Action principle in nonequilibrium statistical dynamics

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We introduce a variational method for approximating distribution functions of dynamics with a ''Liouville operator'' $\hat{L}$, in terms of a *nonequilibrium action functional* for two independent (left and right) trial states. The method is valid for deterministic or stochastic Markov dynamics and for stationary or time-dependent distributions. A practical Rayleigh-Ritz procedure is advanced, whose inputs are a finitely parametrized *Ansatz* for the trial states, leading to a ''parametric action'' for their evolution. The Euler-Lagrange equations of the action principle are Hamiltonian in form (generally noncanonical). This permits a simple identification of fixed points as critical points of the parametric Hamiltonian. We also establish a variational principle for low-order statistics, such as mean values and correlation functions, by means of the *least effective action.* The latter is a functional of the given variable, which is positive and convex as a consequence of Hölder realizability inequalities. Its value measures the ''cost'' for a fluctuation from the average to occur and in a weak-noise limit it reduces to the Onsager-Machlup action. In general, the effective action is shown to arise from the nonequilibrium action functional by a constrained variation. This result provides a Rayleigh-Ritz scheme for calculating just the desired low-order statistics, with internal consistency checks less demanding than for the full distribution. [S1063-651X(96)02710-9]

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I. INTRODUCTION

The Rayleigh-Ritz variational method is a well-established technique in quantum mechanics (e.g., see [1]). In this method one solves approximately the stationary Schrödinger equation by making a physically motivated trial *Ansatz* for the ground-state wave function and then varying the energy-expectation functional with respect to its parameters. A similar method is available for solving the time-dependent Schrödinger equation, based upon the Dirac-Frenkel dynamic variational principle [2–5]. These methods are among the very few tools in the arsenal of theoretical physics able to assault systematically strong-coupling problems of quantum dynamics. They are especially useful in quantum field theory and many-body theory, where alternative numerical approaches are expensive or unfeasible. In some cases, such as the BCS theory of superconductivity, the variational principle has been the stepping stone to an exact solution of the problem.

In our opinion, nonequilibrium statistical mechanics has been lacking a variational principle of the same flexibility and scope as in quantum theory, capable of determining the probability density function (PDF) for both the steady-state and the time-dependent solution to the initial-value problem. This is particularly true for problems such as high Reynolds number turbulence and large scale dynamics of multiphase fluids, where there is no small parameter in which to make a perturbation expansion or asymptotic development and strong fluctuations dominate the phenomena on a wide range of length scales. An obvious analogy exists between Schrödinger's equation for the wave function and the *Liouville equation* for the PDF in the nonequilibrium problems:

$$\partial_t P = \hat{L} P. \tag{1.1}$$

This analogy has been used before to express classical statistical dynamics as a formal quantum field theory in the work of Martin, Siggia, and Rose [6]. It was noted in [6] that variational principles could be formulated, without any further details. However, a mathematical obstacle exists to applying by analogy the quantum principles because the formal ''Hamiltonian'' $\hat{L}$ is generally non-Hermitian for the dissipative dynamical systems of interest. Variational methods of the standard form as in quantum mechanics have been employed in special cases where $\hat{L}$ can be transformed to a Hermitian form [7–9] or else based upon the Hermitian squared operator $\hat{L}^\dagger \hat{L}$ [7,10]. These methods seem to be either too restrictive or too cumbersome to be as useful as the corresponding quantum principles. Recently, we have observed in the turbulence context that a variational method may be developed for nonequilibrium dynamics, which preserves the principal advantages of the quantum method [11]. The key idea in the recent formulation is to vary jointly over *independent left and right trial states*. Although this Rayleigh-Ritz method seems to be most natural for a non-Hermitian operator, it does not seem to have been previously used for nonequilibrium dynamics. It is our purpose here to develop this method in a general context and in some formal detail.

One advantage of the variational method in our formulation is that it yields, by a procedure of *constrained variation*, a characterization of the *effective action* for any selected statistic of interest, such as a mean value or a two-point correlation. The effective action is a non-negative, convex functional whose minimum is achieved by the true ensemble-average value. In quantum field theory the concept has it roots in the early work of Heisenberg and Euler [12] and Schwinger [13] in QED. In nonequilibrium statistical mechanics, the first such action principle seems to have been Onsager's ''principle of least dissipation'' [14], which applies to systems subject to thermal or molecular noise, gov-

erned by a fluctuation-dissipation relation. A formulation of the least-dissipation principle by an action functional on histories was developed by Onsager and Machlup [15]. The effective action we consider coincides in a weak-noise limit with the Onsager-Machlup action, as discussed some time ago by Graham [16]. For vanishing noise, a path-integral formula for the effective action can be evaluated by steepest descent, yielding the ''classical'' action of Onsager-Machlup. However, in the strong-noise case, efficient calculational tools remain to be developed. We show here that the Rayleigh-Ritz method provides one such computational scheme. The basis of this method is a generalization of Symanzik's theorem in Euclidean field theory [17] (see also [18]), which characterizes the static effective action, or, ''effective potential,'' by a constrained variation of the quantum energy-expectation functional. This theorem has been extended by us to Martin-Siggia-Rose field theory with a non-Hermitian Hamiltonian operator [11]. Here we shall, for completeness, briefly recapitulate that result and then expound in detail the corresponding Rayleigh-Ritz method. We also establish a Symanzik-type theorem for the time-dependent effective action, extending the earlier result of Jackiw and Kerman in quantum theory [19] to the initial-value problem in nonequilibrium statistical dynamics.

The methods we develop here are quite general and apply, indeed, to the solution of any large scale stochastic system, not only those in nonequilibrium statistical physics, but also to population dynamics in biology, to stochastic market models in mathematical finance, etc. The advantages of a variational scheme are well known. For example, we quote the following:

> The great virtue of the variational treatment, ''Ritz's method,'' is that it permits efficient use in the process of calculation, of any experimental or intuitive insight which one may possess concerning the problem which is to be solved by calculation. It is important to realize that this is not possible, or possible to a much smaller extent, if one performs the calculation by using the original form of the equations of motion . . . . Ritz's method, on the other hand, is definitely a method of successive approximations, and one which converges better in the later stages of the approximation. Any information therefore which one may possess—no matter whether it comes from experiments, from intuition, or from general experience obtained in previous works on similar problems— can be made useful by using it in formulating the point of departure, the ''zeroeth [*sic*] approximation'' [20].

The present paper elaborates the theoretical foundation of such a variational scheme for stochastic dynamical systems. In future work we shall apply the method to various concrete systems of practical interest. In particular, the paper [21] demonstrates the feasibility of the Rayleigh-Ritz method for numerical computation of the effective potential and [22] applies the action principle to the problem of moment closures in turbulence modeling.

II. THE VARIATIONAL METHOD FOR DISTRIBUTIONS

Our problem is to calculate the probability distribution functions, denoted by P, for nonequilibrium Markov dynamics, governed by an equation of the form of Eq. (1.1), where $\hat{L}$ is the (forward) Markov generator. Concrete examples of practical interest are the nonequilibrium master equations [23] and, as a particular case, the Fokker-Planck equations [7], with

$$\hat{L} = -\frac{\partial}{\partial x_i}[K_i(\mathbf{x})\cdot] + \frac{1}{2}\frac{\partial^2}{\partial x_i \partial x_j}[D_{ij}(\mathbf{x})\cdot], \tag{2.1}$$

in which $\mathbf{K}$ is the drift vector and $\mathbf{D}$ is the diffusion tensor. A degenerate case of the latter of special interest occurs for zero noise ($\mathbf{D}=\mathbf{0}$), which is

$$\hat{L} = -\frac{\partial}{\partial x_i}[K_i(\mathbf{x})\cdot], \tag{2.2}$$

the ''Liouville operator'' of the deterministic dynamical system $\dot{\mathbf{x}}=\mathbf{K}(\mathbf{x})$.

We develop here a simple variational method to calculate approximately the solutions of Eq. (1.1) for P, both for the stationary PDF P_s and for time-dependent solutions P_t with prescribed initial data P_0. Our methods are analogous to Rayleigh-Ritz procedures traditional in quantum mechanics, but with a modification due to the fact that the operator $\hat{L}$ is non-self-adjoint:

$$\hat{L}^\dagger \neq \hat{L}. \tag{2.3}$$

Although the spectra of $\hat{L}$ and $\hat{L}^\dagger$ are the same (because $\hat{L}$ is a real operator $\hat{L}^*=\hat{L}$), their eigenstates are distinct. Equivalently, the left and right eigenstates of $\hat{L}$ are distinct [1,24]. This is particularly true for the ''ground states''

$$\hat{L}|\Omega^R\rangle = 0 \quad \hat{L}^\dagger|\Omega^L\rangle = 0. \tag{2.4}$$

Because of the fundamental asymmetry of the problem, Hilbert space or L^2 methods are not as useful as in quantum theory. Instead, the standard mathematical formulation (see [25]) is to take $\hat{L}$ as an operator on L^1, considered as a space of ''normalizable states,'' and $\hat{L}^\dagger$ as an operator on L^∞, considered as a space of ''bounded observables.'' [The mathematical notation is, unfortunately, the opposite of that generally adopted in the physics literature: what we have called $\hat{L},\hat{L}^\dagger$ are in mathematics usually denoted as L^*,L (forward and backward Markov operators, respectively)]. Although the inequality of the two ground states is a complication, there are special features that largely compensate for this. The ''right ground state'' Ω^R is the main unknown of the problem, the stationary PDF P_s, and it can always be taken to be non-negative

$$\Omega^R(\mathbf{x}) \geqslant 0. \tag{2.5}$$

This is part of the statement of the Perron-Frobenius theorem, since e^{tL} is an operator with strictly positive kernel; see [26], or Theorem 3.3.2 of [27]. On the other hand, the ''left ground state'' is known *exactly a priori*:

$$\Omega^L(\mathbf{x}) \equiv 1. \tag{2.6}$$

This latter fact turns out to be of great utility in our method. We discuss first the stationary problem and thereafter consider the time-dependent case.

A. Stationary distributions

Define a functional $\mathcal{H}$ of left and right state vectors as

$$\mathcal{H}[\Psi^R,\Psi^L]\equiv\langle\Psi^L,\hat{L}\Psi^R\rangle. \tag{2.7}$$

Then it is easy to see that Ω^R,Ω^L are uniquely characterized as the joint extremal point of the functional $\mathcal{H}$

$$\delta\mathcal{H}[\Psi^R,\Psi^L]=0\leftrightarrow(\Psi^R,\Psi^L)=(\Omega^R,\Omega^L). \tag{2.8}$$

In fact,

$$\delta\mathcal{H}[\Psi^R,\Psi^L]=\langle\delta\Psi^L,\hat{L}\Psi^R\rangle+\langle\Psi^L,\hat{L}\delta\Psi^R\rangle=0 \tag{2.9}$$

if and only if

$$\hat{L}|\Psi^R\rangle=0,\quad \hat{L}^\dagger|\Psi^L\rangle=0. \tag{2.10}$$

As stated above, we take $\Psi^R\in L^1$ (''states'') and $\Psi^L\in L^\infty$ (''observables''), with

$$\langle\Psi^L,\Psi^R\rangle\equiv\int d\mathbf{x}\Psi^L(\mathbf{x})^*\Psi^R(\mathbf{x}). \tag{2.11}$$

The ''inner product'' notation is always used in this paper as the canonical sesquilinear association of $\Psi^R\in L^1$ and $\Psi^L\in L^\infty$ with the complex number $\langle\Psi^L,\Psi^R\rangle$ defined in Eq. (2.11).

This simple variational characterization of the ground states can be made the basis of a Rayleigh-Ritz method of approximation. To initiate this method, one must make *trial Ansätze*

$$\Psi^R=\Psi^R(\boldsymbol{\alpha}),\quad \Psi^L=\Psi^L(\boldsymbol{\alpha}) \tag{2.12}$$

for the ground states. (Since we know Ω^L to be exactly equal to one, it may seem unnecessary to make an *Ansatz* for it at all. However, variation over the ''observables'' is required to characterize the ''state,'' or right ground state Ω^R.) The vector $\boldsymbol{\alpha}=(\alpha_1,\ldots,\alpha_N)$ denotes a set of N real parameters (where possibly $N=\infty$). In certain cases, we wish to have some parameters dependence only on one of the vectors $\Psi^H,H=L,R$ and we denote the corresponding parameters as $\boldsymbol{\alpha}^H=(\alpha_1^H,\ldots,\alpha_{N^H}^H)$ for $H=L,R$ respectively. We then use $\boldsymbol{\alpha}$ to denote only the common parameters in both trial vectors. An interesting special case is when there are no such common parameters, i.e.,

$$\Psi^R=\Psi^R(\boldsymbol{\alpha}^R),\quad \Psi^L=\Psi^L(\boldsymbol{\alpha}^L), \tag{2.13}$$

and $N^L=N^R$, i.e., with equal numbers of the left and right parameters. The *Ansätze* provide an explicit, but arbitrary, reduction of the original variational problem in an infinite-dimensional function space to an analogous problem in N-dimensional Euclidean space. A given assumed form of the trial *Ansatz* provides, in essence, a ''nonlinear projection'' of the original time-independent stationarity equations. This is the same general strategy proposed explicitly by Bayly under the term ''parametric PDF closures'' [28] (and used implicitly by others before). Here we simply explain how this strategy may be implemented variationally.

For any particular *Ansatz*, we denote

$$\mathcal{H}(\boldsymbol{\alpha})\equiv\langle\Psi^L(\boldsymbol{\alpha}),\hat{L}\Psi^R(\boldsymbol{\alpha})\rangle, \tag{2.14}$$

which we call the *(parametric) Hamiltonian*. We may now seek the extremal, or critical, points of $\mathcal{H}$:

$$\frac{\partial\mathcal{H}}{\partial\alpha_i}(\boldsymbol{\alpha}_*)=0. \tag{2.15}$$

This condition may be written more explicitly as

$$\langle\psi_i^L(\boldsymbol{\alpha}_*),\hat{L}\Psi^R(\boldsymbol{\alpha}_*)\rangle+\langle\Psi^L(\boldsymbol{\alpha}_*),\hat{L}\psi_i^R(\boldsymbol{\alpha}_*)\rangle=0 \tag{2.16}$$

for each $i=1,\ldots,N$, where, in general, for $H=L,R$

$$\psi_i^H(\boldsymbol{\alpha})=\frac{\partial\Psi^H}{\partial\alpha_i}(\boldsymbol{\alpha}). \tag{2.17}$$

One may take the corresponding state vectors as the approximations to the ground states:

$$\Omega_*^R(\mathbf{x})=\Psi^R(\mathbf{x};\boldsymbol{\alpha}_*),\quad \Omega_*^L(\mathbf{x})=\Psi^L(\mathbf{x};\boldsymbol{\alpha}_*). \tag{2.18}$$

In the special case Eq. (2.13) with no common parameters, the variational equations become simply

$$0=\frac{\partial\mathcal{H}}{\partial\alpha_i^R}=\langle\Psi^L(\boldsymbol{\alpha}_*^L),\hat{L}\psi_i^R(\boldsymbol{\alpha}_*^R)\rangle \tag{2.19}$$

and

$$0=\frac{\partial\mathcal{H}}{\partial\alpha_i^L}=\langle\psi_i^L(\boldsymbol{\alpha}_*^L),\hat{L}\Psi^R(\boldsymbol{\alpha}_*^R)\rangle, \tag{2.20}$$

with $i=1,\ldots,N$ $(=N^R=N^L)$. We may also write out the general equation (2.16) more explicitly as separate equations for the variations under each of $\boldsymbol{\alpha}^R$, $\boldsymbol{\alpha}^L$, and $\boldsymbol{\alpha}$. However, we have not found this version of the equations to be as useful, so that we relegate it to the Appendix.

In general, the function $\mathcal{H}(\boldsymbol{\alpha})$ may have more than one critical point. Some *a priori* criteria for selection of the critical point(s) of interest arise from the *exact* information for the problem that $\mathcal{H}[\Omega^R,\Omega^L]=0$ and that $\Omega^L\equiv1$. Hence, among the possible critical points, we should only accept those for which

$$\mathcal{H}(\boldsymbol{\alpha}_*)\approx0 \tag{2.21}$$

and

$$\Psi^L(\mathbf{x};\boldsymbol{\alpha}_*)\approx1. \tag{2.22}$$

The second condition generally implies the first. Hence we should only accept those critical points for which $\Omega^L{}_*$ is close to the constant 1. We refer to such critical points as ''acceptable.'' Because of the acceptability condition, we see that the *Ansätze* need really only explore the region near $\Psi^L\approx1$. Thus we may, without loss of generality, assume that $\alpha_i^L\ll1$ and expand to linear order

$$\Psi^L(\boldsymbol{\alpha},\boldsymbol{\alpha}^L)=1+\sum_{i=1}^{N^L}\alpha_i^L\psi_i^L(\boldsymbol{\alpha}), \tag{2.23}$$

where, now, for $H=L,R$, $\psi_i^H(\boldsymbol{\alpha},\boldsymbol{\alpha}^H)=(\partial\Psi^H/\partial\alpha_i^H)(\boldsymbol{\alpha},\boldsymbol{\alpha}^H)$, rather than Eq. (2.17). Correspondingly,

$$\mathcal{H}(\boldsymbol{\alpha}^R,\boldsymbol{\alpha}^L,\boldsymbol{\alpha})=\alpha_i^L\langle\psi_i(\boldsymbol{\alpha}),\hat{L}\Psi^R(\boldsymbol{\alpha},\boldsymbol{\alpha}^R)\rangle \tag{2.24}$$

(summation convention implied). To guarantee $\Psi^L\in L^\infty$, we should really take

$$\Psi^L(\alpha,\alpha^L)=\exp\left[i\sum_{i=1}^{N^L}\alpha_i^L\psi_i^L(\alpha)\right]. \tag{2.25}$$

However, this leads to results equivalent to Eq. (2.23).

It is useful to consider the special case Eq. (2.13) with no common parameters, for which the variational equations (2.19) and (2.20) become simply

$$\alpha_i^L\langle\psi_i^L,\hat{L}\psi_j^R(\boldsymbol{\alpha}^R)\rangle=0 \tag{2.26}$$

and

$$\langle\psi_i^L,\hat{L}\Psi^R(\boldsymbol{\alpha}^R)\rangle=0 \tag{2.27}$$

for $i,j=1,\ldots,N$. If the matrix in Eq. (2.26) is nonsingular

$$\det[\langle\psi_i^L,\hat{L}\psi_j^R(\boldsymbol{\alpha}^R)\rangle]\neq 0, \tag{2.28}$$

then the first of the variational equations has as its *unique* solution

$$\boldsymbol{\alpha}_*^L\equiv\mathbf{0}. \tag{2.29}$$

In that case, Eq. (2.27) is the only remaining equation and it determines the critical value $\boldsymbol{\alpha}_*^R$. Thus the condition determining $P_s=\Omega^R$ in this approximation is the stationarity condition

$$\langle\hat{L}^\dagger\psi_i^L\rangle_{\boldsymbol{\alpha}_*^R}=0 \tag{2.30}$$

for the finite set of moment functions ψ_i^L, $i=1,\ldots,N^L$. In that case, the variational method does not differ from the projection of the dynamics onto a finite set of moments. If one permits a more general dependence of Ψ^L on the parameters $\boldsymbol{\alpha}^L$ than the linear *Ansätze* Eq. (2.23), then the variational method does not generally coincide with the moment projection. However, we see no advantage at this point to allowing a nonlinear dependence on $\boldsymbol{\alpha}^L$.

It is possible to obtain the moment projection condition in a slightly more general form, i.e., so that the moments ψ_i^L depend upon the same set of parameters $\boldsymbol{\alpha}$ as the trial state $\Psi^R=\Psi^R(\boldsymbol{\alpha})$. Formally, we take $N^R=0$ and $N=N^L$. We may obtain for the N parameters $\boldsymbol{\alpha}$ determining equations of the form

$$\langle\psi_i^L(\boldsymbol{\alpha}),\hat{L}\Psi_j^R(\boldsymbol{\alpha})\rangle=0 \tag{2.31}$$

or, equivalently,

$$\langle\hat{L}^\dagger\psi_i^L(\boldsymbol{\alpha})\rangle_{\boldsymbol{\alpha}}=0. \tag{2.32}$$

This is accomplished by making the variational *Ansätze*

$$\Psi^L=1+\sum_{i=1}^{N}\alpha_i^L\psi_i^L(\boldsymbol{\alpha}),\quad \Psi^R=\Psi^R(\boldsymbol{\alpha}). \tag{2.33}$$

There may be some advantage in permitting the moments to vary along with the trial state. Hence this more general version is worked out in the Appendix.

A simple example of such *Ansätze* as discussed above may be devised based upon a *trial weight* $w=w(\mathbf{x})$, which is a normalized probability density, and an adapted set of *orthogonal polynomials* $p_n(\mathbf{x})$:

$$\int d\mathbf{x}w(\mathbf{x})p_n(\mathbf{x})p_{n'}(\mathbf{x})=\delta_{nn'}. \tag{2.34}$$

See [29,30]. A natural form of the trial *Ansatz* then takes $N^R=N^L$ $(\equiv N)$ and

$$\Psi^R(\mathbf{x};\boldsymbol{\alpha}^R)=w(\mathbf{x})\sum_{n=0}^{N-1}\alpha_n^R p_n(\mathbf{x}) \tag{2.35}$$

and

$$\Psi^L(\mathbf{x};\boldsymbol{\alpha}^L)=\sum_{n=0}^{N-1}\alpha_n^L p_n(\mathbf{x}). \tag{2.36}$$

This *Ansatz* is a simple case of the type of Eq. (2.13), with no common parameters. Here the stationarity condition becomes simply

$$\mathbf{L}_N\boldsymbol{\alpha}_*^R=0,\quad \boldsymbol{\alpha}_*^L\mathbf{L}_N=0, \tag{2.37}$$

with

$$(\mathbf{L}_N)_{nn'}\equiv\langle p_n,\hat{L}(wp_{n'})\rangle \tag{2.38}$$

for $0\leqslant n,\ n'<N$. In other words, the $\boldsymbol{\alpha}_*^R$ and $\boldsymbol{\alpha}_*^L$ should be, respectively, right and left eigenvectors of the matrix $\mathbf{L}_N$ with eigenvalue zero. It is easy to check that a left eigenvector of $\mathbf{L}_N$ for the eigenvalue zero always exists and is given simply by

$$\alpha_{*n}^L=\delta_{n,0}. \tag{2.39}$$

It is possible to generalize the orthogonal polynomial *Ansatz* by choosing the trial weight $w(\boldsymbol{\alpha})$, depending upon some additional M parameters α_i, $i=1,\ldots,M$. In that case, the adapted orthogonal polynomials will depend also upon $\boldsymbol{\alpha}$. After initial variation over $\boldsymbol{\alpha}^R,\boldsymbol{\alpha}^L$, a second variation may be made to optimize the choice of $\boldsymbol{\alpha}$.

An advantage of the orthogonal polynomial scheme is that it may converge in the limit $N\to\infty$; for an example, see [21]. Some sufficient conditions for convergence are discussed in [11]. It is necessary for convergence that $\int d\mathbf{x}[P_s^2(\mathbf{x})/w(\mathbf{x})]<\infty$ [29]. Unfortunately, the expansion *Ansatz* Eq. (2.35) for the state need not be positive at all values of $\mathbf{x}$. Instead, *realizability* can be guaranteed by making an *Ansatz*

$$\Psi^R=w(\boldsymbol{\alpha},\boldsymbol{\alpha}^R), \tag{2.40}$$

in which

$$w(\mathbf{x};\boldsymbol{\alpha},\boldsymbol{\alpha}^R)\geqslant 0,\quad \int d\mathbf{x}w(\mathbf{x};\boldsymbol{\alpha},\boldsymbol{\alpha}^R)=1. \tag{2.41}$$

This ensures realizability whenever such an *Ansatz*, along with Eq. (2.23), yields an acceptable critical point. The criterion of realizability is especially important for a few parameter *Ansatz*, incorporating certain physical insights and ideas as a test of those beliefs. On the other hand, for the case where $N\rightarrow\infty$, it may be preferable to impose the criterion of *convergence*. This might be done even at the price of loss of realizability if convergence for a statistic of particular interest is rapid enough. The dual criteria of realizability and convergence ought to be regarded as complementary in their applicability.

B. Time-dependent distributions

We first observe how the evolution equation (1.1) may be formulated variationally. Let us define

$$\Gamma[\Psi^R,\Psi^L]\equiv\int_0^\infty dt\langle\Psi^L(t),(\partial_t-\hat{L})\Psi^R(t)\rangle, \quad (2.42)$$

as a functional of ''trajectories'' $\Psi^H(t)$, $H=L,R$. We refer to this functional as the *nonequilibrium action*. It is easy to see formally that the stationarity condition

$$\delta\Gamma[\Psi^R,\Psi^L]=0 \quad (2.43)$$

is equivalent to

$$(\partial_t-\hat{L})|\Psi^R(t)\rangle=0, \quad (\partial_t+\hat{L}^\dagger)|\Psi^L(t)\rangle=0, \quad (2.44)$$

the variation being performed with the constraint

$$\langle\Psi^L(\infty),\Psi^R(\infty)\rangle=\langle\Psi^L(0),\Psi^R(0)\rangle. \quad (2.45)$$

In other words, a pair of trajectories is an extremal point of the action if and only if the ''right trajectory'' is a solution of the evolution equation (1.1) and the ''left trajectory'' is a solution of the adjoint equation, subject to the ''end-point constraint'' Eq. (2.45). It is important to note a particular exact solution of the adjoint equation

$$\Psi^L(\mathbf{x},t)\equiv 1. \quad (2.46)$$

In that case, the end-point constraint becomes

$$\int d\mathbf{x}\Psi^R(\mathbf{x},\infty)=\int d\mathbf{x}\Psi^R(\mathbf{x},0), \quad (2.47)$$

which is automatically satisfied by any solution of the evolution equation. In other words, $\Psi^L(t)\equiv 1$ together with any solution $\Psi^R(t)$ of the evolution equation provides an extremal point of the action $\Gamma[\Psi^R,\Psi^L]$. In this important special case $\Gamma[\Psi^R,\Psi^L]=0$. We may note the equivalent form of the nonequilibrium action

$$\Gamma[\Psi^R,\Psi^L]\equiv\int_0^\infty dt\{\langle\Psi^L(t),\dot{\Psi}^R(t)\rangle-\mathcal{H}[\Psi^R(t),\Psi^L(t)]\}, \quad (2.48)$$

which shows that Ψ^L is formally a momentum Π^R canonically conjugate to Ψ^R. In that case, the evolution equation and its adjoint are formally restated as ''Hamilton's equations''

$$\dot{\Psi}^R(\mathbf{x})=\frac{\delta}{\delta\Psi^L(\mathbf{x})}\mathcal{H}[\Psi^R,\Psi^L],$$

$$\dot{\Psi}^L(\mathbf{x})=-\frac{\delta}{\delta\Psi^R(\mathbf{x})}\mathcal{H}[\Psi^R,\Psi^L]. \quad (2.49)$$

This makes it obvious that the Hamiltonian is invariant along an extremal set of trajectories of the action Eq. (2.48).

In the same manner as for the stationary case, we may use the previous variational principle as the basis of an approximation method for the time-dependent PDF. The basic idea is similar to time-dependent variational principles of standard use in quantum mechanics [2,3], going back to the early work of Dirac [4] and Frenkel [5]. The procedure is initiated by making trial *Ansätze* for the trajectories, in the form

$$\Psi^H(t)=\Psi^H(\boldsymbol{\alpha}(t)), \quad (2.50)$$

with $H=L,R$. In other words, the reduction to a finite number of degrees of freedom is made with the same functional form as for the stationary case and all of the time dependence is contained in the parameters $\boldsymbol{\alpha}(t)$. This is the same idea as in the general method of parametric PDF closure, except that here we derive equations for the closure parameters variationally. Indeed, we may substitute the trial trajectories into the action to obtain a reduced or *parametric action*

$$\Gamma[\boldsymbol{\alpha}]\equiv\int_0^\infty dt[\pi_i(\boldsymbol{\alpha}(t))\dot{\alpha}_i(t)-\mathcal{H}(\boldsymbol{\alpha}(t))], \quad (2.51)$$

with

$$\pi_i(\boldsymbol{\alpha})\equiv\left\langle\Psi^L(\boldsymbol{\alpha}),\frac{\partial}{\partial\alpha_i}\Psi^R(\boldsymbol{\alpha})\right\rangle. \quad (2.52)$$

The Euler-Lagrange equations of the variational principle have the special form

$$\{\alpha_i,\alpha_j\}\dot{\alpha}_j=\frac{\partial\mathcal{H}}{\partial\alpha_i}, \quad (2.53)$$

in which

$$\{\alpha_i,\alpha_j\}\equiv\left\langle\frac{\partial\Psi^L}{\partial\alpha_i}(\boldsymbol{\alpha}),\frac{\partial\Psi^R}{\partial\alpha_j}(\boldsymbol{\alpha})\right\rangle-\left\langle\frac{\partial\Psi^L}{\partial\alpha_j}(\boldsymbol{\alpha}),\frac{\partial\Psi^R}{\partial\alpha_i}(\boldsymbol{\alpha})\right\rangle. \quad (2.54)$$

This is an infinite-dimensional generalization of the *Lagrange bracket* of classical mechanics; see [3] and [31], p. 250. It is easily checked to have the properties

$$\{\alpha_j,\alpha_i\}=-\{\alpha_i,\alpha_j\} \quad (2.55)$$

and

$$\frac{\partial}{\partial\alpha_i}\{\alpha_j,\alpha_k\}+\frac{\partial}{\partial\alpha_j}\{\alpha_k,\alpha_i\}+\frac{\partial}{\partial\alpha_k}\{\alpha_i,\alpha_j\}=0. \quad (2.56)$$

Let us first verify the stated form of the Euler-Lagrange equations (2.53). The verification follows from the result that

$$\frac{\delta}{\delta\alpha_i}\int dt\,\pi_i(\boldsymbol{\alpha})\dot{\alpha}_i=\{\alpha_i,\alpha_j\}\dot{\alpha}_j. \tag{2.57}$$

By a simple calculation

$$\frac{\delta}{\delta\alpha_i}\int dt\,\pi_i(\boldsymbol{\alpha})\dot{\alpha}_i=\left\langle\frac{\partial\Psi^L}{\partial\alpha_i},\frac{\partial\Psi^R}{\partial\alpha_j}\right\rangle\dot{\alpha}_j+\left\langle\Psi^L,\frac{\partial^2\Psi^R}{\partial\alpha_i\partial\alpha_j}\right\rangle\dot{\alpha}_j - \frac{d}{dt}\pi_i(\boldsymbol{\alpha}). \tag{2.58}$$

However,

$$\frac{d}{dt}\pi_i(\boldsymbol{\alpha})=\left\langle\frac{\partial\Psi^L}{\partial\alpha_j},\frac{\partial\Psi^R}{\partial\alpha_i}\right\rangle\dot{\alpha}_j+\left\langle\Psi^L,\frac{\partial^2\Psi^R}{\partial\alpha_i\partial\alpha_j}\right\rangle\dot{\alpha}_j. \tag{2.59}$$

This yields Eq. (2.57). The property Eq. (2.55) of Lagrange brackets is obvious. Equation (2.56) follows from the expression (2.54) by a simple calculation.

If the matrix of Lagrange brackets ($\{\alpha_i,\alpha_j\}$) is nondegenerate, that is, $\det(\{\alpha_i,\alpha_j\})\neq 0$, then we may introduce a corresponding *Poisson bracket* $[\alpha_i,\alpha_j]$ as the elements of the inverse matrix

$$([\alpha_i,\alpha_j])=(\{\alpha_i,\alpha_j\})^{-1}. \tag{2.60}$$

It is straightforward to show that the Poisson bracket has properties implied by those of the Lagrange bracket Eqs. (2.55) and (2.56), namely,

$$[\alpha_j,\alpha_i]=-[\alpha_i,\alpha_j] \tag{2.61}$$

and

$$[\alpha_i,[\alpha_j,\alpha_k]]+[\alpha_j,[\alpha_k,\alpha_i]]+[\alpha_k,[\alpha_i,\alpha_j]]=0. \tag{2.62}$$

The latter is the well known Jacobi identity. The bracket may be extended to arbitrary functions f and g of coordinates $\boldsymbol{\alpha}$ via the definition

$$[f,g]\equiv\sum_{p,q}\frac{\partial f}{\partial\alpha_p}\frac{\partial g}{\partial\alpha_q}[\alpha_p,\alpha_q]. \tag{2.63}$$

With this definition, the Poisson bracket satisfies Eqs. (2.61) and (2.62) for all functions. Note that the Jacobi identity for general functions follows by the argument of [31], p. 257. The parametric equations may then be written as

$$\dot{\alpha}_i=[\alpha_i,\mathcal{H}], \tag{2.64}$$

which are in Hamiltonian form. In general, canonically conjugate variables do not exist for this Hamiltonian (i.e., the system is a noncanonical Hamiltonian). Notice that the Poisson brackets $[\alpha_i,\alpha_j]$ of the system depend only upon the parametrization (i.e., the trial *Ansatz*) and that the dynamics enters solely through the Hamiltonian $\mathcal{H}(\boldsymbol{\alpha})$. We now see very simply that the fixed points of the parametric evolution equations coincide with the critical points of the corresponding Hamiltonian. (Even without the nondegeneracy condition the fixed points would include all of the critical points of $\mathcal{H}$, although there might be additional fixed points.) Furthermore, the parametric Hamiltonian is an integral of motion for the evolution equations. Notice that if the nondegeneracy condition failed at finite time, then the solutions themselves to the parametric equations might become ill defined.

A case of special interest is that in which $\Psi^H=\Psi^H(\boldsymbol{\alpha}^H)$, $H=L,R$, with an equal number of $\boldsymbol{\alpha}^R$ and $\boldsymbol{\alpha}^L$ parameters. Observe that the Lagrange brackets are now given simply as

$$\{\alpha_i^L,\alpha_j^R\}=\langle\psi_i^L(\boldsymbol{\alpha}^L),\psi_j^R(\boldsymbol{\alpha}^R)\rangle \tag{2.65}$$

and

$$\{\alpha_i^R,\alpha_j^L\}=-\langle\psi_j^L(\boldsymbol{\alpha}^L),\psi_i^R(\boldsymbol{\alpha}^R)\rangle, \tag{2.66}$$

with all other brackets vanishing. It is easy to check that the variables $\boldsymbol{\pi}^R$ introduced as

$$\pi_i^R(\boldsymbol{\alpha}_R,\boldsymbol{\alpha}_L)\equiv\left\langle\Psi^L(\boldsymbol{\alpha}^L),\frac{\partial}{\partial\alpha_i^R}\Psi^R(\boldsymbol{\alpha}^R)\right\rangle \tag{2.67}$$

satisfy

$$[\alpha_i^R,\pi_j^R]=\delta_{ij}, \tag{2.68}$$

that is, $\boldsymbol{\pi}^R$ is the momentum canonically conjugate to $\boldsymbol{\alpha}^R$. If $\pi_i^R(\boldsymbol{\alpha}^R,\boldsymbol{\alpha}^L)=\pi_i^R$ is invertible at each fixed $\boldsymbol{\alpha}^R$ for $\boldsymbol{\alpha}^L$ in terms of $\boldsymbol{\pi}^R$ and $\boldsymbol{\alpha}^R$, then by a change of variables the system has canonical Hamiltonian form.

As in the static case, there is a criterion of acceptability of solutions, which requires that $\Psi^L(t)\approx 1$ for all time t. Let us consider first, for simplicity, the previous special case with $\Psi^H=\Psi^H(\boldsymbol{\alpha}^H)$, $H=L,R$. Just as for the statics, we are motivated to adopt the linear *Ansatz*

$$\Psi^L(\mathbf{x};\boldsymbol{\alpha}^L)=1+\sum_{i=1}^{N}\alpha_i^L\psi_i^L(\mathbf{x}). \tag{2.69}$$

In this case, the equations for $\boldsymbol{\alpha}^L(t)$ become

$$-\langle\psi_j^L,\psi_i^R(\boldsymbol{\alpha}^R)\rangle\dot{\alpha}_j^L=\alpha_j^L\langle\psi_j^L,\hat{L}\psi_i^R(\boldsymbol{\alpha}^R)\rangle, \tag{2.70}$$

$i=1,\ldots,N$, which have as an *exact solution*

$$\boldsymbol{\alpha}^L(t)\equiv\mathbf{0}. \tag{2.71}$$

Within this same *Ansatz* the equation remaining to be solved for $\boldsymbol{\alpha}^R(t)$ reduces to

$$\langle\psi_i^L,\psi_j^R(\boldsymbol{\alpha}^R)\rangle\dot{\alpha}_j^R=\langle\psi_i^L,\hat{L}\Psi^R(\boldsymbol{\alpha}^R)\rangle. \tag{2.72}$$

For this case, a further simplification is possible by introducing *moment averages*

$$m_i(\boldsymbol{\alpha}^R)\equiv\langle\psi_i^L\rangle_{\boldsymbol{\alpha}^R} \tag{2.73}$$

and the *dynamical vector*

$$V_i(\boldsymbol{\alpha}^R)\equiv\langle\hat{L}^\dagger\psi_i^L\rangle_{\boldsymbol{\alpha}^R}. \tag{2.74}$$

Because $\{\alpha^L,\alpha^R\}=(\partial m_i/\partial\alpha_j^R)(\boldsymbol{\alpha}^R)$ for the *Ansatz* Eq. (2.69), it follows that

$$\{\alpha_i^L,\alpha_j^R\}\dot{\alpha}_j^R=\frac{\partial m_i}{\partial \alpha_j^R}\dot{\alpha}_j^R=\dot{m}_i. \tag{2.75}$$

Therefore, the equation of motion Eq. (2.72) expressed in terms of the moments $\mathbf{m}$ becomes simply

$$\dot{m}_i=V_i(\mathbf{m}), \tag{2.76}$$

where $\mathbf{V}(\mathbf{m})\equiv\mathbf{V}(\boldsymbol{\alpha}(\mathbf{m}))$. In this way we see how ''moment closures,'' as they have been traditionally employed in nonequilibrium dynamics, are obtained in our scheme. Closure is achieved by calculating all averages with respect to the PDF *Ansatz* $P(\mathbf{x},t)=\Psi^R(\mathbf{x};\boldsymbol{\alpha}^R(t))$ and then eliminating the parameters $\boldsymbol{\alpha}^R(t)$ in terms of the (equal number of) moments $\mathbf{m}(t)$. As we shall discuss in Sec. III, this variational method of moment closure has definite theoretical advantages.

More generally, we may employ the *Ansatz* Eq. (2.33), $\Psi^L=1+\Sigma_{i=1}{}^N\alpha_i^L\psi_i^L(\boldsymbol{\alpha})$, and $\Psi^R=\Psi^R(\boldsymbol{\alpha})$, allowing for some parameter dependence of the moment functions $\psi_i^L(\boldsymbol{\alpha})$. This choice is considered in the Appendix, so here we just report the results. As with the case previously considered, it is not hard to check that $\boldsymbol{\alpha}^L(t)\equiv\mathbf{0}$ is an *exact solution* of its equation. The remaining equation for $\boldsymbol{\alpha}$ takes the form

$$\{\alpha_i^L,\alpha_j\}\dot{\alpha}_j=V_i(\boldsymbol{\alpha}), \tag{2.77}$$

with

$$V_i(\boldsymbol{\alpha})\equiv\langle\hat{L}^\dagger\psi_i^L(\boldsymbol{\alpha})\rangle_{\boldsymbol{\alpha}}, \tag{2.78}$$

generalizing Eq. (2.74), and

$$\{\alpha_i^L,\alpha_j\}=\left\langle\psi_i^L(\boldsymbol{\alpha}),\frac{\partial\Psi^R}{\partial\alpha_j}(\boldsymbol{\alpha})\right\rangle. \tag{2.79}$$

By an easy calculation one can see also that

$$\{\alpha_i^L,\alpha_j\}=\frac{\partial}{\partial\alpha_j}\langle\psi_i^L(\boldsymbol{\alpha})\rangle_{\boldsymbol{\alpha}}-\left\langle\frac{\partial\psi_i^L}{\partial\alpha_j}(\boldsymbol{\alpha})\right\rangle_{\boldsymbol{\alpha}}. \tag{2.80}$$

A comparison with Eq. (2.11) in the work of Bayly [28] reveals that the equation (2.77) obtained via the *Ansatz* Eq. (2.33) is equivalent to the dynamical equations obtained by ''moment projection'' in the parametric PDF closure scheme. Here these equations are simply shown to have a variational formulation.

As in the static case, a useful *Ansatz* is provided by a fixed trial weight $w(\mathbf{x})$ and orthogonal expansions

$$\Psi^R(\boldsymbol{\alpha}^R)=w\sum_{n=0}^{N-1}\alpha_n^R p_n \tag{2.81}$$

and

$$\Psi^L(\boldsymbol{\alpha}^L)=\sum_{n=0}^{N-1}\alpha_n^L p_n. \tag{2.82}$$

In that case it is easy to calculate that

$$\{\alpha_n^L,\alpha_m^R\}=-\{\alpha_m^R,\alpha_n^L\}=\delta_{nm} \tag{2.83}$$

and

$$\mathcal{H}(\boldsymbol{\alpha}^R,\boldsymbol{\alpha}^L)=\sum_{n,m}\alpha_n^L(\mathbf{L}_N)_{nm}\alpha_m^R. \tag{2.84}$$

Therefore we see that $\boldsymbol{\alpha}^R$ and $\boldsymbol{\pi}^R=\boldsymbol{\alpha}^L$ are canonically conjugate and the parametric action is a quadratic form

$$\Gamma[\boldsymbol{\alpha}^R,\boldsymbol{\alpha}^L]=\int dt[\boldsymbol{\alpha}^L\cdot\dot{\boldsymbol{\alpha}}^R-\boldsymbol{\alpha}^L\cdot\mathbf{L}_N\boldsymbol{\alpha}^R]. \tag{2.85}$$

In consequence, the evolution equations are linear

$$\dot{\boldsymbol{\alpha}}^R=\mathbf{L}_N\boldsymbol{\alpha}^R,\quad \dot{\boldsymbol{\alpha}}^L=-\boldsymbol{\alpha}^L\mathbf{L}_N \tag{2.86}$$

for this particular *Ansatz*. The second equation has exact solution $\alpha_n^L(t)\equiv\delta_{n0}$. The first equation is a standard Galerkin truncation of the linear Liouville dynamics Eq. (1.1).

III. CONSTRAINED VARIATION AND EFFECTIVE ACTION

A. The principle of least effective action

For spatially extended systems, or for any system with large numbers of degrees of freedom, it is certainly too ambitious to try to calculate the full PDF. Such a calculation would put any trial *Ansatz* to an extremely severe test and could hardly be expected to succeed, in general, with a few number of parameters. In any case, the physical interest is usually in some special low-order statistic, such as a mean field or a correlation function. Such quantities are represented by random variables $\mathbf{z}$ on microscopic phase space, that is, by functions $\mathbf{z}=\mathbf{z}(\mathbf{x})$ of the dynamical variables $\mathbf{x}$. In practice, one will be mostly interested in some simple low-order moments of the dynamical variables $\mathbf{x}$ themselves, e.g., $\mathbf{z}=\mathbf{x}$, $\mathbf{x}\otimes\mathbf{x}$, etc. It should be possible to successfully calculate a statistic of this type with a simpler Ansatz with just a few parameters, if those are insightfully chosen. However, the variational method, as we have described it so far, allows one to calculate such a low-order statistic only as the by-product of calculating the full distribution. One would like to have a more direct variational method for any statistic of interest.

In fact, it is well known in various contexts that statistical quantities such as expectations and correlations, are characterized by a minimum principle for a certain functional. In (Euclidean) field theory this functional is called the ''effective action,'' and was originally rigorously investigated by Symanzik in [17]. In nonequilibrium statistical mechanics the variational principle associated with the effective action was pointed out some time ago by Graham [16]. The fact that averages of suitable distributions are characterized by a minimum principle is also standard in probability theory; see Sec. 3 of [32]. Such a principle has a very general basis and indeed its origin is the same as that of the familiar equilibrium variational principles of maximum entropy, minimum free energy, etc. Closely related ideas have been exploited recently to develop moment-closure hierarchies for kinetic theories [33]. We shall give here a self-contained discussion of the least-action principle, following the accounts in [17,32].

The main requirement for its validity is *finite exponential moments* of the statistical distribution. Let us denote by $\mathcal{P}$ the probability measure on *histories* of our stochastic dynamics. Thus, P_t is just the projection (or marginal) at time t of the distribution $\mathcal{P}$. Then, what is required is that, integrating over the ensemble of histories $\{\mathbf{x}(t): -\infty < t < +\infty\}$,

$$\int \mathcal{DP}(\mathbf{x}) e^{[\mathbf{f},\mathbf{z}(\mathbf{x})]} < \infty, \tag{3.1}$$

where $\mathbf{f}(t)$ is a real-vector valued test function and $(\mathbf{f},\mathbf{z}) = \int dt \mathbf{f}(t)\mathbf{z}(t)$. If Eq. (3.1) holds, we may define

$$W[\mathbf{f}] \equiv \ln\left[\int \mathcal{DP}(\mathbf{x}) e^{(\mathbf{f},\mathbf{z})}\right], \tag{3.2}$$

which is a cumulant-generating functional of the distribution $\mathcal{P}$. It is a consequence of the positivity of the distribution and the Hölder inequality that

$$\int \mathcal{DP}(\mathbf{x}) e^{[\lambda \mathbf{f}_1 + (1-\lambda)\mathbf{f}_2, \mathbf{z}]} \leqslant \left(\int \mathcal{DP}(\mathbf{x}) e^{(\mathbf{f}_1,\mathbf{z})}\right)^{\lambda} \left(\int \mathcal{DP}(\mathbf{x}) e^{(\mathbf{f}_2,\mathbf{z})}\right)^{1-\lambda}, \tag{3.3}$$

for $0 < \lambda < 1$, or

$$W[\lambda \mathbf{f}_1 + (1-\lambda)\mathbf{f}_2] \leqslant \lambda W[\mathbf{f}_1] + (1-\lambda) W[\mathbf{f}_2]. \tag{3.4}$$

In other words, $W[\mathbf{f}]$ is a globally convex functional of its argument. Observe that this is a result just of a simple realizability inequality for the distribution $\mathcal{P}$. The corresponding conjugate convex functional is

$$\Gamma[\mathbf{z}] = \sup_{\mathbf{f}} \{(\mathbf{f},\mathbf{z}) - W[\mathbf{f}]\}. \tag{3.5}$$

This is the definition of the *effective action* for $\mathbf{z}$ histories. Since $\Gamma[\mathbf{z}]$ is also globally convex under the assumption Eq. (3.1), it follows that it has an absolute minimum (possibly nonunique if Γ is not strictly convex). In fact,

$$\Gamma[\mathbf{z}] \geqslant 0, \quad \Gamma[\overline{\mathbf{z}}] = 0, \tag{3.6}$$

where

$$\overline{\mathbf{z}(t)} = \int \mathcal{DP}(\mathbf{x}) \mathbf{z}[\mathbf{x}(t)]. \tag{3.7}$$

The positivity of Γ follows from the fact that $(\mathbf{f},\mathbf{z}) - W[\mathbf{f}] = 0$ in Eq. (3.5) for $\mathbf{f} = \mathbf{0}$. Furthermore, by Jensen's inequality $\ln[\int \mathcal{DP}(\mathbf{x}) e^{(\mathbf{f},\mathbf{z})}] \geqslant (\mathbf{f},\overline{\mathbf{z}})$. Thus $(\mathbf{f},\overline{\mathbf{z}}) - W[\mathbf{f}] \leqslant 0$ for all $\mathbf{f}$ and so $\Gamma[\overline{\mathbf{z}}] = 0$. That the mean is characterized as the point at which Γ achieves its minimum is just the precise statement of the *principle of least effective action*.

All the derivations we have given for the distribution on histories $\mathcal{P}$, could just as well be given for the single-time stationary distribution P_s. However, since the latter is hard to specify, it is easier to work with a quantity derived from the effective action introduced above, which is commonly referred to as the *effective potential*. This is obtained from the full action by defining, for any time-independent $\mathbf{z}$, the time-extended history $\mathbf{z}_T(t)$ by

$$\mathbf{z}_T(t) \equiv \begin{cases} \mathbf{z} & \text{if } 0 < t < T \\ \overline{\mathbf{z}} & \text{otherwise.} \end{cases} \tag{3.8}$$

Then the effective potential $V[\mathbf{x}]$ is defined as the infinite-time limit

$$V[\mathbf{z}] = \lim_{T \to +\infty} \frac{\Gamma[\mathbf{z}_T]}{T}. \tag{3.9}$$

The effective potential is appropriate to determine expected values in the time-invariant ground state of the theory $\Omega^R = P_s$.

The effective potential has a direct significance in terms of the statistics of the *empirical time average*

$$\overline{\mathbf{z}_T} \equiv \frac{1}{T}\int_0^T dt \mathbf{z}(t). \tag{3.10}$$

For an ergodic process, this random variable converges as $T \to \infty$ to the ensemble average, $\overline{\mathbf{z}_T} \to \overline{\mathbf{z}}$, almost surely in every realization. However, fluctuations away from the expected behavior should furthermore occur with a small probability, decaying asymptotically for large T as

$$\text{Prob}(\overline{\mathbf{z}_T} \approx \mathbf{z}) \sim \exp(-TV[\mathbf{z}]). \tag{3.11}$$

This is a refinement of the standard ergodic hypothesis. It will hold when the limit in Eq. (3.9) exists or, equivalently, if the similar limit $\lim_{T\to+\infty}(1/T)W[\mathbf{h}_T] = \lambda[\mathbf{h}]$ exists. These are standard results of ''large deviations'' in probability theory [34,35]. In fact, what is in physics referred to as the ''effective potential'' coincides for stochastic dynamics with the (level-1) rate function in the Donsker-Varadhan large-deviations theory for ergodic Markov processes. The probabilistic interpretation of the effective potential seems to have been first pointed out in quantum field theory by Jona-Lasinio [36]. Such a large-deviations hypothesis as Eq. (3.11) was conjectured some time ago by Takahashi for deterministic dynamical systems with sufficiently chaotic solutions [37], and rigorous theorems have been proved under suitable hypotheses (e.g., see [38,39]). In this context the effective potential is simply related to the Kolmogorov-Sinai entropy. The earliest origins of the above fluctuation hypothesis in statistical physics appear in the ''Onsager principle,'' as discussed by Oono in [40].

It follows from our assumptions that the effective potential is non-negative $V(\mathbf{z}) \geqslant 0$, convex $\lambda_1 V(\mathbf{z}_1) + \lambda_2 V(\mathbf{z}_2) \geqslant V(\lambda_1 \mathbf{z}_1 + \lambda_2 \mathbf{z}_2)$, $\lambda_1 + \lambda_2 = 1$, and vanishes only at the ensemble mean $V(\overline{\mathbf{z}}) = 0$. [The structure of the effective potential may be more complex if there is ''ergodicity breaking'' associated with multiple ergodic measures. In that case, there may be a convex set of points $\mathbf{z}$ with a nonempty interior on which $V(\mathbf{z})$ vanishes. This would be the case if a so-called nonequilibrium phase transition occurred. The important applications of the effective potential in quantum field theory appeared precisely in this type of situation, where basic symmetries of the quantum Hamiltonian are spontaneously broken by the occurrence of multiple ground states. Similiar

phenomena may be expected in infinite-volume nonequilibrium systems, especially in the parameter range after the first bifurcation from a unique laminar solution but before the transition to fully developed turbulence has occurred.] In Sec. III B we develop a practical method for approximately calculating the effective potential. Because of the connection of the effective potential with fluctuations of the empirical mean Eq. (3.11), it is very unlikely that a closure approximation that violates the basic positivity and convexity properties of the effective potential can yield a reasonable result for the ensemble average itself.

B. Variational characterization of effective potential

We now show how the effective potential $V[\mathbf{z}]$ is related to the Hamiltonian $\mathcal{H}[\Psi^R,\Psi^L]$ discussed before by means of a *constrained variation*. A similar result was proved by Symanzik in Euclidean field theory [17]. In our case, a modification is required associated with the non-self-adjoint character of $\hat{L}$. More precisely, we have the following.

Theorem 1. The effective potential

$$V[\mathbf{z}]=\lim_{T\to+\infty}\frac{1}{T}\Gamma[\mathbf{z}_T] \tag{3.12}$$

for a stationary Markov process is the value at the extremum point of the functional

$$V[\Psi^R,\Psi^L]=-\mathcal{H}[\Psi^R,\Psi^L], \tag{3.13}$$

varying over all pairs of state vectors Ψ^R,Ψ^L subject to the constraints

$$\langle\Psi^L,\Psi^R\rangle=1 \tag{3.14}$$

and

$$\langle\Psi^L,\hat{\mathbf{Z}}\Psi^R\rangle=\mathbf{z}. \tag{3.15}$$

Here $\hat{\mathbf{Z}}$ is the operator of multiplication by $\mathbf{z}(\mathbf{x})$. Although the original version of the theorem required just one trial state, there now must be *two independent trial states.*

Nevertheless, the proof is similar to the original one of Symanzik [17]. Let $\Omega^R=P_s$, $\Omega^L\equiv 1$. Then the generating functional $W[\mathbf{h}]$ introduced above may be represented in the operator formulation by

$$W[\mathbf{h}]=\ln\left\langle\Omega^L,T\exp\left(\int_0^T dt\hat{L}_{\mathbf{h}}(t)\right)\Omega^R\right\rangle, \tag{3.16}$$

where T denotes time ordering (increasing from right to left) and

$$\hat{L}_{\mathbf{h}}(t)=\hat{L}+\mathbf{h}(t)\cdot\hat{\mathbf{Z}}. \tag{3.17}$$

No time dependence is required for the coordinate operators because the exponential factors automatically introduce the correct Heisenberg picture operators after differentiating and setting $\mathbf{h}$ to zero. We note then that for a *static* field $\mathbf{h}$ in the limit $T\to+\infty$,

$$\begin{aligned}\exp(W[\mathbf{h}_T])&=\langle\Omega^L,\exp(T\hat{L}_{\mathbf{h}})\Omega^R\rangle\\&\approx\langle\Omega^L,\Omega^R[\mathbf{h}]\rangle\langle\Omega^L[\mathbf{h}],\Omega^R\rangle\exp(T\lambda[\mathbf{h}]),\end{aligned} \tag{3.18}$$

where $\lambda[\mathbf{h}]$ is the eigenvalue of the ''perturbed operator''

$$\hat{L}_{\mathbf{h}}=\hat{L}+\mathbf{h}\cdot\hat{\mathbf{Z}} \tag{3.19}$$

with the *largest real part* and $\Omega^R[\mathbf{h}],\Omega^L[\mathbf{h}]$ are the associated right and left ground-state eigenvectors

$$\hat{L}_{\mathbf{h}}|\Omega^R[\mathbf{h}]\rangle=\lambda[\mathbf{h}]|\Omega^R[\mathbf{h}]\rangle \tag{3.20}$$

and

$$\hat{L}_{\mathbf{h}}^{\dagger}|\Omega^L[\mathbf{h}]\rangle=\lambda^*[\mathbf{h}]|\Omega^L[\mathbf{h}]\rangle. \tag{3.21}$$

Furthermore, we can see that

$$\frac{\partial W[\mathbf{h}_T]}{\partial h_n}=Tz_n[\mathbf{h}]+o(T), \tag{3.22}$$

with

$$z_n[\mathbf{h}]=\langle\Omega^L[\mathbf{h}],\hat{Z}_n\Omega^R[\mathbf{h}]\rangle. \tag{3.23}$$

This can be obtained from the formula

$$\begin{aligned}\exp(W[\mathbf{h}_T])\frac{\partial W[\mathbf{h}_T]}{\partial h_n}&=\left\langle\Omega^L,\frac{\partial}{\partial h_n}\exp(T\hat{L}_{\mathbf{h}})\Omega^R\right\rangle\\&=\langle\Omega^L,\Omega^R[\mathbf{h}]\rangle\langle\Omega^L[\mathbf{h}],\Omega^R\rangle\\&\quad\times\left\langle\Omega^L[\mathbf{h}],\frac{\partial}{\partial h_n}\exp(T\hat{L}_{\mathbf{h}})\Omega^R[\mathbf{h}]\right\rangle\\&\quad+O(e^{-T\Delta\lambda}),\end{aligned} \tag{3.24}$$

where $\Delta\lambda$ is the spectral gap between the real parts of the ground-state eigenvalue and the next highest eigenvalue. We have used the well known fact that, for any one-parameter family of operators $\hat{L}(h)$ depending smoothly on a parameter h,

$$\frac{\partial}{\partial h}\exp[\hat{L}(h)]=\exp[\hat{L}(h)]\varphi[-\mathrm{Ad}\hat{L}(h)]\left[\frac{\partial\hat{L}(h)}{\partial h}\right], \tag{3.25}$$

where $\mathrm{Ad}\hat{L}$ denotes the ''adjoint operator'' defined by the commutator

$$(\mathrm{Ad}\hat{L})[\hat{O}]=[\hat{L},\hat{O}], \tag{3.26}$$

and $\varphi(z)$ is the entire function $\varphi(z)=(e^z-1)/z=1+(1/2!)z+(1/3!)z^2s\cdots$. See [41]. Since

$$\langle\Omega^L[\mathbf{h}],[\hat{L}_{\mathbf{h}},\hat{O}]\Omega^R[\mathbf{h}]\rangle=0 \tag{3.27}$$

for any operator $\hat{O}$, only the first term survives in the expansion of φ when substituted into the first term of formula (3.24). This yields Eq. (3.22).

Now let us consider the variational problem. If we incorporate the constraints by suitable Lagrange multipliers, then the variational equation is just

$$\delta[-\langle\Psi^L,\hat{L}\Psi^R\rangle-\mathbf{h}\cdot\langle\Psi^L,\hat{\mathbf{Z}}\Psi^R\rangle+\lambda\langle\Psi^L,\Psi^R\rangle]=0 \tag{3.28}$$

or

$$\langle\delta\Psi^L,(\hat{L}_{\mathbf{h}}-\lambda)\Psi^R\rangle+\langle\Psi^L,(\hat{L}_{\mathbf{h}}-\lambda)\delta\Psi^R\rangle=0. \tag{3.29}$$

In other words, there are infinitely many stationary points of the functional $V[\Psi^R,\Psi^L]$ subject to the constraints. They consist precisely of pairs $(\Psi^R_\nu[\mathbf{h}],\Psi^L_\nu[\mathbf{h}])$ of eigenvectors of $\hat{L}_{\mathbf{h}}$,

$$\hat{L}_{\mathbf{h}}|\Psi^R_\nu[\mathbf{h}]\rangle=\lambda_\nu[\mathbf{h}]|\Psi^R_\nu[\mathbf{h}]\rangle \tag{3.30}$$

and

$$\hat{L}^\dagger_{\mathbf{h}}|\Psi^L_\nu[\mathbf{h}]\rangle=\lambda^*_\nu[\mathbf{h}]|\Psi^L_\nu[\mathbf{h}]\rangle, \tag{3.31}$$

corresponding to different branches of eigenvalues $\lambda_\nu[\mathbf{h}],\nu=0,1,2,\ldots$. To be precise, we should consider the stationary point corresponding to the branch with largest real part for each $\mathbf{h}$, that is, the pair of ground-state eigenvectors $(\Omega^R[\mathbf{h}],\Omega^L[\mathbf{h}])$ introduced above. For small enough $\mathbf{h}$ this corresponds to the eigenvalue branch with $\lambda(\mathbf{0})=0$ because the spectrum of $\hat{L}$ is all in the left half of the complex λ plane, $\mathrm{Re}\lambda<0$, except for a simple eigenvalue at $\lambda=0$. See [25] and [26]. We refer to this as the ''zero branch'' of eigenvalues.

Applying then the left eigenvector to the eigenequation of the right vector and using the constraints gives

$$\langle\Omega^L[\mathbf{h}],\hat{L}\Omega^R[\mathbf{h}]\rangle+\mathbf{h}\cdot\mathbf{z}[\mathbf{h}]=\lambda[\mathbf{h}] \tag{3.32}$$

and thus

$$\begin{aligned}-\langle\Omega^L[\mathbf{h}],\hat{L}\Omega^R[\mathbf{h}]\rangle&=\mathbf{h}\cdot\mathbf{z}[\mathbf{h}]-\lambda[\mathbf{h}]\\&=\frac{1}{T}\left[\left\langle\mathbf{h}_T,\frac{\delta W}{\delta\mathbf{h}}[\mathbf{h}_T]\right\rangle-W[\mathbf{h}_T]\right]+o(1)\\&=\frac{1}{T}\Gamma[\mathbf{z}_T]+o(1).\end{aligned} \tag{3.33}$$

The first quantity is independent of T, so that we see, taking the limit $T\to+\infty$, that

$$-\langle\Omega^L[\mathbf{h}],\hat{L}\Omega^R[\mathbf{h}]\rangle=V[\mathbf{z}], \tag{3.34}$$

as was claimed. □

We have given only a formal proof of the theorem without a careful statement of the conditions, which would certainly involve spectral properties of the Liouville operator $\hat{L}$, etc. The assumption of a spectral gap may be stronger than required. The above variational characterization of the effective potential is, in fact, equivalent to a spectral characterization of the potential that has been rigorously established in the Donsker-Varadhan theory [35,34,32]. In that case it is shown, under suitable conditions, that $V[\mathbf{z}]=\sup_{\mathbf{h}}(\mathbf{z}\cdot\mathbf{h}-\lambda[\mathbf{h}])$, where $\lambda[\mathbf{h}]$ is the ''principal eigenvalue'' of the operator $\hat{L}_{\mathbf{h}}=\hat{L}+\mathbf{h}\cdot\hat{\mathbf{Z}}$. The equivalence of these two characterizations follows from the preceding formal proof. The representation of the potential $V[\mathbf{z}]$ as a Legendre transform of $\lambda[\mathbf{h}]$ is entirely analogous to the representation of the entropy in equilibrium lattice spin systems as the Legendre transform of the free energy, where the latter is determined as the leading eigenvalue of the transfer matrix. For deterministic dynamics the existence of a spectral gap in the so-called Perron-Frobenius operator has been established only for a few special cases, such as the work of Pollicot and Ruelle on Axiom A systems [44]. The eigenvalue $\lambda[\mathbf{h}]$ in that context is a particular case of the topological pressure $P(\varphi)$; see [39] (or [43] for an introduction). For example, in the work of Ruelle [42] on expanding maps f of compact spaces X, the effective potential would coincide with $P(\varphi)$ for the choice $\varphi(\mathbf{x})=-\ln|f'(\mathbf{x})|+\mathbf{h}\cdot\mathbf{z}(\mathbf{x})$. Here $|f'(\mathbf{x})|$ is the Jacobian determinant of the map and its logarithm $\ln|f'(\mathbf{x})|$ is the Hamiltonian in the thermodynamic formalism for expanding maps.

C. Rayleigh-Ritz approximation of the effective potential

We outline a simple variational method of Rayleigh-Ritz type to approximate the effective potential and thereby the ensemble means. The *Ansatz* used previously for Ψ^R,Ψ^L may need to be replaced by ''augmented *Ansatz*'' $\overline{\Psi}^R,\overline{\Psi}^L$. The reason is that the left ground state under the imposed constraint, is no longer 1 identically and the constant component must be allowed to vary. In other words, we must augment the linear *Ansatz* Eq. (2.33) for the left ground state, by setting

$$\overline{\Psi}^L(\boldsymbol{\alpha},\boldsymbol{\alpha}^L)=\sum_{i=0}^{N}\alpha^L_i\psi^L_i(\boldsymbol{\alpha}). \tag{3.35}$$

Here the test function

$$\psi^L_0(\mathbf{x};\boldsymbol{\alpha})\equiv 1 \tag{3.36}$$

is included with an adjustable parameter α^L_0. Of course, with the orthogonal expansion *Ansatz* Eqs. (2.35) and (2.36), the constant term (zero-degree polynomial) is already included. However, if it was not originally, it should now be added, and an additional free parameter α_0 should be added to the PDF *Ansatz* $P=\Psi^R(\boldsymbol{\alpha})$ as well. The most natural way to do so is to simply replace the normalized density $\Psi^R\geqslant 0$ by

$$\overline{\Psi}^R(\mathbf{x};\overline{\boldsymbol{\alpha}})=\alpha_0\Psi^R(\mathbf{x};\boldsymbol{\alpha}), \tag{3.37}$$

where α_0 denotes an arbitrary normalization factor

$$\int d\mathbf{x}\overline{\Psi}^R(\mathbf{x};\overline{\boldsymbol{\alpha}})=\alpha_0. \tag{3.38}$$

Because $\overline{\Psi}^L\neq 1$ under the constraint, unit normalization of $\overline{\Psi}^R$ is no longer required, but instead the overlap condition $\langle\overline{\Psi}^L,\overline{\Psi}^R\rangle=1$ must be maintained. Notice that we use the notations $\overline{\boldsymbol{\alpha}},\overline{\boldsymbol{\alpha}}^L$ simply to indicate the parameter vectors $\boldsymbol{\alpha},\boldsymbol{\alpha}^L$ along with the additional zero components α_0,α^L_0. We shall refer to the *Ansatz* Eqs. (3.37) and (3.35) as the *natural augmentation*. While others can be contrived, this is the sim-

plest extended *Ansatz* and likely to be the most generally useful. (Despite this, some of our arguments below do not apply to the natural augmentation. We will point out where this occurs later in the discussion. This is really a technical issue, since all of the *results* discussed hereinafter still hold for the natural augmentation and it is only the proofs that need to be changed somewhat. Rather than complicate the discussion, we have decided to present proofs under the simplest assumptions. These are satisfied, for example, by the orthogonal expansion *Ansatz*. The natural augmentation is discussed in detail elsewhere [45].) Note that it is not necessary to have a closed-form expression for Ψ^R, but it is enough only to be able to calculate averages such as

$$\overline{m_i}(\overline{\boldsymbol{\alpha}}) = \langle \psi_i^L(\overline{\boldsymbol{\alpha}}) \rangle_{\overline{\boldsymbol{\alpha}}} \tag{3.39}$$

and

$$\overline{V_i}(\overline{\boldsymbol{\alpha}},\mathbf{h}) = \langle \hat{L}_{\mathbf{h}}^{\dagger} \psi_i^L(\overline{\boldsymbol{\alpha}}) \rangle_{\overline{\boldsymbol{\alpha}}}, \tag{3.40}$$

with $i=0,1,\ldots,N$. In the most practical PDF closures, the *Ansatz* $\Psi^R(\mathbf{x};\boldsymbol{\alpha})$ will be given, not explicitly, but instead by averages with respect to ''surrogate'' random variables $\mathbf{X}_{\boldsymbol{\alpha}}$ whose distributions are parametrized by $\boldsymbol{\alpha}$. From the joint *Ansatz* for Ψ^H, $H=L,R$, an approximation to the effective potential is then obtained:

$$V_*(\mathbf{z}) = -\langle \overline{\Psi}_*^L, \hat{L} \overline{\Psi}_*^R \rangle, \tag{3.41}$$

where $\overline{\Psi}_*^L = \overline{\Psi}^L(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}), \overline{\boldsymbol{\alpha}}_*^L(\mathbf{h}))$ and $\overline{\Psi}_*^R = \overline{\Psi}^R(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}))$ and the parameters $\overline{\boldsymbol{\alpha}}_*^L(\mathbf{h}), \overline{\boldsymbol{\alpha}}_*(\mathbf{h})$, and $\mathbf{h}=\mathbf{h}_*(\mathbf{z})$ are to be determined as follows.

Incorporating as before the constraints by suitable Lagrange multipliers λ and $\mathbf{h}$, the extremum point within the Ansatz is obtained by varying the function

$$F(\overline{\boldsymbol{\alpha}},\overline{\boldsymbol{\alpha}}^L) \equiv -\langle \overline{\Psi}^L(\overline{\boldsymbol{\alpha}},\overline{\boldsymbol{\alpha}}^L), \hat{L}_{\mathbf{h}} \overline{\Psi}^R(\overline{\boldsymbol{\alpha}}) \rangle + \lambda \langle \overline{\Psi}^L(\overline{\boldsymbol{\alpha}},\overline{\boldsymbol{\alpha}}^L), \overline{\Psi}^R(\overline{\boldsymbol{\alpha}}) \rangle \tag{3.42}$$

of the parameters $\overline{\boldsymbol{\alpha}},\overline{\boldsymbol{\alpha}}^L$. First, by variation of the $\overline{\boldsymbol{\alpha}}$ parameters, one obtains the equation

$$\mathbf{A}(\overline{\boldsymbol{\alpha}},\mathbf{h}) \cdot \overline{\boldsymbol{\alpha}}^L = \lambda \mathbf{B}(\overline{\boldsymbol{\alpha}}) \cdot \overline{\boldsymbol{\alpha}}^L, \tag{3.43}$$

with the matrices $\mathbf{A}(\overline{\boldsymbol{\alpha}},\mathbf{h})$ and $\mathbf{B}(\overline{\boldsymbol{\alpha}})$ defined by

$$A_{ij}(\overline{\boldsymbol{\alpha}},\mathbf{h}) = \frac{\partial}{\partial \overline{\alpha}^j} \overline{V}_j(\overline{\boldsymbol{\alpha}},\mathbf{h}) \tag{3.44}$$

and

$$B_{ij}(\overline{\boldsymbol{\alpha}}) = \frac{\partial}{\partial \overline{\alpha}^j} \overline{m}_j(\overline{\boldsymbol{\alpha}}) \tag{3.45}$$

for $i,j=0,1,\ldots,N$. Equation (3.43) has the form of a *generalized eigenvalue problem* [24,46]. The parameter vector $\overline{\boldsymbol{\alpha}}^L(\overline{\boldsymbol{\alpha}},\mathbf{h})$ is to be determined as the generalized eigenvector associated to the leading eigenvalue.

However, the proper definition of this last quantity requires some discussion. In the original infinite-dimensional setting, the ''leading'' eigenvalue was defined to be that with largest real part and for $\mathbf{h}$ small enough it coincides with the zero branch passing through 0 for $\mathbf{h}=\mathbf{0}$. On the other hand, within an approximation such as that we consider here, these two quantities need no longer coincide, although both exist. An eigenvalue branch $\lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})$ such that $\lambda(\overline{\boldsymbol{\alpha}},\mathbf{0})=0$ exists always with the associated eigenvector $\overline{\alpha}_i^L=\delta_{i0}$ at $\mathbf{h}=\mathbf{0}$. Likewise, an eigenvalue with a real part, denoted $\Lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})$, of largest value will certainly exist. Because the two quantities $\lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})$ and $\Lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})$ are possibly distinct, either may be plausibly used as the basis of an approximate calculation. However, there are compelling reasons to prefer the use of $\lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})$. Most importantly, it is only due to $\lambda(\overline{\boldsymbol{\alpha}},\mathbf{0})=0$ that $\overline{\boldsymbol{\alpha}}_*(\mathbf{0})=\overline{\boldsymbol{\alpha}}_*$ coincides with one of the fixed points of the $\mathbf{h}=\mathbf{0}$ vector field $\overline{\mathbf{V}}(\overline{\boldsymbol{\alpha}})$ (see below). Also, as a practical matter, it will generally be easier to compute $\lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})$ than $\Lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})$, whose calculation requires a determination of the entire spectrum of $\mathbf{A}(\overline{\boldsymbol{\alpha}},\mathbf{h})$. Actually, all of these considerations are rather academic. If $\Lambda(\overline{\boldsymbol{\alpha}},\mathbf{h}) > \lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})=0$ at $\mathbf{h}=\mathbf{0}$, then the stability matrix $(\partial\overline{\mathbf{V}}/\partial\overline{\boldsymbol{\alpha}})(\overline{\boldsymbol{\alpha}}) = [\mathbf{A}(\overline{\boldsymbol{\alpha}},\mathbf{0})]^{\top}$ has an eigenvalue with positive real part. If this were to occur at the starting point $\overline{\boldsymbol{\alpha}}_*$, that point would be linearly unstable under the dynamical flow of the vector field $\overline{\mathbf{V}}(\overline{\boldsymbol{\alpha}})$. That alone would be enough to disqualify the point $\overline{\boldsymbol{\alpha}}_*$ from physical interest. On the other hand, if $\Lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})=\lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})$ at $\mathbf{h}=\mathbf{0}$, then, except for degenerate cases, this will also be true in a small interval of $\mathbf{h}$ about $\mathbf{0}$ and no distinction need be made. It will be explained below that the approximate potential $V_*(\mathbf{z})$ calculated from $\lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})$ necessarily has the approximate mean

$$\overline{\mathbf{z}}_* \equiv \int d\mathbf{x} \mathbf{z}(\mathbf{x}) \Omega_*^R(\mathbf{x}) \tag{3.46}$$

as a critical point, with $V_*(\overline{\mathbf{z}}_*)=0$, but that $V_*(\mathbf{z})$ need no longer be convex at $\overline{\mathbf{z}}_*$.

Returning, then, to the specification of the approximation scheme, we next determine $\overline{\boldsymbol{\alpha}}_*(\mathbf{h})$ as the value of $\overline{\boldsymbol{\alpha}}$ satisfying the variational equation under the parameters $\overline{\boldsymbol{\alpha}}^L$:

$$\overline{V_i}(\overline{\boldsymbol{\alpha}},\mathbf{h}) = \lambda(\overline{\boldsymbol{\alpha}},\mathbf{h}) \overline{m_i}(\overline{\boldsymbol{\alpha}}), \tag{3.47}$$

$i=0,1,\ldots,N$. This may be thought of as a type of ''nonlinear eigenvalue condition'' and $\overline{\boldsymbol{\alpha}}_*(\mathbf{h})$ as the associated eigenvector. Since $\lambda(\overline{\boldsymbol{\alpha}},\mathbf{0})=0$, it is a consequence of this definition that

$$\overline{\boldsymbol{\alpha}}_*(\mathbf{0}) = \overline{\boldsymbol{\alpha}}_*, \tag{3.48}$$

with $\overline{\boldsymbol{\alpha}}_*$ a fixed point of the dynamical vector $\overline{\mathbf{V}}(\overline{\boldsymbol{\alpha}})$ defined in Eq. (2.74). As long as the stability matrix $(\partial\overline{\mathbf{V}}/\partial\overline{\boldsymbol{\alpha}})(\overline{\boldsymbol{\alpha}}_*)$ is nonsingular, the implicit function theorem guarantees that Eq. (3.47) has a solution for at least some small interval of $\mathbf{h}$ about $\mathbf{0}$. (This is the property that is not satisfied by the ''natural augmentation.'' In fact, it is not hard to show that with that choice

$$\frac{\partial\overline{\mathbf{V}}}{\partial\overline{\alpha}}(\overline{\alpha}_*) = \begin{pmatrix} 0 & \mathbf{0} \\ \mathbf{0} & \dfrac{\partial\mathbf{V}}{\partial\alpha}(\alpha_*) \end{pmatrix}. \tag{3.49}$$

Clearly, this matrix is singular. However, as we have already noted, it is only the present proofs that fail and the results themselves, proved here assuming nonsingularity, still hold

for the natural augmentation [45].) For practical computation, a Newton-Raphson or other root-finding algorithm may be employed (see [47], Chap. 9), starting with $\overline{\boldsymbol{\alpha}}_*$ at $\mathbf{h}=\mathbf{0}$ and tracking a sequence of roots $\overline{\boldsymbol{\alpha}}_*(\mathbf{h}_k)$ iteratively for $\mathbf{h}_k$ of increasing magnitude. If the starting *Ansatz* $\overline{\Psi}^R,\overline{\Psi}^L$ has more than one acceptable fixed point, then any of them may be used as a basis for the calculation. Next, $\overline{\boldsymbol{\alpha}}_*{}^L(\mathbf{h})$ is defined as $\overline{\boldsymbol{\alpha}}^L(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}),\mathbf{h})$ with its normalization fixed by the constraint $\langle\Psi_*{}^L,\Psi^R{}_*\rangle=1$. This allows one to define the function

$$\mathbf{z}_*(\mathbf{h})\equiv\langle\overline{\Psi}^L(\overline{\boldsymbol{\alpha}}_*{}^L(\mathbf{h}),\overline{\boldsymbol{\alpha}}_*(\mathbf{h})),\hat{\mathbf{Z}}\overline{\Psi}^R(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}))\rangle \quad (3.50)$$

and to determine $\mathbf{h}$ thereby as the value $\mathbf{h}_*(\mathbf{z})$ of its inverse function at $\mathbf{z}$. It should be remarked that both $\overline{\boldsymbol{\alpha}}_*(\mathbf{h})$ and $\overline{\boldsymbol{\alpha}}^L_*(\mathbf{h})$ are real vectors, at least for small enough $\mathbf{h}$, and therefore $\mathbf{z}_*[\mathbf{h}]$ is a real vector too. The eigenvalue $\lambda(\overline{\boldsymbol{\alpha}},\mathbf{h})$ will be real for $\mathbf{h}$ sufficiently near $\mathbf{0}$ and, in that case, the associated generalized eigenvector $\overline{\boldsymbol{\alpha}}^L(\overline{\boldsymbol{\alpha}},\mathbf{h})$ for the real matrices $\mathbf{A}(\overline{\boldsymbol{\alpha}},\mathbf{h}),\mathbf{B}(\overline{\boldsymbol{\alpha}})$ will also be real. We observe for $\mathbf{h}=\mathbf{0}$ that $\mathbf{z}_*[\mathbf{0}]=\overline{\mathbf{z}}_*$.

These prescriptions complete our recipe for the Rayleigh-Ritz approximation to the effective potential $V(\mathbf{z})$. We now establish an important representation for $V_*(\mathbf{z})$. Let us define

$$\lambda_*(\mathbf{h})\equiv\lambda(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}),\mathbf{h}) \quad (3.51)$$

in terms of the quantities introduced above. We now prove the following

Proposition 1. The approximate effective potential $V_*(\mathbf{z})$ is a formal Legendre transform of $\lambda_*(\mathbf{h})$ that is,

$$\frac{\partial\lambda_*}{\partial\mathbf{h}}(\mathbf{h})=\mathbf{z}_*(\mathbf{h}) \quad (3.52)$$

and

$$V_*(\mathbf{z})=\mathbf{z}_*(\mathbf{h})\cdot\mathbf{h}-\lambda_*(\mathbf{h}) \quad (3.53)$$

for $\mathbf{h}=\mathbf{h}_*(\mathbf{z})$.

Proof. Setting

$$\overline{\Psi}^L_*(\mathbf{x};\mathbf{h})=\sum_{i=0}^N\overline{\alpha}^L_{*i}(\mathbf{h})\psi_i^L(\overline{\boldsymbol{\alpha}}_*(\mathbf{h})) \quad (3.54)$$

and

$$\overline{\Psi}^R_*(\mathbf{x};\mathbf{h})=\overline{\Psi}(\mathbf{x};\overline{\boldsymbol{\alpha}}_*(\mathbf{h})), \quad (3.55)$$

we observe the overlap condition $\langle\overline{\Psi}^L_*(\mathbf{h}),\overline{\Psi}^R_*(\mathbf{h})\rangle=1$ becomes simply

$$\sum_{i=0}^N\overline{\alpha}^L_{*i}(\mathbf{h})\overline{m_i}(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}))=1. \quad (3.56)$$

We next show that

$$\langle\overline{\Psi}^L_*(\mathbf{h}),\hat{L}_{\mathbf{h}}\overline{\Psi}^R_*(\mathbf{h})\rangle=\lambda_*(\mathbf{h}). \quad (3.57)$$

In fact,

$$\begin{aligned}\langle\overline{\Psi}^L_*(\mathbf{h}),\hat{L}_{\mathbf{h}}\overline{\Psi}^R_*(\mathbf{h})\rangle&=\sum_{i=0}^N\overline{\alpha}^L_{*i}(\mathbf{h})\overline{V_i}(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}),\mathbf{h})\\&=\lambda_*(\mathbf{h})\sum_{i=0}^N\overline{\alpha}^L_{*i}(\mathbf{h})\overline{m_i}(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}))\\&=\lambda_*(\mathbf{h}),\end{aligned} \quad (3.58)$$

where the first line follows using the linear *Ansatz*, Eq. (3.54) above, the second line follows from the nonlinear eigenvalue condition Eq. (3.47), and the last line follows from the overlap condition Eq. (3.56). Now it is easy to see that

$$\begin{aligned}V_*(\mathbf{z})&=-\langle\overline{\Psi}^L_*(\mathbf{h}),\hat{L}\overline{\Psi}^R_*(\mathbf{h})\rangle=\langle\overline{\Psi}^L_*(\mathbf{h}),\hat{\mathbf{Z}}\overline{\Psi}^R_*(\mathbf{h})\rangle\cdot\mathbf{h}\\&\quad-\langle\overline{\Psi}^L_*(\mathbf{h}),\hat{L}_{\mathbf{h}}\overline{\Psi}^R_*(\mathbf{h})\rangle=\mathbf{z}_*(\mathbf{h})\cdot\mathbf{h}-\lambda_*(\mathbf{h}),\end{aligned} \quad (3.59)$$

which is Eq. (3.53).

The verification of Eq. (3.52) is a straightforward but somewhat tedious calculation. Using once more the basic expression Eq. (3.57) for $\lambda_*(\mathbf{h})$, one finds by differentiation that

$$\begin{aligned}\frac{\partial\lambda_*}{\partial\mathbf{h}}(\mathbf{h})&=\mathbf{z}_*(\mathbf{h})+\left\langle\frac{\partial\overline{\Psi}^L_*}{\partial\mathbf{h}}(\mathbf{h}),\hat{L}_{\mathbf{h}}\overline{\Psi}^R_*(\mathbf{h})\right\rangle\\&\quad+\left\langle\overline{\Psi}^L_*(\mathbf{h}),\hat{L}_{\mathbf{h}}\frac{\partial\overline{\Psi}^R_*}{\partial\mathbf{h}}(\mathbf{h})\right\rangle.\end{aligned} \quad (3.60)$$

Furthermore, calculation yields for the second term

$$\begin{aligned}&\left\langle\frac{\partial\overline{\Psi}^L_*}{\partial\mathbf{h}}(\mathbf{h}),\hat{L}_{\mathbf{h}}\overline{\Psi}^R_*(\mathbf{h})\right\rangle\\&\quad=\sum_{i=0}^N\left(\frac{\partial}{\partial\mathbf{h}}\overline{\alpha}^L_{*i}(\mathbf{h})\right)\lambda_*(\mathbf{h})\overline{m_i}(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}))+\sum_{i,j=0}^N\overline{\alpha}^L_{*i}(\mathbf{h})\\&\qquad\times\left\langle\hat{L}^\dagger_{\mathbf{h}}\frac{\partial\psi_i^L}{\partial\overline{\alpha}^j}(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}))\right\rangle_{\overline{\boldsymbol{\alpha}}_*(\mathbf{h})}\frac{\partial\overline{\alpha}_{*j}}{\partial\mathbf{h}}(\mathbf{h}),\end{aligned} \quad (3.61)$$

where the nonlinear eigenvalue condition Eq. (3.47) was used in the first sum on the right-hand side. Likewise, for the third term in Eq. (3.60)

$$\begin{aligned}\left\langle\overline{\Psi}^L_*(\mathbf{h}),\hat{L}_{\mathbf{h}}\frac{\partial\overline{\Psi}^R_*}{\partial\mathbf{h}}(\mathbf{h})\right\rangle&=\sum_{i=0}^N\overline{\alpha}^L_{*i}(\mathbf{h})\lambda_*(\mathbf{h})\left(\frac{\partial}{\partial\mathbf{h}}\overline{m_i}(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}))\right)\\&\quad-\sum_{i,j=0}^N\overline{\alpha}^L_{*i}(\mathbf{h})\\&\quad\times\left\langle\hat{L}^\dagger_{\mathbf{h}}\frac{\partial\psi_i^L}{\partial\overline{\alpha}^j}(\overline{\boldsymbol{\alpha}}_*(\mathbf{h}))\right\rangle_{\overline{\boldsymbol{\alpha}}_*(\mathbf{h})}\\&\quad\times\frac{\partial\overline{\alpha}_{*j}}{\partial\mathbf{h}}(\mathbf{h}),\end{aligned} \quad (3.62)$$

where the generalized eigenvalue equation (3.43) was used in the first sum on the right-hand side. Adding the two contributions, the last terms of each cancel and the result is

$$\left\langle \frac{\partial\overline{\Psi^L_*}}{\partial\mathbf{h}}(\mathbf{h}),\hat{L}_{\mathbf{h}}\overline{\Psi^R_*}(\mathbf{h})\right\rangle+\left\langle \overline{\Psi^L_*}(\mathbf{h}),\hat{L}_{\mathbf{h}}\frac{\partial\overline{\Psi^R_*}}{\partial\mathbf{h}}(\mathbf{h})\right\rangle$$
$$=\sum_{i=0}^{N}\left[\left(\frac{\partial}{\partial\mathbf{h}}\overline{\alpha^L_{*i}}(\mathbf{h})\right)\lambda_*(\mathbf{h})\overline{m_i}(\overline{\boldsymbol{\alpha}_*}(\mathbf{h}))+\overline{\alpha^L_{*i}}(\mathbf{h})\lambda_*(\mathbf{h})\right.$$
$$\left.\times\left(\frac{\partial}{\partial\mathbf{h}}\overline{m_i}(\overline{\boldsymbol{\alpha}_*}(\mathbf{h}))\right)\right]$$
$$=\lambda_*(\mathbf{h})\frac{\partial}{\partial\mathbf{h}}\left[\sum_{i=0}^{N}\overline{\alpha^L_{*i}}(\mathbf{h})\overline{m_i}(\overline{\boldsymbol{\alpha}_*}(\mathbf{h}))\right]$$
$$=0. \tag{3.63}$$

The constant overlap Eq. (3.56) was invoked in the last line. Thus $(\partial\lambda_*/\partial\mathbf{h})(\mathbf{h})=\mathbf{z}_*(\mathbf{h})$. It may be worth remarking that this result is a nonlinear generalization of the Hellmann-Feynman theorem used in quantum-mechanical perturbation theory. □

It is a consequence of this proposition that

$$V_*(\overline{\mathbf{z}_*})=0,\quad \frac{\partial V_*}{\partial\mathbf{z}}(\overline{\mathbf{z}_*})=\mathbf{0}. \tag{3.64}$$

Indeed, since $\mathbf{z}_*(\mathbf{0})=\overline{\mathbf{z}_*}$ and $\lambda_*(\mathbf{0})=0$, the first follows directly from Eq. (3.53). For the second, we use the simple result of Eq. (3.53) that

$$\frac{\partial V_*}{\partial\mathbf{z}}(\mathbf{z})=\mathbf{h}_*(\mathbf{z}) \tag{3.65}$$

and $\mathbf{h}_*(\overline{\mathbf{z}_*})=\mathbf{0}$. Hence we conclude that the properties Eq. (3.64), which hold for the *exact* effective potential, are automatically guaranteed to hold in the Rayleigh-Ritz approximation. However, the important property of *convexity* of $V_*(\mathbf{z})$ is not guaranteed. All that can be inferred from Eq. (3.53) is that $V_*(\mathbf{z})$ is convex in $\mathbf{z}$ if and only if $\lambda_*(\mathbf{h})$ is convex in $\mathbf{h}$.

Let us first note, however a useful simplification. As discussed in Sec. II B, it is very convenient here also to replace the parameters $\overline{\boldsymbol{\alpha}}$ by the moments $\overline{\mathbf{m}}$. Assuming that the matrix $\mathbf{B}(\overline{\boldsymbol{\alpha}})=\partial\overline{\mathbf{m}}/\partial\overline{\boldsymbol{\alpha}}$ defined in Eq. (3.45) is nonsingular, then the relation $\overline{\mathbf{m}}=\overline{\mathbf{m}}(\overline{\boldsymbol{\alpha}})$ may be inverted, at least locally, to give $\overline{\boldsymbol{\alpha}}(\overline{\mathbf{m}})$ as a function of $\overline{\mathbf{m}}$. Therefore, the $\overline{\mathbf{m}}$ may be used as parameters instead of the $\overline{\boldsymbol{\alpha}}$, writing as well $\psi^L(\overline{\mathbf{m}})=\psi^L(\boldsymbol{\alpha}(\overline{\mathbf{m}}))$ and $\overline{\Psi^R}(\overline{\mathbf{m}})=\overline{\Psi^R}(\overline{\boldsymbol{\alpha}}(\overline{\mathbf{m}}))$ without any possibility of confusion. In this case, the equation obtained under variation of the $\overline{\mathbf{m}}$ parameters reduces to an ordinary eigenvalue problem

$$\mathbf{A}(\overline{\mathbf{m}},\mathbf{h})\cdot\overline{\boldsymbol{\alpha}^L}=\lambda\,\overline{\boldsymbol{\alpha}^L}, \tag{3.66}$$

with the matrix $\mathbf{A}(\overline{\mathbf{m}},\mathbf{h})$ defined similarly as before:

$$A_{ij}(\overline{\mathbf{m}},\mathbf{h})\equiv\frac{\partial}{\partial\overline{m^i}}\overline{V_j}(\overline{\mathbf{m}},\mathbf{h}) \tag{3.67}$$

and

$$\overline{V_i}(\overline{\mathbf{m}},\mathbf{h})\equiv\langle\hat{L}^\dagger_{\mathbf{h}}\psi^L_i(\overline{\mathbf{m}})\rangle_{\overline{\mathbf{m}}}, \tag{3.68}$$

Once again, $\lambda(\overline{\mathbf{m}},\mathbf{h})$ may be taken as the leading eigenvalue and $\overline{\boldsymbol{\alpha}^L}(\overline{\mathbf{m}},\mathbf{h})$ its associated eigenvector. Likewise, an equation may be obtained for $\overline{\mathbf{m}}_*(\mathbf{h})$ by varying $\overline{\boldsymbol{\alpha}^L}$, which is now simply

$$\overline{\mathbf{V}}(\overline{\mathbf{m}},\mathbf{h})=\lambda(\overline{\mathbf{m}},\mathbf{h})\overline{\mathbf{m}}. \tag{3.69}$$

With these additional simplifications, the procedure to calculate $V_*(\mathbf{z})$ is otherwise the same as before.

In calculating the approximation $V_*(\mathbf{z})$ by the Rayleigh-Ritz method, one obtains as well approximations to Ω^H, $H=L,R$. Since it requires more work to impose the constraints, it may seem that nothing has been gained and even something has been lost. However, a moderately good *Ansatz* $\Psi^H(\boldsymbol{\alpha},\boldsymbol{\alpha}^H)$ may yield rather poor results for Ω^R and yet quite good results for $\overline{\mathbf{z}}$. It is useful to calculate the effective potential from the *Ansatz* as a diagnostic since the qualitative features should be reproduced such that $V_*(\mathbf{z})\geqslant 0$ and that $\overline{\mathbf{z}_*}$ is a minimum point of V_* with $V_*(\overline{\mathbf{z}_*})=0$. If one's only interest is in the mean values, then these are more realistic criteria of acceptability of the approximation than to insist, e.g., that ${\Psi_*}^R\geqslant 0$ everywhere. Negative density in an insignificant region of $\mathbf{x}$ space might have very little effect on the approximate average $\overline{\mathbf{z}_*}$, which could be quite close to the true average $\overline{\mathbf{z}}$. On the other hand, a failure of convexity of $V_*(\mathbf{z})$ would doubtless indicate serious errors in $\overline{\mathbf{z}_*}$ as an approximation to $\overline{\mathbf{z}}$. Such a ''prediction'' would need to be discarded as spurious. The condition of convexity of the effective potential is not contained in any property of the closure dynamics and it incorporates important additional information from the exact Liouville dynamics.

D. Variational characterization of the effective action

We now show that the time-dependent effective action can also be obtained by a constrained variation of the nonequilibrium action functional $\Gamma[\Psi^R,\Psi^L]$. The proof of this theorem is almost the same as the proof of a corresponding result in quantum field theory due to Jackiw and Kerman [19]. Just as the Symanzik theorem is a constrained version of the familiar quantum variational principle for energy eigenvalues and eigenvectors, the Jackiw-Kerman theorem can be seen as a constrained version of Dirac's [4] variational formulation of the Schrödinger equation (a quantum analog of Hamilton's principle). In addition to providing a basis for time-dependent Rayleigh-Ritz calculations, the Jackiw-Kerman-type theorem establishes the existence of a Lagrangian functional for the effective action.

Theorem 2. The effective action $\Gamma[\mathbf{z}]$ for the initial-value problem is the value at the extremum point of the functional

$$\Gamma[\Psi^R,\Psi^L]=\int_0^\infty dt\langle\Psi^L(t),(\partial_t-\hat{L})\Psi^R(t)\rangle \tag{3.70}$$

when that is independently varied over all pairs of time-dependent state vectors subject to the constraints for each time t,

$$\langle \Psi^L(t), \Psi^R(t)\rangle = 1 \tag{3.71}$$

and

$$\langle \Psi^L(t), \hat{\mathbf{Z}}\Psi^R(t)\rangle = \mathbf{z}(t), \tag{3.72}$$

and also to the boundary conditions

$$|\Psi^R(0)\rangle = P_0, \quad |\Psi^L(\infty)\rangle \equiv 1. \tag{3.73}$$

Proof. As in the static case, we use the representation

$$W[\mathbf{h}] = \ln\left\langle \Omega^L, T\exp\left(\int_0^\infty dt \hat{L}_{\mathbf{h}}(t)\right)\Omega^R\right\rangle, \tag{3.74}$$

where $\hat{L}_{\mathbf{h}}(t) = \hat{L} + \mathbf{h}(t)\cdot\hat{\mathbf{Z}}$ as before but now $\Omega^R = P_0$, $\Omega^L \equiv 1$. In other words,

$$W[\mathbf{h}] = \ln\langle \Omega^L(t), \Omega^R(t)\rangle, \tag{3.75}$$

where

$$|\Omega^R(t)\rangle = T\exp\left(\int_0^t ds \hat{L}_{\mathbf{h}}(s)\right)|\Omega^R\rangle \tag{3.76}$$

and, if $\overline{T}$ denotes ''antitime ordering,''

$$|\Omega^L(t)\rangle = \overline{T}\exp\left(\int_t^\infty ds \hat{L}^\dagger_{\mathbf{h}}(s)\right)|\Omega^L\rangle. \tag{3.77}$$

These trajectories are the solutions, respectively, of the initial-value problem

$$\partial_t|\Omega^R(t)\rangle = \hat{L}_{\mathbf{h}}(t)|\Omega^R(t)\rangle, \quad \Omega^R(0) = P_0 \tag{3.78}$$

and of the final-value problem

$$\partial_t|\Omega^L(t)\rangle = -\hat{L}^\dagger_{\mathbf{h}}(t)|\Omega^L(t)\rangle, \quad \Omega^L(\infty) \equiv 1. \tag{3.79}$$

On the other hand, the variational problem can be solved by the use of Lagrange multipliers for the time-dependent constraints

$$\delta\Big(\Gamma[\Psi^R, \Psi^L] - \int_0^\infty dt[\mathbf{h}(t)\cdot\langle \Psi^L(t), \hat{\mathbf{Z}}\Psi^R(t)\rangle - \lambda(t) \times\langle \Psi^L(t), \Psi^R(t)\rangle]\Big) = 0, \tag{3.80}$$

yielding

$$[\partial_t - \hat{L}_{\mathbf{h}}(t)]|\Psi^R(t)\rangle = -\lambda(t)|\Psi^R(t)\rangle \tag{3.81}$$

and

$$[\partial_t + \hat{L}^\dagger_{\mathbf{h}}(t)]|\Psi^L(t)\rangle = \lambda^*(t)|\Psi^L(t)\rangle. \tag{3.82}$$

In that case we see that

$$|\Omega^R(t)\rangle = \exp\left[\int_0^t ds\lambda(s)\right]|\Psi^R(t)\rangle \tag{3.83}$$

and

$$|\Omega^L(t)\rangle = \exp\left[\int_t^\infty ds\lambda^*(s)\right]|\Psi^L(t)\rangle. \tag{3.84}$$

Substituting these into Eq. (3.75) and using the overlap constraint, we obtain the expression for the cumulant-generating function,

$$W[\mathbf{h}] = \int_0^\infty dt\lambda(t) = \int dt\langle \Psi^L(t), [-\partial_t + \hat{L} + \mathbf{h}(t)\cdot\hat{\mathbf{Z}}]\Psi^R(t)\rangle. \tag{3.85}$$

The last equation was obtained by applying $\Psi^L(t)$ on the left-hand side to Eq. (3.81). Note that, indeed, $\delta W[\mathbf{h}]/\delta\mathbf{h}(t) = \mathbf{z}(t)$ by a simple calculation

$$\begin{aligned}\frac{\delta W[\mathbf{h}]}{\delta\mathbf{h}(t)} &= \mathbf{z}(t) + \int_0^\infty ds\left[\lambda(s)\left\langle \frac{\delta\Psi^L(s)}{\delta\mathbf{h}(t)}, \Psi^R(s)\right\rangle + \lambda(s) \times\left\langle \Psi^L(s), \frac{\delta\Psi^R(s)}{\delta\mathbf{h}(t)}\right\rangle\right] \\ &= \mathbf{z}(t) + \int_0^\infty ds\lambda(s)\frac{\delta}{\delta\mathbf{h}(t)}\langle \Psi^L(s), \Psi^R(s)\rangle \\ &= \mathbf{z}(t).\end{aligned} \tag{3.86}$$

To obtain the first line we used Eqs. (3.81) and (3.82) and to obtain the last line we used again the overlap condition. We therefore get directly from Eq. (3.85) that

$$\begin{aligned}\Gamma[\mathbf{z}] &\equiv \int_0^\infty dt\mathbf{h}(t)\cdot\mathbf{z}(t) - W[\mathbf{h}] \\ &= \int_0^\infty dt\langle \Psi^L(t), (\partial_t - \hat{L})\Psi^R(t)\rangle,\end{aligned} \tag{3.87}$$

as was claimed. □

As remarked above, the quantity

$$\mathcal{L}(t) \equiv \langle \Psi^L(t), (\partial_t - \hat{L})\Psi^R(t)\rangle \tag{3.88}$$

can be taken as a Lagrangian functional in terms of which $\Gamma = \int_{-\infty}^{+\infty} dt\mathcal{L}(t)$, i.e., a time density for the effective action.

On the basis of this theorem a practical Rayleigh-Ritz scheme may be devised. If the variation described in the theorem is carried out within a finite-parameter *Ansatz* such as Eq. (2.50) for Ψ^H, $H = L, R$, then the problem reduces to determining stationary points of a parametric action

$$\Gamma[\overline{\boldsymbol{\alpha}}; \mathbf{h}] \equiv \int_0^\infty dt\{\pi_i(\overline{\boldsymbol{\alpha}}(t))\dot{\overline{\alpha}}_i(t) - \mathcal{H}(\overline{\boldsymbol{\alpha}}(t)) - \mathbf{h}(t)\cdot \times[\mathcal{Z}(\overline{\boldsymbol{\alpha}}(t)) - \mathbf{z}(t)] + \lambda(t)[\mathcal{N}(\overline{\boldsymbol{\alpha}}(t)) - 1]\}, \tag{3.89}$$

which incorporates the constraints by Lagrange multipliers $\mathbf{h}(t), \lambda(t)$. We have defined

$$\mathcal{Z}_\mu(\overline{\boldsymbol{\alpha}}) = \langle \overline{\Psi^L}(\overline{\boldsymbol{\alpha}}), \hat{Z}_\mu \overline{\Psi^R}(\overline{\boldsymbol{\alpha}}) \rangle \tag{3.90}$$

and

$$\mathcal{N}(\overline{\boldsymbol{\alpha}}) = \langle \overline{\Psi^L}(\overline{\boldsymbol{\alpha}}), \overline{\Psi^R}(\overline{\boldsymbol{\alpha}}) \rangle. \tag{3.91}$$

As in the static case, the *Ansatz* Eqs. (2.50) may need to be ''augmented'' to allow for the fact that $\Psi^L(t) \neq 1$ when $\mathbf{h}(t) \neq \mathbf{0}$. We will consider here briefly just the simplest situation, where $\overline{\Psi^H} = \overline{\Psi^H}(\overline{\boldsymbol{\alpha}^H})$, $H = L, R$, with $\overline{\Psi^L}$ given by Eq. (3.35) and the $\overline{\boldsymbol{\alpha}^R}$ parameters taken just to be the corresponding moments $\overline{\mathbf{m}}$, as in Eqs. (3.66)–(3.69). In this case, the parametric action takes the form

$$\Gamma[\overline{\mathbf{m}}, \overline{\boldsymbol{\alpha}^L}; \mathbf{h}] \equiv \int_0^\infty dt [\overline{\boldsymbol{\alpha}^L}(t) \cdot \dot{\overline{\mathbf{m}}}(t) - \overline{\boldsymbol{\alpha}^L}(t) \cdot \overline{\mathbf{V}}(\overline{\mathbf{m}}(t), \mathbf{h}(t)) + \lambda(t)(\overline{\boldsymbol{\alpha}^L}(t) \cdot \overline{\mathbf{m}}(t) - 1)], \tag{3.92}$$

neglecting some terms independent of the parameters being varied. The corresponding Euler-Lagrange equations are

$$\dot{\overline{\mathbf{m}}}(t) = \overline{\mathbf{V}}(\overline{\mathbf{m}}(t), \mathbf{h}(t)) - \lambda(t) \overline{\mathbf{m}}(t), \tag{3.93}$$

$$\dot{\overline{\boldsymbol{\alpha}}}^L(t) + \mathbf{A}(\overline{\mathbf{m}}(t), \mathbf{h}(t)) \overline{\boldsymbol{\alpha}^L}(t) = \lambda(t) \overline{\boldsymbol{\alpha}^L}(t), \tag{3.94}$$

$$\overline{\boldsymbol{\alpha}^L}(t) \cdot \overline{\mathbf{m}}(t) = 1, \tag{3.95}$$

with the boundary conditions at initial and final times

$$\overline{\mathbf{m}}(0) = \overline{\mathbf{m}}_0, \quad \overline{\boldsymbol{\alpha}^L}(+\infty) = (1, \mathbf{0}), \quad \lambda(+\infty) = 0. \tag{3.96}$$

These equations should be compared with their static counterparts Eqs. (3.66) and (3.69). For a specified $\mathbf{h}(t)$, this *two-point boundary value problem* may be solved numerically by standard methods; see [47], Chap. 17. For small $\mathbf{h}(t)$, the best numerical scheme is probably the relaxation method because an exact solution is known for the system at $\mathbf{h}(t) \equiv \mathbf{0}$, corresponding to a solution $\overline{\mathbf{m}}(t)$ of the moment-closure dynamics with specified initial data $\overline{\mathbf{m}}(0) = \overline{\mathbf{m}}_0$ and to $\overline{\boldsymbol{\alpha}^L}(t) \equiv (1, \mathbf{0})$, $\lambda(t) \equiv 0$. This known solution for $\mathbf{h}_0(t) \equiv \mathbf{0}$ may then be input as an initial guess into a relaxation algorithm to find the solution with some small $\mathbf{h}_1(t)$, and, iteratively, a sequence of solutions with $\mathbf{h}_k(t)$ of increasing magnitude constructed. In this way, the fluctuations around the predicted dynamical trajectory $\overline{\mathbf{m}}(t)$ of the moment closure may be explored in the Rayleigh-Ritz method by varying $\mathbf{h}(t)$. The method then yields an approximate effective action

$$\Gamma_*[\mathbf{z}] = \int_0^\infty dt [\overline{\boldsymbol{\alpha}^L_*}(t) \cdot \dot{\overline{\mathbf{m}}}_*(t) - \overline{\boldsymbol{\alpha}^L_*}(t) \cdot \overline{\mathbf{V}}(\overline{\mathbf{m}}_*(t))], \tag{3.97}$$

in which $\overline{\mathbf{m}}_*(t), \overline{\boldsymbol{\alpha}^L_*}(t), \lambda_*(t)$ are solutions of the initial-final value problem Eqs. (3.94) and (3.95), with $\mathbf{h}(t)$ selected so that

$$z_{*\mu}(t) \equiv \overline{\boldsymbol{\alpha}^L_*}(t) \cdot \overline{\mathbf{Z}}_{*\mu}(t) \tag{3.98}$$

equals the specified $z_\mu(t)$. We have defined $\overline{\mathbf{Z}}_{*\mu}(\overline{\mathbf{m}}) = \langle \hat{Z}_\mu \overline{\boldsymbol{\psi}^L} \rangle_{\overline{\mathbf{m}}}$.

Equivalently, the approximate action may be written as

$$\Gamma_*[\mathbf{z}] = \int_0^\infty dt [\mathbf{z}_*(t) \cdot \mathbf{h}(t) - \lambda_*(t)]. \tag{3.99}$$

This can be compared with the approximate effective potential in Proposition 1. If we define the approximate generating functional $W_*[\mathbf{h}] = \int_0^\infty dt \lambda_*(t)$, then it also follows as in Proposition 1 that

$$\frac{\delta W_*[\mathbf{h}]}{\delta h_\mu(t)} = z_{*\mu}(t). \tag{3.100}$$

Thus the approximate effective action from the Rayleigh-Ritz method, Eq. (3.97) or (3.99), retains the Legendre transform structure of the true effective action. It is not hard to derive from this fact that

$$\Gamma_*[\overline{\mathbf{z}_*}] = 0, \quad \frac{\delta \Gamma_*}{\delta \mathbf{z}(t)}[\overline{\mathbf{z}_*}] = \mathbf{0}, \tag{3.101}$$

where $\overline{\mathbf{z}_*}(t) = \langle \mathbf{z} \rangle_{\overline{\mathbf{m}}(t)}$ is the expected value of $\mathbf{z}$ in the PDF *Ansatz* calculated along the trajectory $\overline{\mathbf{m}}(t)$ of the moment closure. Hence the predicted mean history $\overline{\mathbf{z}_*}(t)$ is guaranteed to be a stationary point of $\Gamma_*[\mathbf{z}]$, but not necessarily a minimum point.

Recently, an alternative nonperturbative approximation to the nonequilibrium effective action has been developed by Crisanti and Marconi [48] via a dynamical Hartree approximation. While the two approximation schemes are similar in spirit, there are essential differences between them. We present here no detailed comparison of the two techniques. However, we believe it is a virtue of the present method that it allows an approximation of the effective action and effective potential within *any* PDF *Ansatz* that may be proposed. Furthermore, it makes direct connection with the moment-closure equations that have been traditionally used in nonequilibrium statistical dynamics. We believe that the combination of flexibility to incorporate intuitive guesses and transparency of the physical interpretation should give the present method far-reaching applications.

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APPENDIX: GENERAL VARIATIONAL EQUATIONS

The most general trial *Ansatz* has the form $\Psi^H = \Psi^H(\boldsymbol{\alpha}, \boldsymbol{\alpha}^H)$, $H = L, R$, with $N^L = N + N^R$. In this case, the parametric Hamiltonian is calculated as

$$\mathcal{H}(\boldsymbol{\alpha}, \boldsymbol{\alpha}^R, \boldsymbol{\alpha}^L) = \langle \Psi^L(\boldsymbol{\alpha}, \boldsymbol{\alpha}^L), \hat{L} \Psi^R(\boldsymbol{\alpha}, \boldsymbol{\alpha}^R) \rangle. \tag{A1}$$

Correspondingly, the fixed point conditions are

$$\frac{\partial \mathcal{H}}{\partial \alpha_i^L}(\boldsymbol{\alpha},\boldsymbol{\alpha}^R,\boldsymbol{\alpha}^L)=\langle \psi_i^L(\boldsymbol{\alpha},\boldsymbol{\alpha}^L),\hat{L}\Psi^R(\boldsymbol{\alpha},\boldsymbol{\alpha}^R)\rangle = 0, \tag{A2}$$

$$\frac{\partial \mathcal{H}}{\partial \alpha_i^R}(\boldsymbol{\alpha},\boldsymbol{\alpha}^R,\boldsymbol{\alpha}^L)=\langle \Psi^L(\boldsymbol{\alpha},\boldsymbol{\alpha}^L),\hat{L}\psi_i^R(\boldsymbol{\alpha},\boldsymbol{\alpha}^R)\rangle = 0, \tag{A3}$$

and

$$\frac{\partial \mathcal{H}}{\partial \alpha_i}(\boldsymbol{\alpha},\boldsymbol{\alpha}^R,\boldsymbol{\alpha}^L)=\left\langle \frac{\partial \Psi^L}{\partial \alpha_i}(\boldsymbol{\alpha},\boldsymbol{\alpha}^L),\hat{L}\Psi^R(\boldsymbol{\alpha},\boldsymbol{\alpha}^R)\right\rangle + \left\langle \Psi^L(\boldsymbol{\alpha},\boldsymbol{\alpha}^L),\hat{L}\frac{\partial \Psi^R}{\partial \alpha_i}(\boldsymbol{\alpha},\boldsymbol{\alpha}^R)\right\rangle = 0, \tag{A4}$$

with $\psi_i^H=(\partial\Psi^H/\partial\alpha_i^H)$, $H=R,L$. Within the same *Ansatz*, the parametric evolution equations have the form

$$\{\alpha_i,\alpha_j\}\dot{\alpha}_j+\{\alpha_i,\alpha_j^R\}\dot{\alpha}_j^R+\{\alpha_i,\alpha_j^L\}\dot{\alpha}_j^L=\frac{\partial \mathcal{H}}{\partial \alpha_i}(\boldsymbol{\alpha},\boldsymbol{\alpha}^R,\boldsymbol{\alpha}^L), \tag{A5}$$

$$\{\alpha_i^R,\alpha_j\}\dot{\alpha}_j+\{\alpha_i^R,\alpha_j^L\}\dot{\alpha}_j^L=\frac{\partial \mathcal{H}}{\partial \alpha_i^R}(\boldsymbol{\alpha},\boldsymbol{\alpha}^R,\boldsymbol{\alpha}^L), \tag{A6}$$

and

$$\{\alpha_i^L,\alpha_j\}\dot{\alpha}_j+\{\alpha_i^L,\alpha_j^R\}\dot{\alpha}_j^R=\frac{\partial \mathcal{H}}{\partial \alpha_i^L}(\boldsymbol{\alpha},\boldsymbol{\alpha}^R,\boldsymbol{\alpha}^L). \tag{A7}$$

The most general *Ansatz* of any obvious utility is that given in Eq. (2.33):

$$\Psi^L=1+\sum_{i=1}^N \alpha_i^L\psi_i^L(\boldsymbol{\alpha}),\quad \Psi^R=\Psi^R(\boldsymbol{\alpha}). \tag{A8}$$

This may be thought to correspond to the previous *Ansatz* with $N^R=0$, $N^L=N$, and a linear dependence of Ψ^L on the $\boldsymbol{\alpha}^L$. For this case, the parametric Hamiltonian is

$$\mathcal{H}(\boldsymbol{\alpha},\boldsymbol{\alpha}^L)=\sum_{i=1}^N \alpha_i^L V_i(\boldsymbol{\alpha}), \tag{A9}$$

with $V_i(\boldsymbol{\alpha})=\langle \hat{L}^\dagger\psi_i^L(\boldsymbol{\alpha})\rangle_{\boldsymbol{\alpha}}$ the dynamical vector field in the parameter space, as in Eq. (2.78). The fixed point conditions are simply

$$V_i(\boldsymbol{\alpha})=0 \tag{A10}$$

and

$$\alpha_j^L\frac{\partial V_j}{\partial \alpha_i}(\boldsymbol{\alpha})=0 \tag{A11}$$

for $i=1,\ldots,N$. When the stability matrix at a fixed point $\boldsymbol{\alpha}_*$ of Eq. (A10) is nonsingular, $\det[(\partial\mathbf{V}/\partial\boldsymbol{\alpha})(\boldsymbol{\alpha}_*)]\neq 0$, then the only solution of Eq. (A11) is $\boldsymbol{\alpha}^L=\mathbf{0}$. The parametric evolution equations within the same *Ansatz* are

$$\{\alpha_i,\alpha_j\}\dot{\alpha}_j+\{\alpha_i^L,\alpha_j\}\dot{\alpha}_j=V_i(\boldsymbol{\alpha}) \tag{A12}$$

and

$$\{\alpha_i,\alpha_j^L\}\dot{\alpha}_j^L=\alpha_j^L\frac{\partial V_j}{\partial \alpha_i}(\boldsymbol{\alpha}), \tag{A13}$$

where the Lagrange brackets are

$$\{\alpha_i,\alpha_j\}=\sum_{k=1}^N \alpha_k^L\left[\left\langle \frac{\partial \psi_k^L}{\partial \alpha_i}(\boldsymbol{\alpha}),\psi_j^R(\boldsymbol{\alpha})\right\rangle-\left\langle \frac{\partial \psi_k^L}{\partial \alpha_j}(\boldsymbol{\alpha}),\psi_i^R(\boldsymbol{\alpha})\right\rangle\right] \tag{A14}$$

and

$$\{\alpha_i^L,\alpha_j\}=\langle \psi_i^L(\boldsymbol{\alpha}),\psi_j^R(\boldsymbol{\alpha})\rangle, \tag{A15}$$

with now $\psi_i^R\equiv\partial\Psi^R/\partial\alpha_i$. Equation (A13) clearly has the constant solution $\boldsymbol{\alpha}^L(t)\equiv\mathbf{0}$. Equation (A12) then has the same form as Eq. (2.77). It is also identical to Eq. (2.11) in the work of Bayly [28], but here derived by the variational method.

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