*^\top. \tag{4.13}$$

Needless to say, we have now arrived at exactly the same linear Langevin model that we obtained before from the Rayleigh-Ritz approximation with a ''Markovian'' *Ansatz*. The present derivation should make clearer the physical assumptions involved in that more formal derivation.

The quadratic Onsager-Machlup term in the Rayleigh-Ritz effective action will dominate in the vicinity of the mean history, barring degenerate cases where the quadratic term vanishes. As seen earlier, the realizability of the effective action in that region will be essentially equivalent to the realizability of the linear Langevin model (2.41). The latter property is really a consistency check on the validity of the physical hypotheses underlying the Langevin model, in particular the consistency of employing the PDF *Ansatz* for an ensemble conditioned on the past history. In general, this depends upon the particular situation considered. In particular, enough variables must be included in the moment closure that the Markovian assumption inherent in the approximation is justifiable.

This is perhaps the proper place to remind the reader that if a vector Markov process $\boldsymbol{\psi}(t)$ is divided into two subsets $[\overline{\boldsymbol{\psi}}(t), \boldsymbol{\psi}'(t)]$, then, in general, the separate subprocesses $\overline{\boldsymbol{\psi}}(t)$ and $\boldsymbol{\psi}'(t)$ will not be Markov. Thus, if the Rayleigh-Ritz effective action is determined not for the *complete* set of moment variables $\boldsymbol{\psi}(t)$ but instead only for a subset $\overline{\boldsymbol{\psi}}(t)$, then it will not ordinarily have the Onsager-Machlup form. However, there are special cases in which this is true. For example, suppose that the PDF *Ansatz* is such that the two variable sets are uncorrelated at equal times:

$$\langle \boldsymbol{\psi}'(t)\overline{\boldsymbol{\psi}}^\top(t)\rangle - \langle \boldsymbol{\psi}'(t)\rangle\langle \overline{\boldsymbol{\psi}}^\top(t)\rangle = \mathbf{O}. \tag{4.14}$$

Suppose also that the closure equation of the ignored set of moments $\mathbf{m}'(t)$ is independent of the retained set $\overline{\mathbf{m}}(t)$, that is,

$$\dot{\mathbf{m}}'(t) = \mathbf{V}'(\mathbf{m}'(t), t), \tag{4.15}$$

where $\mathbf{V}'$ is a function of $\mathbf{m}'$ alone. This would be realistic for cases such as fluid turbulence with a passive scalar contaminant. In that case, the exact velocity dynamics is independent of the passive scalar. In cases where these two conditions hold, the Rayleigh-Ritz action $\Gamma_*[\overline{\boldsymbol{\psi}}]$ would still have a quadratic part of the Onsager-Machlup form. This is straightforward to show by arguments such as those used before. Needless to say, the two conditions are quite restrictive.

V. RELATION TO PRINCIPAL OSCILLATION PATTERN (POP) ANALYSIS

There is a very close relation of the foregoing theory with the principal oscillation pattern (POP) analysis, particularly as it was developed by Penland [6]. In her approach, the POP method is a procedure to derive directly from the empirical time-series data for a selected set of variables the linear Langevin dynamics whose stochastic solution has the same mean and covariance as those empirically derived, if such a Langevin model exists. Her method can be explained in terms of the equations used above. Indeed, assuming the validity of a Langevin equation such as Eq. (1.5), it is easy to show that, for any $t>t'$,

$$\frac{d}{dt}\mathbf{C}(t,t')=\mathbf{A}(t)\mathbf{C}(t,t'), \tag{5.1}$$

where $\mathbf{C}(t,t'):=\langle\hat{\boldsymbol{\psi}}(t)\hat{\boldsymbol{\psi}}^{\top}(t')\rangle$ is the *empirical* two-time covariance matrix. Thus, the linear dynamical matrix $\mathbf{A}(t)$ can be obtained as

$$\mathbf{A}(t)=\frac{d}{dt}\mathbf{C}(t,t')\bigg|_{t'=t-}\mathbf{C}^{-1}(t), \tag{5.2}$$

where, as before, $\mathbf{C}(t):=\mathbf{C}(t,t)$. Once $\mathbf{A}(t)$ is known, the FDT relation analogous to Eq. (4.13) can be used to determine $\mathbf{Q}(t)$ from $\mathbf{A}(t)$ and $\mathbf{C}(t)$. This is essentially the procedure proposed by Penland to deduce the Langevin model from the data, with appropriate changes having been made to allow for the general case of time-dependent statistics considered here.

A remark on terminology is in order. Although the procedure outlined above is the most natural generalization to the time-dependent case, the rationale for the term ''POP'' is no longer apparent. In fact, the ''principal oscillation patterns'' in the standard approach for stationary time series are the (right) eigenvectors $\mathbf{u}_i$, $i=1,\ldots,n$ of the linear propagator $\mathbf{G}(\tau):=e^{\tau\mathbf{A}}$, for some $\tau>0$. The corresponding eigenvalues are of the form $\mu_i(\tau)=e^{\tau\lambda_i}$ in terms of the eigenvalues λ_i of $\mathbf{A}$. If a linear Langevin model is assumed valid for the two-time covariance $\mathbf{C}(t,t'):=\mathbf{S}(t-t')$, then the propagator can be obtained from $\mathbf{G}(\tau)=\mathbf{S}(\tau)\mathbf{S}^{-1}(0)$. In the standard POP method, the linear dynamical matrix $\mathbf{A}$ is reconstituted by taking $\lambda_i:=1/\tau\ln\mu_i(\tau)$ and then writing

$$\mathbf{A}:=\sum_{i=1}^{n}\lambda_i\mathbf{u}_i\mathbf{v}_i^{\top}, \tag{5.3}$$

where $\mathbf{v}_i$ are the corresponding left eigenvectors, satisfying the biorthogonality relation $\mathbf{v}_i^{\top}\mathbf{u}_j=\delta_{ij}$. (It has been assumed here that complete sets of eigenvectors exist, which holds generically.) In the limit as $\tau\to 0$, it is not hard to see that this procedure is equivalent to the one we described above, when the latter is specialized to the case of stationary time series. There are good reasons why the ''POP'' method is employed in meteorology and climatology, rather than the method we have described. In those problem areas, the resolution of observation times is generally too coarse to allow a numerical evaluation of the necessary derivatives for our formula (5.2). Thus, the above spectral decomposition is required. On the other hand, it should be emphasized that construction of the linear Langevin model in the general time-dependent case will *require* time derivatives. One can still define ''time-dependent POP's'' as eigenvectors of the two-time Green's function $\mathbf{G}(t,t')$, but there is no simple operation analogous to taking the logarithm to allow one to construct therefrom the dynamical matrix.

Of course, a Langevin model need not exist at all, as pointed out also by Penland. There are some basic consistency properties that must be satisfied, if this is to be possible. First, the computed noise covariance $\mathbf{Q}(t)$ must be positive-definite. This is the same type of realizability condition that was encountered in the Rayleigh-Ritz approach. It is a qualitative check of the Langevin model assumption, basically amounting to a statistical stability condition within that framework. A more stringent and quantitative property for validity of a linear Langevin model is deduced from the inversion formula (5.2). This must hold for *all* $t'<t$. In general, the right-hand side of Eq. (5.2) defines an object $\mathbf{A}(t,t')$ for $t'=t-\tau<t$ which will have a nontrivial dependence upon the time lag τ:

$$\mathbf{A}(t,t'):=\frac{d}{dt}\mathbf{C}(t,t')\cdot\mathbf{C}^{-1}(t,t'). \tag{5.4}$$

To be consistent with a linear Langevin model, however, there should be no such dependence. Hence, the degree of constancy of $\mathbf{A}(t,t')$ in the lag time τ is a quantitative measure of the validity of the linear Langevin modeling assumption. This is Penland's ''τ test'' [6]. We note that there is generally some τ dependence in numerical applications of POP, even for time series *generated* by a Langevin model, with reliability of the results degrading seriously for very large values of τ.

On the other hand, there is also a peculiarity of the ''zero-lag'' or $\tau=0$ prescription embodied in Eq. (5.2), which deserves to be emphasized. If that definition of $\mathbf{A}(t)$ is substituted into the FDT relation (4.13), one finds, as a consequence of the calculus identity

$$\frac{d}{dt}\mathbf{C}(t,t)=\frac{d}{dt}[\mathbf{C}(t,t')+\mathbf{C}(t',t)]_{t'=t}, \tag{5.5}$$

for covariance functions which are continuously differentiable, that

$$\mathbf{Q}(t)=\frac{1}{2}\frac{d}{dt}[\mathbf{C}(t,t)-\mathbf{C}(t,t')-\mathbf{C}(t',t)]_{t'=t-}\equiv\mathbf{O}. \tag{5.6}$$

That is, the noise covariance vanishes *identically* at each instant t. Of course, this shows that the matrix $\mathbf{A}(t,t')$ defined by Eq. (5.2) really does depend upon lag time τ in a special way, under the above continuity assumption on the covariances. In the Langevin model itself the assumption is false, since $\mathbf{C}(t,t')=\mathbf{C}(t)-[\dot{\mathbf{C}}(t)+\mathbf{L}(t)](t-t')+O((t-t')^2)$ for $t>t'$ but $\mathbf{C}(t,t')=\mathbf{C}(t)+\mathbf{L}^\top(t)(t-t')+O((t-t')^2)$ for $t<t'$. Thus, the Langevin model covariances have different values of time derivatives from the right and the left. However, it will often be the case that input empirical covariances will have, approximately, continuous first derivatives and then the computed noise will nearly vanish. Already in the classical Onsager-Machlup theory there is a tricky issue of how such time derivatives should even be calculated. As discussed by those authors [3] (and at greater length by Onsager in [13], pp. 418 and 419), the increment δt for calculating time derivatives should be small compared to macroscopic relaxation times, but nevertheless large compared to microscopic (e.g., mean-free) times. If such time scales are not well-separated, as is often the case, then this condition can only be marginally satisfied. In our case, the proper choice of this increment is related to the optimal choice of time lag τ. Because the true dynamical matrix $\mathbf{A}(t)$ does not depend upon τ at all (assuming it exists), it may be better to choose the value τ_* at which the dependence is smallest, according to a ''principle of minimal sensitivity.'' That is, rather than the zero-lag prescription (5.2), it may be better to take $\mathbf{A}_*(t):=\mathbf{A}(t,t-\tau_*)$, where τ_* is the value of the lag which minimizes some matrix norm $\|(d/d\tau)\mathbf{A}(t,t-\tau)\|$. These issues belong to the general rubric of POP practice, and we shall not discuss them further here.

Although the Rayleigh-Ritz and POP methods are seen to be closely related, they have almost opposite points of view. The Rayleigh-Ritz approach is an *a priori* theoretical method, whereas the POP approach is *a posteriori* and empirical. That is, the Rayleigh-Ritz method uses the underlying dynamical equations of motion computationally, in conjunction with physically inspired guesses for the system statistics. Thus, it deduces the linear Langevin model without any direct empirical input (aside from experimental knowledge which may have been exploited to develop suitable PDF *Ansätze* for the problem). On the other hand, the POP method makes no use of the dynamical equation of motion, and, indeed, could be applied to time series generated by very different means than a dynamical equation. POP is blind to theoretical considerations, except through the choice of relevant variables $\hat{\boldsymbol{\psi}}(t)$ to be used in the analysis. Because the two approaches have such different philosophies but yet a close formal relationship, they should be quite complementary in assaulting a given problem. In both cases, a linear Langevin model is obtained which is supposed to reproduce faithfully all first- and second-order correlators of the selected set of variables. Thus, the Langevin model deduced theoretically by the Rayleigh-Ritz approximation may be compared directly with that deduced from the experimental data via POP. On the other hand, a successful application of the empirical POP procedure for a given set of variables—with ''success'' meaning here that realizability of the noise covariance is satisfied and that lag dependence of the deduced matrix $\mathbf{A}(t,t')$ is weak—would imply the possibility of carrying out a successful Rayleigh-Ritz approximation with the same set of variables.

Although POP is an *a posteriori* method, relying upon a substantial empirical input, it has predictive power. This capability rests upon a basic hypothesis: that the POP Langevin model, while constructed only to reproduce partially the second-order statistics, may also be used to predict other statistical properties of the system with some accuracy. In particular, quantities such as transition probability densities $P(\boldsymbol{\psi},t|\boldsymbol{\psi}_0,t_0)$ can be deduced from the POP Langevin model. For many problems of weather and climate prediction, such probabilities would yield crucial information. For example, a measure of the spread of the predictions, such as Penland's *relative discrepancy,*

$$\delta(t,t_0):=\frac{\langle\|\hat{\boldsymbol{\psi}}(t)-\mathbf{G}(t,t_0)\hat{\boldsymbol{\psi}}(t_0)\|^2\rangle}{\langle\|\hat{\boldsymbol{\psi}}(t_0)\|^2\rangle}, \tag{5.7}$$

can be estimated. This quantity is itself second-order, but not one used in the derivation of the POP Langevin model and thus not one that the model is guaranteed to predict successfully for arbitrary time lags $\tau=t-t_0$.

The Rayleigh-Ritz method has the potential for superior predictive ability, particularly with regard to non-Gaussian statistics and large fluctuations. As we have noted, the full Rayleigh-Ritz calculation predicts nonvanishing higher-order cumulants of the moment variables, as required for non-Gaussian statistics. Thus, when the statistics of the problem—such as the transition probabilities—have a very non-Gaussian form, the Rayleigh-Ritz approximation may still derive them successfully. Previous work on simple systems has already shown that very large fluctuations, far outside the Gaussian core, may be successfully captured by a Rayleigh-Ritz calculation. See the examples in [11]. Thus, the Rayleigh-Ritz method can yield crucial information about such large fluctuations, not available by a POP analysis. When the system is strongly fluctuating, and the most probable future event is only weakly selected, realizations deviating from that predicted event by percentages $\gg\delta(t,t_0)$ would have sizable probability. In that case, a Gaussian transition density, such as always yielded by a linear Langevin model, would yield very misleading estimates of event probabilities. The Rayleigh-Ritz method has the potential to predict better the non-Gaussian probabilities of such large-deviation events.

VI. FLUCTUATION-DISSIPATION RELATIONS

A basic premise of our work is that the dynamical system considered is statistically stable, i.e., that the probability measures $\mathcal{P}(t)$ which solve the Liouville equation $\partial_t\mathcal{P}(t)=\hat{\mathcal{L}}\mathcal{P}(t)$ for all initial conditions $\mathcal{P}_0$ converge to a unique invariant measure $\mathcal{P}_\infty$ as $t\to\infty$. (This remark applies to autonomous evolution only, in which the Liouville operator $\hat{\mathcal{L}}$ has no explicit time dependence.) Of course, such statistical stability is not precluded—indeed, is even assisted—by chaotic instability of the underlying microdynamics. In this context, one expects that a generalized second law of thermodynamics should apply, appropriate to dissipative dynamical systems that are driven by external forces or open to the environment. In such a circumstance, the usual thermodynamic entropy of the system proper obviously need not increase, but only the overall entropy of the system plus environment. An entropy function appropriate to describe the irreversible decay of the system to its stable, dissipative steady state is provided by the *relative entropy* introduced in Sec. II. Its production rate (or, rather, destruction rate, with our sign convention) is zero in the steady state itself, and thus does not account for the dissipative processes occurring therein. The latter have been subtracted out in the definition of the relative entropy. However, the relative or generalized entropy turns out to be the most useful concept in the dynamical description of the system proper, since it provides a *Lyapunov functional* for the irreversible decay to the statistical steady state. Furthermore, the usual relations between random fluctuations and mean dissipation—the *fluctuation-dissipation relations*—are valid in terms of this generalized or ''excess'' entropy production within the Rayleigh-Ritz approximation, subject to satisfaction of realizability constraints. Such results for statistical steady states, under hypotheses paralleling those made here, are due originally to Schlögl [14]. In view of the generality of these results, it is appropriate to give here a brief account.

The generalized entropy relative to the predicted mean history $\mathbf{m}_*(t)$ is defined by

$$H_*(\boldsymbol{\mu},t) := H(\boldsymbol{\mu}|\mathbf{m}_*(t),t), \tag{6.1}$$

where H on the right-hand side is given by Eq. (2.15) in the text. The generalized entropy production or excess dissipation is then defined by $\eta_*(\boldsymbol{\mu},t) := (d/dt')H_*(\mathbf{m}(t'),t')|_{t'=t}$, where $\mathbf{m}(\ )$ is the solution of the closure equation which satisfies $\mathbf{m}(t)=\boldsymbol{\mu}$. Thus, a simple calculation gives

$$\eta_*(\boldsymbol{\mu},t) = \mathbf{h}_*(\boldsymbol{\mu},t)\cdot\mathbf{V}(\boldsymbol{\mu},t) + \frac{\partial H_*}{\partial t}(\boldsymbol{\mu},t). \tag{6.2}$$

It is not hard to show that, to quadratic order accuracy in small deviations,

$$\eta_* := -\left(\mathbf{L}_*^s + \frac{1}{2}\dot{\mathbf{C}}_*\right):\delta\mathbf{h}\delta\mathbf{h} + O(\delta h^3). \tag{6.3}$$

We shall sketch the proof below. First, however, let us recall the relation between the noise covariance $\mathbf{Q}_*(t)$ and the Onsager matrix $\mathbf{L}_*(t) = -\mathbf{A}_*(t)\mathbf{C}_*(t)$, already given in Eq. (2.39):

$$\mathbf{Q}_* = \mathbf{L}_*^s + \frac{1}{2}\dot{\mathbf{C}}_*. \tag{6.4}$$

This is the *fluctuation-dissipation relation (FDR) of the first type*. Along with Eq. (6.3) it allows one to express the quadratic part of the entropy production (or dissipation) directly in terms of the noise covariance $\mathbf{Q}_*$:

$$\eta_* := -\mathbf{Q}_*:\delta\mathbf{h}\delta\mathbf{h} + O(\delta h^3). \tag{6.5}$$

Thus, the FDR of the first type expresses a direct connection between the noise characteristics and the dissipative part of the linear dynamics. The generalized entropy $H_*(\boldsymbol{\mu},t)$ is a non-negative, convex function, vanishing at $\mathbf{m}_*(t)$. When the noise covariance $\mathbf{Q}_*(t)$ is positive-definite, Eq. (6.5) implies that the generalized entropy is a Lyapunov function for the closure dynamics. At least for small deviations $\delta\mathbf{m}(t)$ from the solution $\mathbf{m}_*(t)$, where the linearized dynamics $\delta\dot{\mathbf{m}}(t) = -\mathbf{L}_*(t)\delta\mathbf{h}(t)$ applies, the entropy $H_*(t)$ is guaranteed to decrease in time, $dH_*(t)/dt<0$. This implies a ''stability'' of the history $\mathbf{m}_*(t)$ under the closure dynamics, generalizing the results of Schlögl [14] to nonsteady states of strongly fluctuating systems. [Strictly speaking, only in the steady-state case does stability follow, by Lyapunov's theorem. Simple counterexamples show that the conditions adduced are not in general sufficient for stability of the solution trajectory $\mathbf{m}_*(t)$ under the closure dynamics. For example, level sets of $H_*(\boldsymbol{\mu},t)$ may expand outward from the solution trajectory at an exponential rate, allowing nearby trajectories to diverge at a smaller exponential rate.]

The proof of Eq. (6.3) is as follows: Expanding the generalized entropy in a power series about $\mathbf{m}_*(t)$ yields, with $\delta\boldsymbol{\mu}(t) := \boldsymbol{\mu} - \mathbf{m}_*(t)$,

$$H_*(\boldsymbol{\mu},t) = \frac{1}{2}\boldsymbol{\Gamma}_*(t):\delta\boldsymbol{\mu}(t)\delta\boldsymbol{\mu}(t) + \frac{1}{3!}\boldsymbol{\Gamma}_*^{(3)}(t)\vdots\,\delta\boldsymbol{\mu}(t)\delta\boldsymbol{\mu}(t)\delta\boldsymbol{\mu}(t) + O(\delta\mu^4). \tag{6.6}$$

Recall that $\boldsymbol{\Gamma}_*^{(p)}(t) := \partial^p H_*/\partial\boldsymbol{\mu}^p(\mathbf{m}_*(t),t)$. Taking one derivative of Eq. (6.6) with respect to $\boldsymbol{\mu}$ gives

$$\mathbf{h}_*(\boldsymbol{\mu},t) = \boldsymbol{\Gamma}_*(t)\cdot\delta\boldsymbol{\mu}(t) + \frac{1}{2}\boldsymbol{\Gamma}_*^{(3)}(t):\delta\boldsymbol{\mu}(t)\delta\boldsymbol{\mu}(t) + O(\delta\mu^3). \tag{6.7}$$

Introducing $\delta\mathbf{h}(t) := \boldsymbol{\Gamma}_*(t)\cdot\delta\boldsymbol{\mu}(t)$, the latter becomes

$$\mathbf{h}_*(\boldsymbol{\mu},t) = \delta\mathbf{h}(t) + \frac{1}{2}\boldsymbol{\Gamma}_*^{(3)}(t):\delta\boldsymbol{\mu}(t)\delta\boldsymbol{\mu}(t) + O(\delta\mu^3). \tag{6.8}$$

A similar Taylor expansion of the dynamical vector field $\mathbf{V}$ gives

$$\begin{aligned}\mathbf{V}(\boldsymbol{\mu},t) &= \mathbf{V}_*(t) + \mathbf{A}_*(t)\delta\boldsymbol{\mu}(t) + O(\delta\mu^2)\\ &= \mathbf{V}_*(t) - \mathbf{L}_*(t)\delta\mathbf{h}(t) + O(\delta h^2),\end{aligned} \tag{6.9}$$

with $\mathbf{V}_*(t) := \mathbf{V}(\mathbf{m}_*(t),t)$. Now the Taylor expansion of the first part of the excess dissipation (the force-flux quadratic form) can be obtained by direct substitution of Eqs. (6.8) and (6.9):

$$\mathbf{h}_*\cdot\mathbf{V} = \delta\mathbf{h}\cdot\mathbf{V}_* - \mathbf{L}_*:\delta\mathbf{h}\delta\mathbf{h} + \frac{1}{2}\boldsymbol{\Gamma}_*^{(3)}\vdots\,\delta\boldsymbol{\mu}\delta\boldsymbol{\mu}\mathbf{V}_* + O(\delta h^3). \tag{6.10}$$

The second part of the entropy production is obtained by partial differentiation of Eq. (6.6):

$$\frac{\partial H_*}{\partial t} = -\delta\mathbf{h}\cdot\mathbf{V}_* + \frac{1}{2}\frac{\partial\mathbf{\Gamma}_*}{\partial t}(\mathbf{m}_*(t),t):\delta\boldsymbol{\mu}\delta\boldsymbol{\mu} + \frac{1}{3!}\frac{\partial\mathbf{\Gamma}_*^{(3)}}{\partial t}(\mathbf{m}_*(t),t)\vdots\,\delta\boldsymbol{\mu}\delta\boldsymbol{\mu}\delta\boldsymbol{\mu} + O(\delta\mu^4). \tag{6.11}$$

We made use of the facts that $(\partial/\partial t)\,\delta\boldsymbol{\mu}(t) = (\partial/\partial t)\,(\boldsymbol{\mu} - \mathbf{m}_*(t)) = -\mathbf{V}_*(t)$ and that, for every non-negative integer p, $\mathbf{\Gamma}_*^{(p+1)}(\mathbf{m}_*(t),t) = \partial\mathbf{\Gamma}^{(p)}/\partial\boldsymbol{\mu}\,(\mathbf{m}_*(t),t)$. Adding together the two parts of the entropy production from Eqs. (6.10) and (6.11) then gives

$$\eta_* = -\mathbf{L}_*:\delta\mathbf{h}\delta\mathbf{h} + \frac{1}{2}\left(\mathbf{\Gamma}_*^{(3)}\cdot\mathbf{V}_* + \frac{\partial\mathbf{\Gamma}_*}{\partial t}\right):\delta\boldsymbol{\mu}\delta\boldsymbol{\mu} + O(\delta h^3). \tag{6.12}$$

If one recalls that $(d/dt)\mathbf{\Gamma}_* = \mathbf{\Gamma}_*^{(3)}\cdot\mathbf{V}_* + \partial\mathbf{\Gamma}_*/\partial t$, as in Eq. (2.32), then we obtain finally

$$\begin{aligned}\eta_* &= -\mathbf{L}_*:\delta\mathbf{h}\delta\mathbf{h} + \frac{1}{2}\dot{\mathbf{\Gamma}}_*:\delta\boldsymbol{\mu}\delta\boldsymbol{\mu} + O(\delta h^3)\\ &= -\left(\mathbf{L}_*^s + \frac{1}{2}\dot{\mathbf{C}}_*\right):\delta\mathbf{h}\delta\mathbf{h} + O(\delta h^3),\end{aligned} \tag{6.13}$$

where $\dot{\mathbf{\Gamma}}_* = -\mathbf{\Gamma}_*\dot{\mathbf{C}}_*\mathbf{\Gamma}_*$ was employed in the last line. This is just Eq. (6.3), as was claimed.

There is another result, *the fluctuation-dissipation relation of the second type*, which holds for a general linear Langevin model. This relation expresses a proportionality between the mean response function to an appropriately coupled force and a time derivative of the two-time correlation function. The equation to be considered is

$$\delta\dot{\boldsymbol{\psi}} = -\mathbf{L}_*(t)[\delta\mathbf{h} - \mathbf{f}(t)] + \mathbf{q}(t), \tag{6.14}$$

where $\mathbf{f}(t)$ is a deterministic external force. Because of the linearity of this equation, it follows immediately that the corresponding response function $\mathbf{H}(t,t_0) := \delta\boldsymbol{\psi}(t)/\delta\mathbf{f}(t_0)$ is *non-random* and its average $\mathbf{H}_*(t,t_0) := \langle\mathbf{H}(t,t_0)\rangle$ is thus given just by the solution of

$$\frac{\partial}{\partial t}\mathbf{H}_*(t,t_0) = \mathbf{A}_*(t)\mathbf{H}_*(t,t_0) + \mathbf{L}_*(t_0)\,\delta(t-t_0). \tag{6.15}$$

It is not hard to see that the latter solution is

$$\mathbf{H}_*(t,t_0) = \mathbf{G}_*(t,t_0)\mathbf{L}_*(t_0), \tag{6.16}$$

with $\mathbf{G}_*$ the matrix Green's function defined in Eq. (4.9). On the other hand, by using the same Green's function to solve Eq. (5.1) for $\mathbf{C}_*(t,t_0)$ starting from time t_0, it is determined that

$$\mathbf{C}_*(t,t_0) = \mathbf{G}_*(t,t_0)\mathbf{C}_*(t_0). \tag{6.17}$$

Because $\mathbf{L}_*(t_0) := -\mathbf{A}_*(t_0)\mathbf{C}_*(t_0)$ and because $(\partial/\partial t_0)\,\mathbf{G}_*(t,t_0) = -\mathbf{G}_*(t,t_0)\mathbf{A}_*(t_0)$ for $t > t_0$, it follows from Eqs. (6.16) and (6.17) that

$$\frac{\partial}{\partial t_0}[\mathbf{C}_*(t,t_0)\mathbf{\Gamma}(t_0)] = \mathbf{H}_*(t,t_0)\mathbf{\Gamma}(t_0) \tag{6.18}$$

for $t > t_0$. This proportionality is termed an FDR of the second type. [The reader should be cautioned at this point that there is a great divergence of terminology in the literature. One finds often the following terms used instead: *FDR of the first kind* to indicate what we called FDR of the second type and *FDR of the second kind* to indicate our FDR of the first type. There are also authors who call Eq. (6.17) the FDR of the second type (first kind) rather than Eq. (6.19). For further discussion of these matters, see [15], Secs. 3.2, 4.1, and Appendix D.] The intuitive content is better seen from the corresponding integral relation,

$$\mathbf{C}_*(t,t_0) = \left[\mathbf{I} - \int_{t_0}^{t} ds\,\mathbf{H}_*(t,s)\mathbf{\Gamma}_*(s)\right]\mathbf{C}_*(t_0), \tag{6.19}$$

which expresses the two-time correlation as the summed mean response to infinitesimal perturbations at intervening times.

Another relation of the ''second type'' exists within the Rayleigh-Ritz formalism. This has a slightly different character, in that the external perturbation field is now added to the *deterministic* equation. As the simplest example, consider the following perturbation of the moment-closure equations:

$$\dot{\mathbf{m}} = \mathbf{V}(\mathbf{m},t) + \mathbf{C}(\mathbf{m},t)\cdot\mathbf{h}(t), \tag{6.20}$$

in which $\mathbf{C}(\mathbf{m},t)$ is the model single-time covariance matrix provided by the PDF ansatz. Then, if $\mathbf{R}(t,t_0) := \delta\mathbf{m}(t)/\delta\mathbf{h}(t_0)\,|_{\mathbf{h}=\mathbf{0}}$ is the corresponding response function, it is easy to see by functional differentiation that, for initial conditions $\mathbf{m}(t_0) = \mathbf{m}_{*0}$ in the above equation, $\mathbf{R}_*$ satisfies

$$\partial_t\mathbf{R}_*(t,t_0) = \mathbf{A}_*(t)\mathbf{R}_*(t,t_0) + \mathbf{C}_*(t_0)\,\delta(t-t_0). \tag{6.21}$$

The solution is just $\mathbf{R}_*(t,t_0) = \mathbf{G}_*(t,t_0)\mathbf{C}_*(t_0)$ for $t > t_0$. Thus, we see by reference to Eq. (6.17) above and the symmetry of the covariance that

$$\mathbf{C}_*(t,t_0) = \mathbf{R}_*(t,t_0) + \mathbf{R}_*^{\top}(t,t_0), \tag{6.22}$$

where $\mathbf{R}_*^{\top}(t,t') := [\mathbf{R}_*(t',t)]^{\top}$. Relation (6.22) might be better termed a *fluctuation-response relation*, in analogy to that of Kraichnan [16]. It turns out that this relation is completely general within the Rayleigh-Ritz method. In fact, Eq. (6.20) above is nothing more than the Euler-Lagrange equation for $\mathbf{m}(t)$ in the Rayleigh-Ritz algorithm, when the expectation constraint (2.5) is incorporated via a Lagrange multiplier $\mathbf{h}(t)$. That is, Eq. (6.20) above is equivalent to Eq. (3.93) in [1]. All of these statements remain true even when the random variables whose two-time covariance is to be approximated by the Rayleigh-Ritz approximation are not the basic moment variables appearing in the closure and the linear Langevin model is not available. The demonstration of this fact will be given elsewhere [17], since it is outside the scope of the present work. The result (6.22) is very useful, because it provides the most efficient numerical procedure to extract the Rayleigh-Ritz predictions for the two-time covariances.

VII. CONCLUSIONS

In this work we have shown how the general Rayleigh-Ritz algorithm for statistical dynamics of nonlinear systems, proposed in [1], gives rise to linear Langevin models. Such stochastic models reproduce the predictions of the full Rayleigh-Ritz calculation for second-order statistics. In general, for higher-order statistics and larger fluctuations, the two methods yield different predictions. Thus, the Rayleigh-Ritz approach also gives a means to assess *a priori* the domain of validity of the linear Langevin models. A more physical derivation of Langevin models was also sketched. The theoretical and *a priori* Rayleigh-Ritz method was compared with the empirical and *a posteriori* POP method of Penland. Finally, some general results on the thermodynamics of statistical moments—law of entropy increase and fluctuation-dissipation relations at the linear level—were derived within the Rayleigh-Ritz formalism.

ACKNOWLEDGMENTS

I wish to thank Frank Alexander, Brian Farrell, Greg Halloway, Petros Ioannou, Jay Taylor, and Victor Yakhot for useful conversations on the subject of this work, and in particular F.A. for informing me of the POP method of Penland. I also wish to thank Shiyi Chen and CNLS for support to attend the 18th Annual International Conference of CNLS on ''Predictability.'' My conversations with many of the participants and their lectures helped considerably in sharpening the focus of this work. Finally, I wish to thank the Center for Turbulence Research (CTR) at Stanford for supporting my work in their 1998 Summer Program. Testing the Rayleigh-Ritz method on homogeneous turbulent flows in their extensive database helped to illuminate some important general issues.

[1] G. L. Eyink, Phys. Rev. E **54**, 3419 (1996).
[2] G. L. Eyink, Prog. Theor. Phys. Suppl. **130**, 77 (1998).
[3] L. Onsager and S. Machlup, Phys. Rev. **91**, 1505 (1953); S. Machlup and L. Onsager, *ibid.* **91**, 1512 (1953).
[4] H. Cramér, Actual. Sci. Ind. **736**, 5 (1938).
[5] C. Itzykson and J.-B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).
[6] C. Penland, Mon. Weather Rev. **117**, 2165 (1989).
[7] B. A. Finlayson, *The Method of Weighted Residuals and Variational Principles* (Academic Press, New York, 1972).
[8] J. L. Lumley, J. Fluid Mech. **41**, 413 (1970).
[9] R. S. Ellis, *Entropy, Large Deviations, and Statistical Mechanics* (Springer-Verlag, New York, 1985).
[10] G. L. Eyink and F. J. Alexander, Phys. Rev. Lett. **78**, 2563 (1997).
[11] G. L. Eyink and F. J. Alexander, J. Stat. Phys. **91**, 221 (1998).
[12] E. Lorenz, Tellus **12**, 243 (1960).
[13] L. Onsager, Phys. Rev. **37**, 405 (1931).
[14] F. Schlögl, Z. Phys. **244**, 199 (1971); **248**, 446 (1971).
[15] G. L. Eyink, J. L. Lebowitz, and H. Spohn, J. Stat. Phys. **83**, 385 (1996).
[16] R. H. Kraichnan, Phys. Rev. **113**, 1181 (1959).
[17] G. L. Eyink (unpublished).