Quantum fields out of thermal equilibrium

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The isoentropic, but energy-nonconserving, time evolution of mixed quantum states is studied in quantum mechanics and quantum field theory. A variational principle, which gives the Liouville–von Neumann equation, is implemented approximately by making a Gaussian *Ansatz* for the density matrix. The dynamical equations governing the parameters that define the *Ansatz* satisfy equations variously analogous to the Schrödinger equation and to mechanical problems. Interesting nonequilibrium evolution is found in special cases, as, for example, when the analog Schrödinger equation gives rise to reflectionless transmission. For field theory in an external, time-dependent metric we obtain equations that were previously derived in the many-field (spherical-model) limit.

I. INTRODUCTION

High-temperature restoration of spontaneously broken field-theoretic symmetries[1] and the calculational method for describing this phenomenon[2] have become widely accepted. Moreover, temperature-induced symmetry-changing phase transitions are crucial ingredients in various cosmological scenarios, e.g., the "slow-rollover" transition effecting the inflationary early Universe,[3] and the "unification" phase transition which may have been accompanied by the appearance of strings/vortices that may have seeded galaxy formation.[4] Establishing the validity of such scenarios requires examining the dynamical evolution of the cosmos in time—before, during, and after the transition—periods when the system was obviously changing and therefore not in thermal equilibrium. However, the methods[2] for studying quantum field theory at finite temperature concern systems in equilibrium, with no time variation. (The "imaginary time" that occurs in some of the formalisms is a fictitious "time" related to temperature—there is no actual time variation.) In the absence of anything better, the static but temperature-dependent effective potential of Ref. 2 has been taken as the potential energy of a dynamical Lagrangian, which is then used to determine time evolution, once the temperature is also allowed to vary in time, according to some physically plausible rule. In this paper we attempt a more firmly based method.

More generally, let us observe that the formulation of quantum field theory in terms of causal Green's functions, which these days comprises a popular approach to the subject, is not especially suited to time-dependent problems that require an initial condition for specific solution. Green's functions contain all the information needed for determining transition rates, S matrices, etc., of systems in equilibrium, where initial data are superfluous. However, following the system's time evolution from a definite initial configuration is more efficiently accomplished in a Schrödinger picture description, where the initial data consist of specifying a pure or mixed state.[5]

II. SCHRÖDINGER PICTURE

The field-theoretic Schrödinger picture is well known,[6] at least for bosonic fields, but not as widely used as the Green's-function method. The reason is that perturbative divergences can be isolated and renormalized more conveniently within the latter framework. However, by now we have become experienced in dealing with field-theoretical infinities, so their occurrence is not an obstacle. Indeed, recent results establish renormalizability of the Schrödinger picture, both for static[7] and time-dependent problems.[8]

Let us review the functional Schrödinger picture for quantum field theory, which we shall employ in this paper. The formalism is a generalization from ordinary quantum mechanics to the infinite number of degrees of freedom that comprise a field. It offers, therefore, the possibility of using physical/mathematical intuition gained in quantum mechanics to analyze approximately the field-theoretic problem.

In the field-theoretic Schrödinger picture, states are described by wave functionals $\Psi(\varphi)$ of a c-number field $\varphi(\mathbf{r})$ at fixed time. The inner product is defined by functional integration:

$$\langle \Psi_1 \mid \Psi_2 \rangle = \int \mathcal{D}\varphi \, \Psi_1^*(\varphi)\Psi_2(\varphi) \, , \tag{2.1}$$

while operators are represented by functional kernels:

$$\mathcal{O} \mid \Psi \rangle \leftrightarrow \int D\tilde{\varphi} \, \mathcal{O}(\varphi,\tilde{\varphi})\Psi(\tilde{\varphi}) \, . \tag{2.2}$$

For the canonical field operator at fixed time, $\Phi(\mathbf{r})$ (the time argument is common to all operators in the Schrödinger picture, so it is suppressed), we use a diago-

nal kernel $\Phi(\mathbf{r})\leftrightarrow\varphi(\mathbf{r})\delta(\varphi-\tilde{\varphi})$; the canonical commutation relations determine the canonical momentum kernel as $\Pi(\mathbf{r})\leftrightarrow(1/i)[\delta/\delta\varphi(\mathbf{r})]\delta(\varphi-\tilde{\varphi})$; both kernels involve a functional δ function. Evidently Φ acts by multiplication on functionals of φ, while Π acts by functional differentiation. In this way, the action of any operator constructed from Π and Φ is

$$\mathcal{O}(\Pi,\Phi)\,|\,\Psi\rangle\leftrightarrow\mathcal{O}\left[\frac{1}{i}\frac{\delta}{\delta\varphi},\varphi\right]\Psi(\varphi)\ . \tag{2.3}$$

The fundamental dynamical equation is the time-dependent Schrödinger equation for a time-dependent functional $|\,\Psi;t\,\rangle\leftrightarrow\Psi(\varphi;t)$. The equation takes definite form, once a Hamiltonian operator $H(\Pi,\Phi)$ is specified:

$$i\frac{\partial}{\partial t}\Psi(\varphi;t)=H\left[\frac{1}{i}\frac{\delta}{\delta\varphi},\varphi\right]\Psi(\varphi;t)\ . \tag{2.4}$$

For time-independent Hamiltonians, the usual separation of variables leads to a functional eigenvalue problem:

$$\Psi(\varphi;t)=e^{-iEt}\Psi_E(\varphi)\ , \tag{2.5}$$

$$H\left[\frac{1}{i}\frac{\delta}{\delta\varphi},\varphi\right]\Psi_E(\varphi)=E\Psi_E(\varphi)\ . \tag{2.6}$$

In particular for quadratic Hamiltonians

$$H=\tfrac{1}{2}\int(\Pi^2+\Phi h\Phi) \tag{2.7}$$

the ground state (vacuum) is a Gaussian functional,

$$\Psi_0(\varphi)=\det{}^{1/4}\omega\exp\left[-\tfrac{1}{2}\int\varphi\omega\varphi\right] \tag{2.8a}$$

with covariance ω determined by the "first quantized" Hamiltonian h,

$$\omega^2=h \tag{2.8b}$$

and vacuum energy

$$E_0=\tfrac{1}{2}\mathrm{tr}\omega\ . \tag{2.9}$$

[Throughout, a self-evident functional/matrix notation is used: ω and h are kernels, $\int\varphi\omega\varphi\equiv\int d\mathbf{r}\,d\mathbf{r}'\varphi(\mathbf{r})\omega(\mathbf{r},\mathbf{r}')\varphi(\mathbf{r}')$, $\mathrm{tr}\omega\equiv\int d\mathbf{r}\,\omega(\mathbf{r},\mathbf{r})$, and the determinant in (2.8a) is functional.]

Equation (2.8) represents the conventional Fock vacuum in the Schrödinger picture. Higher excited (multiparticle) Fock states are represented by polynomials of φ multiplying the vacuum Gaussian (2.8a); they are orthonormalized if taken in linear combinations corresponding to functional Hermite polynomials.

For translationally invariant theories, kernels depend only on differences of coordinates and diagonalization may be achieved by Fourier transformation:

$$h(\mathbf{r},\mathbf{r}')=\int_{\mathrm{p}}e^{-i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}h(\mathbf{p})\ ,$$

$$\omega(\mathbf{r},\mathbf{r}')=\int_{\mathrm{p}}e^{-i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}\omega(\mathbf{p})\ ,$$

and (2.8b) enforces $\omega^2(\mathbf{p})=h(\mathbf{p})$ [$\int_{\mathrm{p}}$ in d=dimensional space denotes $\int d^dp/(2\pi)^d$.] As a consequence our free-field formulas are superpositions over all $\mathbf{p}$ of corresponding quantum-mechanical formulas for harmonic oscillators with frequencies $\omega(\mathbf{p})$, which for a conventional bosonic free field theory, describing particles with mass m, is $\omega(\mathbf{p})=\sqrt{\mathbf{p}^2+m^2}$.

In the translationally invariant case, there are infrared divergences due to the infinite volume V of space, e.g., $\frac{1}{2}\mathrm{tr}\omega=\frac{1}{2}V\int_{\mathrm{p}}\omega(\mathbf{p})$. These we shall ignore. Also there are ultraviolet divergences when the integral over momenta diverges. For the free case, these are trivially renormalized in the energy formula by normal ordering. The fact that the normalization factor of (2.8a) may also diverge,

$$\det{}^{1/4}\omega=\exp(\tfrac{1}{4}\mathrm{tr}\ln\omega)=\exp\left[\frac{V}{4}\int_{\mathrm{p}}\ln\omega(\mathbf{p})\right]\ ,$$

is ignored, because the norm disappears from all matrix elements—it is chosen precisely so that will be the case.[9] More intricate questions of ultraviolet finiteness will be addressed as they arise in our discussion of interacting field theories.

The analogous Schrödinger picture for fermion theories has also been recently developed,[10] but we shall not need it for the models analyzed in this paper.

III. TIME EVOLUTION

When the initial state of a system is a pure state, described by a definite wave functional Ψ, the time-dependent Schrödinger equation (2.4) determines uniquely subsequent evolution.

However, for the collective phenomena that we study, initially the system is likely to be in a mixed state, described by a (functional) density matrix;

$$\rho(\varphi_1,\varphi_2)=\sum_n p_n\Psi_n(\varphi_1)\Psi_n^*(\varphi_2)\ , \tag{3.1a}$$

$$\mathrm{tr}\rho=\int\mathcal{D}\varphi\,\rho(\varphi,\varphi)=1\ . \tag{3.1b}$$

Here $\{\Psi_n\}$ is a complete set of wave functionals and p_n is the probability that the system is in state n. Average values of physical quantities described by operators $\mathcal{O}$, which in turn are represented by kernels $\mathcal{O}(\varphi,\tilde{\varphi})$, are determined by the density matrix

$$\langle\mathcal{O}\rangle=\mathrm{tr}\rho\mathcal{O}=\int\mathcal{D}\varphi\,\mathcal{D}\tilde{\varphi}\,\rho(\tilde{\varphi},\varphi)\mathcal{O}(\varphi,\tilde{\varphi})\ . \tag{3.2}$$

The time development of these averages is determined, once the time dependence of the density matrix is known.

For the equilibrium problems considered in Ref. 2, dynamics is time-translational invariant and energy is conserved. The complete set of wave functionals in (3.1a) comprises the energy eigenstates with eigenvalues E_n and the occupation probabilities are given by the canonical Boltzmann distribution: $p_n=e^{-\beta E_n}/\sum_{n'}e^{-\beta E_{n'}}$ where $1/\beta$ is temperature times Boltzmann's constant k. The initial density matrix corresponds to the canonical ensemble and its time evolution is trivial: it remains constant in time because the p_n's are constant and the time dependence in energy eigenfunctions is a phase that disappears from $\Psi\Psi^*$. In this static situation the Green's-function methods of Ref. 2 become applicable. Calculations become similar to those at zero temperature,

but in space-time, once the analogy between β and (imaginary) time is made.

More generally however, the time evolution is nontrivial. The p_n's need not be Boltzmann factors, and they can change in time. Also the Ψ_n's need not be energy eigenstates; they may have complicated time dependence which we shall assume to be determined by the time-dependent Schrödinger equation, with a time-dependent Hamiltonian. Evidently, a differential equation summarizing this time variation is

$$\frac{d\rho}{dt}=i[\rho,H]+\frac{\partial\rho}{\partial t} . \tag{3.3}$$

The commutator on the right-hand side arises from the time variation of the wave functions, assumed governed by the Hamiltonian H. (Note that the sign is opposite from the Heisenberg equation of motion.) The second term, which by definition is

$$\frac{\partial\rho}{\partial t}\equiv\sum_n\frac{dp_n}{dt}\Psi_n\Psi_n^* \tag{3.4}$$

reflects the possible time dependence of the occupation probabilities.

To solve (3.3), and thereby to determine the time evolution of ρ, we need three pieces of information. In order that (3.3) be a specific equation, the form of H must be given, and also a model for dp_n/dt must be adopted so that something can be said about $\partial\rho/\partial t$. Once (3.3) is well posed, an initial condition is required for a specific solution.

To gain further insight into (3.3), let us relate ρ and its time derivative to a microscopic description in terms of a pure state for a larger, closed system. This discussion will be carried out in the language and formalism of quantum mechanics; the functional Schrödinger picture allows applying the same ideas to quantum field theory. The density matrix $\rho(\mathbf{x}_1,\mathbf{x}_2)$ arises when we consider a system in a pure state described by two sets of variables $\{\mathbf{P},\mathbf{X}\}$ and $\{\mathbf{p},\mathbf{x}\}$ and ignore the former:

$$\rho(\mathbf{x}_1,\mathbf{x}_2)=\int d\mathbf{X}\,\Psi(\mathbf{X},\mathbf{x}_1)\Psi^*(\mathbf{X},\mathbf{x}_2) , \tag{3.5a}$$

$$\mathrm{tr}\rho=\int d\mathbf{x}\,\rho(\mathbf{x},\mathbf{x})=\int d\mathbf{X}\,d\mathbf{x}\,|\,\Psi(\mathbf{X},\mathbf{x})\,|^2=1 . \tag{3.5b}$$

The Hamiltonian for the entire system is taken as

$$\mathbb{H}(\mathbf{P},\mathbf{X};\mathbf{p},\mathbf{x})=\frac{\mathbf{P}^2}{2M}+\frac{\mathbf{p}^2}{2m}+V(\mathbf{X},\mathbf{x}) . \tag{3.6}$$

The time-dependent Schrödinger equation gives a differential equation satisfied by ρ:

$$\begin{aligned}i\frac{d}{dt}\rho=&\int d\mathbf{X}\left[\left[-\frac{\nabla_{\mathbf{X}}^2}{2M}\Psi(\mathbf{X},\mathbf{x}_1)\right]\Psi^*(\mathbf{X},\mathbf{x}_2)+\Psi(\mathbf{X},\mathbf{x}_1)\left[\frac{\nabla_{\mathbf{X}}^2}{2M}\Psi^*(\mathbf{X},\mathbf{x}_2)\right]\right]\\&+\int d\mathbf{X}\left[\left[-\frac{\nabla_{\mathbf{x}_1}^2}{2m}\Psi(\mathbf{X},\mathbf{x}_1)\right]\Psi^*(\mathbf{X},\mathbf{x}_2)+\Psi(\mathbf{X},\mathbf{x}_1)\left[\frac{\nabla_{\mathbf{x}_2}^2}{2m}\Psi^*(\mathbf{X},\mathbf{x}_2)\right]\right]\\&+\int d\mathbf{X}[V(\mathbf{X},\mathbf{x}_1)-V(\mathbf{X},\mathbf{x}_2)]\Psi(\mathbf{X},\mathbf{x}_1)\Psi^*(\mathbf{X},\mathbf{x}_2) .\end{aligned} \tag{3.7a}$$

The first term on the right-hand side of (3.7a) vanishes, because it receives contributions only from the surface boundary of $\mathbf{X}$ space:

$$\begin{aligned}&\int d\mathbf{X}\left[\left[-\frac{\nabla_{\mathbf{X}}^2}{2M}\Psi(\mathbf{X},\mathbf{x}_1)\right]\Psi^*(\mathbf{X},\mathbf{x}_2)+\Psi(\mathbf{X},\mathbf{x}_1)\left[\frac{\nabla_{\mathbf{X}}^2}{2M}\Psi^*(\mathbf{X},\mathbf{x}_2)\right]\right]\\&\qquad=\frac{1}{2M}\int d\mathbf{X}\,\nabla_{\mathbf{X}}\cdot[\Psi(\mathbf{X},\mathbf{x}_1)\nabla_{\mathbf{X}}\Psi^*(\mathbf{X},\mathbf{x}_2)-\nabla_{\mathbf{X}}\Psi(\mathbf{X},\mathbf{x}_1)\Psi^*(\mathbf{X},\mathbf{x}_2)] .\end{aligned}$$

The second and third terms in (3.7a) may be rewritten as

$$\frac{d}{dt}\rho=i[\rho,H]+\int d\mathbf{X}\{[V(\mathbf{X},\mathbf{x}_1)-V(\mathbf{x}_1)]-[V(\mathbf{X},\mathbf{x}_2)-V(\mathbf{x}_2)]\}\Psi(\mathbf{X},\mathbf{x}_1)\Psi^*(\mathbf{X},\mathbf{x}_2) . \tag{3.7b}$$

Here

$$H=\frac{\mathbf{p}^2}{2m}+V(\mathbf{x}) \tag{3.7c}$$

and $V(\mathbf{x}_i)$ is some suitable average of $V(\mathbf{X},\mathbf{x}_i)$ over the complete wave functions $\Psi(\mathbf{X},\mathbf{x}_1)\Psi^*(\mathbf{X},\mathbf{x}_2)$.

Comparison of (3.3) with (3.7) shows that the former follows from the microscopic theory of the latter, provided there exists an average potential $V(\mathbf{x})$ which permits (i) using a Hamiltonian exclusively for the $\mathbf{p},\mathbf{x}$ variables and (ii) replacing the last term in (3.7b) by the last term of (3.3). Let us observe that $V(\mathbf{x})$ will in general be time dependent since $\Psi(\mathbf{X},\mathbf{x})$ is. Hence the effective Hamiltonian (3.7c) describes an isolated system in the sense that it makes reference only to the relevant variables $\mathbf{p}$ and $\mathbf{x}$, but the effect of the environment is still felt through the time dependence of H. Moreover, further effects of the

environment are coded in the last term of (3.3), which represents the last term of (3.7b).

Presumably for a specific many-body system, the physical situation may be carefully examined, at least in principle, so that (3.3) can be justified on the basis of (3.7), and appropriate expressions for H and $\partial\rho/\partial t$ can be derived by this so-called *coarse-graining* procedure. In the cosmological application that we have in mind, such analysis does not appear feasible since we do not have an adequate description of the physical "environment" in which our cosmos evolved through its various phase transitions.

Therefore, we shall *assume* the validity of (3.3), with some time-dependent Hamiltonian H, and also we shall drop the last term, i.e., we take the probabilities p_n not to change in time. This is tantamount to the assumption that entropy S stays constant:

$$S \equiv -k \, \mathrm{tr}\rho \ln\rho = -k \sum_n p_n \ln p_n \ . \tag{3.8}$$

While we are led to our assumption by necessity (we do not know how the probabilities vary in time) the end result describes physically plausible processes in which energy is not conserved, but entropy is. Precisely such transitions are thought to take place in the early Universe. In the language of statistical mechanics we are speaking of *adiabatic* processes—closely related to but not identical with the *quantum adiabatic theorem* discussed later.

The approximations that we employ are realized when interactions between the $\{\mathbf{P},\mathbf{X}\}$ and $\{\mathbf{p},\mathbf{x}\}$ systems may be ignored in the complete Hamiltonian (3.6), so that $\mathbb{H}$ is approximated by

$$\mathbb{H} \approx \frac{\mathbf{P}^2}{2M} + U(\mathbf{X}) + \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \ , \tag{3.9}$$

$U(\mathbf{X})+V(\mathbf{x})$ in formula (3.9) should be viewed as an approximate and average replacement for the exact $V(\mathbf{X},\mathbf{x})$; hence $U(\mathbf{X})+V(\mathbf{x})$ may carry a time dependence that represents the residual influence of one system on the other. With (3.9) the last term in (3.7b) vanishes.

When the Hamiltonian is a sum as in (3.9), the initial wave function $\Psi(\mathbf{X},\mathbf{x})$ is a superposition of factorized orthonormalized wave functions for each subsystem:

$$\Psi(\mathbf{X},\mathbf{x}) = \sum_n c_n \Theta_n(\mathbf{X}) \Psi_n(\mathbf{x}) \ . \tag{3.10}$$

Here c_n are constant and $\mathbf{P}^2/2M + U(\mathbf{X})$ governs the time evolution of $\Theta_n(\mathbf{X})$, while $\mathbf{p}^2/2m + V(\mathbf{x})$ governs $\Psi_n(\mathbf{x})$. Thus the density matrix (3.5a) becomes

$$\rho(\mathbf{x}_1,\mathbf{x}_2) = \sum_n p_n \Psi_n(\mathbf{x}_1) \Psi_n^*(\mathbf{x}_2) \tag{3.11a}$$

with constant probabilities

$$p_n = |\, c_n \,|^2 \ . \tag{3.11b}$$

To summarize, in the absence of the last term in (3.3), we need to solve the quantum Liouville (–von Neumann) equation

$$\frac{d\rho}{dt} = i[\rho, H] \tag{3.12}$$

with a time-dependent Hamiltonian. Because we are interested in time evolution through a phase transition, we shall take the time dependence in H to reside in the quadratic term—most often in the mass term squared for a field theory, in the square of the harmonic frequency for quantum-mechanical examples. We shall allow this quantity to vary in time in a prescribed fashion, for example, passing from one positive value to another, or from positive (stable) to negative (unstable) values. We view this time dependence as occurring in an interval $t_i < t < t_f$. For times earlier than t_i, the Hamiltonian is assumed constant, and the initial data for the Liouville equation will always be specified in this static regime, where we shall take ρ to be given by $\rho_i(\beta_i)$, the initial Hamiltonian's Boltzmann distribution density matrix at some initial β_i, or an approximation thereto. The solution to (3.12) is then examined in the late period $t > t_f$, where the Hamiltonian is again static but perhaps with different parameters. We wish to determine whether at late times ρ is static or not, and if static, whether it is given by a Boltzmann distribution but perhaps at some other temperature. (In some examples $t_{i,f}$ may be $\mp\infty$. Also for field theory in de Sitter space we shall discuss initial data more generally.)

The terminology we shall use is as follows: a time-independent density matrix is said to describe a system in *equilibrium;* if its form corresponds to a Boltzmann distribution, we say that the system is in *thermal equilibrium,* but nonthermal equilibria are also possible; when the density matrix is time dependent, we say that the system is *out of equilibrium.*

Therefore we are considering the problem of a system in thermal equilibrium, which becomes disturbed by the environment so that Hamiltonian parameters change. We wish to know whether there is a return to equilibrium, in particular to thermal equilibrium after the disturbance ceases, and also we wish to follow the behavior of various interesting quantities through the disturbance. Our methods allow considering an arbitrary initial distribution, not necessarily in thermal equilibrium, and we could calculate the time evolution in this more general situation. However, we do not examine such problems here.

IV. VARIATIONAL PRINCIPLES

Our goal is now settled: obtain solutions to the Liouville equation (3.12) with a canonical distribution density matrix as initial condition. But the method for achieving this goal must still be developed because (3.12) cannot be integrated directly, except for linear (noninteracting) problems described by a quadratic Hamiltonian. To this end we use a variational principle, first stated in the many-body context by Balian and Vénéroni,[11] which yields, under arbitrary variation, the Liouville equation. An approximate application of this principle with a restricted variational *Ansatz,* in the Rayleigh-Ritz manner, leads to approximate but tractable equations for the density matrix that may be integrated.

The variational principle results in a time-dependent equation; such variational methods are not as familiar as

the static variational principles appropriate to time-independent equations. Therefore, first we survey the subject of time-dependent variational principles.

A. Generalities

Already in classical mechanics, one encounters time-independent and time-dependent variational principles for the relevant dynamical equations of mechanics. Static solutions stationarize the Hamiltonian (energy) as a function of p and q; this is seen from the Hamiltonian equations

$$\dot{q}=0=\frac{\partial H(p,q)}{\partial p}, \quad -\dot{p}=0=\frac{\partial H(p,q)}{\partial q} . \tag{4.1}$$

The full time-dependent Newtonian equations are derived by Hamilton's variational principle, which requires stationarizing the classical action $I_{\rm cl}$, the time integral of the Lagrangian L, and a functional of $q(t)$:

$$I_{\rm cl}=\int dt\, L, \quad \frac{\delta I_{\rm cl}(q)}{\delta q(t)}=0 . \tag{4.2}$$

Notice that the static variations require no boundary conditions, while the time-dependent ones must vanish at the end points of the time integral that defines the action.

Both the static and the time-dependent variation principles of classical physics have their quantum analogs. The former translates into the requirement that expectation values of the Hamiltonian be stationary; this yields the time-independent Schrödinger equation. The latter's analog is Dirac's little-known time-dependent variational principle, which results in the time-dependent Schrödinger equation.[12]

The parallel to classical physics is even closer when generating functionals are used. (We discuss the field-theory case.) On the one hand, generating functionals, the field theory analogs of the Gibbs free energy, generate (single-particle-irreducible) Green's functions. On the other hand, they implement the above two quantum variational principles in two steps: in the first step, the variation is carried out subject to a constraint, in the second the constraint is removed.

Thus we define the *effective energy* $E(\phi)$ as the stationary expectation of the Hamiltonian, in a normalized state $|\Psi\rangle$, subject to the constraint that the expectation of the quantum field operator $\Phi(\mathbf{r})$ is a prescribed static function $\phi(\mathbf{r})$:

$$E(\phi)=\text{stationary value of } \langle\Psi|H|\Psi\rangle , \tag{4.3a}$$

$$\langle\Psi|\Phi(\mathbf{r})|\Psi\rangle=\phi(\mathbf{r}) , \tag{4.3b}$$

$$\langle\Psi|\Psi\rangle=1 . \tag{4.3c}$$

Then removing the constraint (4.3b) requires solving

$$\frac{\delta E(\phi)}{\delta\phi(\mathbf{r})}=0 \tag{4.4}$$

and this point also defines the physical theory.[13] (When ϕ is further restricted to be $\mathbf{r}$ independent, the effective energy functional becomes the *effective potential,* times the volume of space.[14]) The effective energy generates Green's functions at zero energy, the effective potential generates them at zero energy and momentum.

The time-dependent generalization of the above implements Dirac's variational principle in two steps.[15] First, we define the *effective action* Γ as a stationary value subject to the constraint that a matrix element of the quantum field $\Phi(\mathbf{r})$ is held fixed at a prescribed function of space and time $\phi(t,\mathbf{r})$:

$$\Gamma(\phi)=\text{stationary value of}$$

$$\int dt\,\langle\Psi_-;t\,|\,i\frac{d}{dt}-H\,|\,\Psi_+;t\rangle , \tag{4.5a}$$

$$\langle\Psi_-;t\,|\,\Phi(\mathbf{r})\,|\,\Psi_+;t\rangle=\phi(t,\mathbf{r}) , \tag{4.5b}$$

$$\langle\Psi_-;t\,|\,\Psi_+;t\rangle=1 . \tag{4.5c}$$

As befits a time-dependent variation principle, one also needs boundary conditions. Analogously to the classical case, these are set at the end points of the time integral, here $\pm\infty$. One demands that the time-dependent states $|\Psi_\pm;t\rangle$ tend to the ground state $|0\rangle$ of H, and the variations vanish there:

$$\lim_{t\to\mp\infty}|\Psi_\pm;t\rangle=|0\rangle . \tag{4.6}$$

Finally, to regain the physical theory, the constraint is removed,

$$\frac{\delta\Gamma(\phi)}{\delta\phi(t,\mathbf{r})}=0 \tag{4.7}$$

and at this point Γ generates Green's functions, with arbitrary energy or momentum. [When Γ is evaluated on a time-independent function, $\phi(t,\mathbf{r})\to\phi(\mathbf{r})$, the result is the (negative) effective energy, used above, multiplied by the (infinite) time interval.]

B. Liouville equation

A variational principle that gives the Liouville equation (3.12) makes use of a Lagrange multiplier kernel. Consider the actionlike quantity[11]

$$I=-\int dt\,\mathrm{tr}\rho\left[\frac{d}{dt}\Lambda+i[H,A]\right]-\mathrm{tr}(\rho\Lambda)\,|_{t=t_i}$$

$$=-\int dt\left\langle\frac{d}{dt}\Lambda+i[H,\Lambda]\right\rangle-\langle\Lambda\rangle\,|_{t=t_i} . \tag{4.8}$$

Here Λ, ρ, and H are time-dependent kernels and the trace is over these kernels, while the time integral ranges from an initial time t_i to a final time t_f. The Lagrangian multiplier kernel is Λ, whose variation gives

$$\delta_\Lambda I=\int dt\,\mathrm{tr}\left[\frac{d}{dt}\rho+i[H,\rho]\right]\delta\Lambda-\mathrm{tr}(\rho\delta\Lambda)\,|_{t=t_f} . \tag{4.9}$$

Similarly, variation of ρ leaves

$$\delta_\rho I = -\int dt\ \mathrm{tr}\left[\frac{d}{dt}\Lambda + i[H,\Lambda]\right]\delta\rho - \mathrm{tr}(\Lambda\delta\rho)\,|_{t=t_i}\ . \tag{4.10}$$

Next we impose temporal boundary conditions to eliminate the last terms in (4.9) and (4.10). We shall require that

$$\Lambda\,|_{t=t_f} = \mathbb{1}\ ; \tag{4.11}$$

i.e., the Lagrange multiplier becomes the identity kernel $\delta(\varphi_1-\varphi_2)$ at the final time. Consequently, $\delta\Lambda$ must vanish there. At initial time t_i, the boundary condition is set on the density matrix, and according to our program $\rho\,|_{t=t_i}$ will be given by $\rho_i(\beta_i)$, the canonical Boltzmann distribution density matrix appropriate to $H\,|_{t=t_i}$, with temperature β_i, or an approximation thereto. Hence $\delta\rho$ vanishes at initial time.

Demanding that I be stationary against both variations gives, with the help of our boundary conditions, the Liouville equation (3.12) for ρ, and also for Λ. Moreover, the boundary condition (4.11) on Λ selects the static solution $\Lambda=\mathbb{1}$ for all time. [Note that $\rho_i(\beta_i)$ does not provide a static solution to the Liouville equation for all time, except when H is time independent.] With this development, Λ disappears from the discussion,[16] and we are left with a variational formulation for the Liouville equation, which will be implemented approximately in the subsequent.

Notice that the Liouville equation implies that $\mathrm{tr}\rho$ is constant. Hence proper normalization of ρ is assured, provided $\rho_i(t_i)$ is normalized. It is not necessary to enforce normalization during the variation, though one can do so by adding to (4.8) another Lagrange multiplier times $(\mathrm{tr}\rho-1)$. Upon redefining the phase of Λ, this addition may be removed, leaving (4.8) once again.

Let us further observe that the specific condition (4.11) (viz., Λ becomes the identity rather than some other fixed kernel) is also needed to make contact with the effective action formalism. This is seen by implementing the above variational principle in two steps, where at the first step subsidiary conditions are imposed; compare (4.3b) and (4.3c), (4.5b) and (4.5c):

$$\mathrm{tr}\rho\tfrac{1}{2}\{\Lambda,\Phi\} = \langle\, \tfrac{1}{2}\{\Lambda,\Phi\}\,\rangle = \phi(t,\mathbf{r})\ , \tag{4.12a}$$

$$\mathrm{tr}\rho\Lambda = \langle\,\Lambda\,\rangle = 1\ . \tag{4.12b}$$

(The first of the two above equations reads explicitly

$$\tfrac{1}{2}\int \mathcal{D}\varphi_1\mathcal{D}\varphi_2\{\Lambda(\varphi_1,\varphi_2)\rho(\varphi_2,\varphi_1)[\varphi_1(\mathbf{r})+\varphi_2(\mathbf{r})]\} = \phi(t,\mathbf{r})\ ,$$

with the time dependence arising because Λ and ρ are time-dependent kernels.) We shall show that the *nonequilibrium effective action* $\Gamma(\phi)$, defined as the stationary value of I in (4.8),

$$\Gamma(\phi) = \text{stationary value of } \int dt\ \mathrm{tr}\rho\left[-\frac{d\Lambda}{dt} - i[H,\Lambda]\right]$$
$$= \text{stationary value of } \int dt\left\langle -\frac{d}{dt}\Lambda - i[H,\Lambda]\right\rangle\ , \tag{4.13}$$

subject to the above boundary conditions and constraints, is also the single-particle-irreducible generating functional, obtained as the usual Legendre transform of the connected generating functional, the field theory analog of the Helmholtz free energy. The argument parallels the derivation of the analogous zero-temperature results (4.5)–(4.7) (Ref. 15).

We begin by introducing Lagrange multipliers $J(x)$ and $w(t)$, which ensure the constraints (4.12a) and (4.12b), respectively; that is, we consider the quantity

$$I' = I + \int dx\ J(x)\mathrm{tr}\rho\tfrac{1}{2}\{\Lambda,\Phi\} - \int dt\ w(t)tr\rho\Lambda\ . \tag{4.14}$$

(The collection of variables $t,\mathbf{r}$ is denoted by x.) Variation with respect to Λ and ρ produces, respectively, the equations

$$\frac{d\rho}{dt} + i[H,\rho] + \int d\mathbf{r}\,J(x)\tfrac{1}{2}\{\rho,\Phi\} - w(t)\rho = 0\ , \tag{4.15a}$$

$$\frac{d\Lambda}{dt} + i[H,\Lambda] - \int d\mathbf{r}\,J(x)\tfrac{1}{2}\{\Lambda,\Phi\} + w(t)\Lambda = 0\ . \tag{4.15b}$$

The last elements in both equations may be removed by a redefinition:

$$\tilde{\rho} = \rho\exp\left[-\int_{-\infty}^{t} dt' w(t')\right]\ , \tag{4.16a}$$

$$\tilde{\Lambda} = \Lambda\exp\left[-\int_{t}^{\infty} dt' w(t')\right]\ , \tag{4.16b}$$

while the commutator may be eliminated by introducing the evolution operator U, which satisfies

$$i\frac{\partial}{\partial t}U(t) = HU(t) \tag{4.17}$$

subject to the boundary condition that $U(-\infty)$ is the identity

$$\tilde{\rho} = U\rho_H U^{-1}\ , \tag{4.18a}$$

$$\tilde{\Lambda} = U\Lambda_H U^{-1}\ . \tag{4.18b}$$

The transformation (4.18) is recognized as passage to the Heisenberg picture relative to the Hamiltonian H, where states are still time dependent due to the source J. Evidently, ρ_H obeys the same boundary condition as ρ at $t=-\infty$, similarly Λ_H coincides with Λ at $t=\infty$ *provided the latter becomes the identity.* The equations satisfied by ρ_H and Λ_H are

$$\frac{d\rho_H}{dt} = -\int d\mathbf{r}\,J(x)\tfrac{1}{2}\{\rho_H,\Phi_H\}\ , \tag{4.19a}$$

$$\frac{d\Lambda_H}{dt} = \int d\mathbf{r}\,J(x)\tfrac{1}{2}\{\Lambda_H,\Phi_H\}\ , \tag{4.19b}$$

where $\Phi_H(x)$ is the operator $\Phi(\mathbf{r})$ in the Heisenberg picture $\Phi_H(x) = U^{-1}(t)\Phi(\mathbf{r})U(t)$. The solution to these is

$$\rho_H = T\exp\left[-\tfrac{1}{2}\int_{-\infty}^{t} dx\, J(x)\Phi_H(x)\right]\rho_i(\beta_i) \times T\exp\left[-\tfrac{1}{2}\int_{-\infty}^{t} dx\, J(x)\Phi_H(x)\right], \tag{4.20a}$$

$$\Lambda_H = T\exp\left[-\int_{t}^{\infty} dx\, J(x)\Phi_H(x)\right]. \tag{4.20b}$$

Now we can prove our statement. We define the Helmholtz free energy $W(J)$ by a Heisenberg picture expression, which evidently generates connected Green's functions:

$$e^{-W(J)} = \mathrm{tr}\left[\rho_i(\beta_i) T\exp\left[-\int d^4x\, J(x)\Phi_H(x)\right]\right] = \left\langle T\exp\left[-\int d^4x\, J(x)\Phi_H(x)\right]\right\rangle . \tag{4.21a}$$

As seen from (4.20), the right-hand side is also $\mathrm{tr}\rho_H\Lambda_H$, which may be evaluated with the help of (4.12), (4.16), and (4.18). Thus, we establish that $W(J)$ is related to the Lagrange multiplier $w(t)$:

$$W(J) = \int_{-\infty}^{\infty} dt\, w(t) . \tag{4.21b}$$

The quantity $w(t)$ is obtained from (4.15) either by multiplying (4.15a) by Λ or (4.15b) by ρ and taking the trace. Therefore, with the help of (4.12), $W(J)$ is evaluated as

$$W(J) = \Gamma(\phi) + \int dx\, J(x)\phi(x) . \tag{4.21c}$$

This completes the argument, when it is recognized that (4.21a) implies that

$$\frac{\delta W(J)}{\delta J(x)} = \phi(x) . \tag{4.22}$$

Consequently, from (4.21c) it follows that

$$\frac{\delta\Gamma(\phi)}{\delta\phi(x)} = -J(x) \tag{4.23}$$

which must vanish in the absence of sources.

It is seen that an effective action formalism is available for our problem, indeed it is equivalent to the variational principle, provided trivial boundary conditions on the Lagrange multiplier kernel $[\Lambda\,|_{t=t_f} = \mathbb{1}]$ are imposed. At zero temperature or in equilibrium, the effective-action and effective-energy formulations of the relevant variational principles suggest approximation techniques other than the parametric (Rayleigh-Ritz) restricted variation, which we employ below. Specifically, the loop expansion and semiclassical method give various perspectives on the problem, and allow for systematic improvement of an initial approximation. Thus far, a systematic expansion for the nonequilibrium effective action introduced here has not been developed, but would be most welcome.

V. CALCULATIONS

We shall solve the Liouville equation (3.12) for various time-dependent H, both in quantum mechanics and in simple quantum field theories. For nontrivial problems, H is not quadratic, the dynamics is nonlinear, and (3.12) cannot be solved exactly. However, by making a restricted variational *Ansatz* within the exact variational principle (4.8) formulated above, tractable equations are obtained, which still retain some of the nonlinearity of the complete problem.

A. Gaussian density matrix

The *Ansatz* that we make for ρ is Gaussian. Thus we make contact with the well-known approximations of zero-temperature physics: two-loop effective action, time-dependent Hartree-Fock, large-n limit, etc. In quantum mechanics for n-component vectors $\mathbf{x}$ we take

$$\rho(\mathbf{x}_1,\mathbf{x}_2) = N\exp[-\tfrac{1}{2}(x_1^i A_{ij} x_1^j - 2x_1^i B_{ij} x_2^j + x_2^i C_{ij} x_2^j)] , \tag{5.1}$$

where by virtue of Hermiticity, $\rho(\mathbf{x}_1,\mathbf{x}_2) = \rho^*(\mathbf{x}_2,\mathbf{x}_1)$,

$$A^* = C, \quad B^\dagger = B , \tag{5.2}$$

while the real normalization factor N ensures $\int d\mathbf{x}\,\rho(\mathbf{x},\mathbf{x}) = 1$. To accommodate (5.2) and for later convenience we reparametrize ρ as

$$\rho(\mathbf{x}_1,\mathbf{x}_2) = e^{-\gamma}\exp\left\{-\frac{1}{2}\left[x_1^i\left[\frac{G^{-1}}{2} - 2i\Pi\right]_{ij} x_1^j + x_2^i\left[\frac{G^{-1}}{2} + 2i\Pi\right]_{ij} x_2^j - x_1^i (G^{-1/2}\xi G^{-1})_{ij} x_2^j\right]\right\} . \tag{5.3}$$

The matrices G and Π are real symmetric, and ξ is Hermitian, i.e., $\xi = \xi_R + 4iG^{1/2}\xi_I G^{1/2}$, where ξ_R is real symmetric and ξ_I is real antisymmetric. The density matrix is properly normalized when

$$-\ln N = \gamma = \tfrac{1}{2}\ln\det 2\pi G^{1/2}(1-\xi_R)^{-1}G^{1/2} . \tag{5.4}$$

Observe that nonvanishing ξ is a measure of the amount by which our density matrix differs from a pure state. For $\xi = 0$, $\rho(\mathbf{x}_1,\mathbf{x}_2) = \Psi(\mathbf{x}_1)\Psi^*(\mathbf{x}_2)$, with

$$\Psi(\mathbf{x}) = (\det^{-1/4} 2\pi G)\exp\left[-\frac{1}{2}x^i\left[\frac{G^{-1}}{2} - 2i\Pi\right]_{ij} x^j\right] .$$

Therefore we call ξ the *degree of mixing*.

With the above density matrix, it follows that averages of $\mathbf{x}$ and $\mathbf{p}$ vanish:

$$\langle\mathbf{x}\rangle = \int d\mathbf{x}\,\mathbf{x}\rho(\mathbf{x},\mathbf{x}) = 0 , \tag{5.5a}$$

$$\langle \mathbf{p} \rangle = \int d\mathbf{x} \frac{1}{i} \nabla_{\mathbf{x}} \rho(\mathbf{x},\mathbf{x}') \Big|_{\mathbf{x}'=\mathbf{x}} = 0 \ , \tag{5.5b}$$

while averages of bilinears are

$$\langle x^i p^j \rangle = \int d\mathbf{x}\, x^i x^j \rho(\mathbf{x},\mathbf{x}) = [G^{1/2}(1-\xi_R)^{-1}G^{1/2}]_{ij} \ , \tag{5.6a}$$

$$\langle p^i p^j \rangle = -\int d\mathbf{x} \frac{\partial^2 \rho(\mathbf{x},\mathbf{x}')}{\partial x^i \partial x^j} \Big|_{\mathbf{x}'=\mathbf{x}}$$

$$= \tfrac{1}{4}[G^{-1/2}(1+\xi_R)G^{-1/2}]_{ij} + 4[(\Pi+\xi_I)G^{1/2}(1-\xi_R)^{-1}G^{1/2}(\Pi-\xi_I)]_{ij} \ , \tag{5.6b}$$

$$\langle x^i p^j \rangle = -i \int d\mathbf{x}\, x^i \frac{\partial}{\partial x^j} \rho(\mathbf{x},\mathbf{x}') \Big|_{\mathbf{x}'=\mathbf{x}} = \frac{i}{2}\delta_{ij} + 2[G^{1/2}(1-\xi_R)^{-1}G^{1/2}(\Pi-\xi_I)]_{ij} \ . \tag{5.6c}$$

When we take the dynamics to be invariant against rotations in the n-dimensional vector space, all the symmetric matrices are proportional to δ_{ij}, and the antisymmetric matrix ξ_I vanishes, except for $n=2$, where $(\xi_I)_{ij}$ could be proportional to ϵ_{ij}, but we ignore this exception. (The antisymmetric structure arises, for example, in planar systems moving in a constant magnetic field, perpendicular to the plane.[17])

Formulas for field theory are analogous. We consider an n-tuplet of scalar fields $\Phi^i(\mathbf{r})$, and assume $O(n)$ symmetry throughout. The density matrix becomes

$$\rho(\varphi_1,\varphi_2) = e^{-\gamma} \exp\left\{ -\frac{1}{2}\left[\varphi_1 \left[\frac{G^{-1}}{2} - 2i\Pi \right] \varphi_1 + \varphi_2 \left[\frac{G^{-1}}{2} + 2i\Pi \right] \varphi_2 - \varphi_1 G^{-1/2} \xi G^{-1/2} \varphi_2 \right] \right\} . \tag{5.7}$$

G, Π, and ξ are kernels are $\mathbf{r}$ space and matrices in the n-dimensional component space.

Translation invariance allows diagonalizing the kernels:

$$G(\mathbf{r}_1,\mathbf{r}_2) = \int_{\mathbf{p}} e^{-i\mathbf{p}\cdot(\mathbf{r}_1-\mathbf{r}_2)} G(\mathbf{p}) \ , \tag{5.8a}$$

$$\Pi(\mathbf{r}_1,\mathbf{r}_2) = \int_{\mathbf{p}} e^{-i\mathbf{p}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \Pi(\mathbf{p}) \ , \tag{5.8b}$$

$$\xi(\mathbf{r}_1,\mathbf{r}_2) = \int_{\mathbf{p}} e^{-i\mathbf{p}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \xi(\mathbf{p}) \ , \tag{5.8c}$$

where $G(\mathbf{p})$, $\Pi(\mathbf{p})$, and $\xi(\mathbf{p})$ are still matrices in component space. By $O(n)$ invariance, they are proportional to δ_{ij}, except at $n=2$ where the tensor ϵ_{ij} is also available, but we do not consider that exception. It therefore follows that bilinears of the form $\varphi_1 O \varphi_2 \equiv \int d\mathbf{r}\, d\mathbf{r}' \varphi^i(\mathbf{r}) O_{ij}(\mathbf{r},\mathbf{r}') \varphi^j(\mathbf{r}')$ becomes $\int_{\mathbf{p}} \varphi_1^{*i}(\mathbf{p}) O(\mathbf{p}) \varphi_2^i(\mathbf{p})$, where $\varphi^i(\mathbf{p}) = \int d\mathbf{r}\, e^{i\mathbf{p}\cdot\mathbf{r}} \varphi^i(\mathbf{r})$.

Averages of field operators follow (5.5) and (5.6). Linear averages vanish, bilinear averages are

$$\langle \Phi^i(\mathbf{r}) \Phi^j(\mathbf{r}') \rangle = [G^{1/2}(1-\xi_R)^{-1}G^{1/2}]_{ij}(\mathbf{r},\mathbf{r}') \ , \tag{5.9a}$$

$$\langle \Pi^i(\mathbf{r}) \Pi^j(\mathbf{r}') \rangle = \tfrac{1}{4}[G^{-1/2}(1+\xi_R)G^{-1/2}]_{ij}(\mathbf{r},\mathbf{r}') + 4[(\Pi+\xi_I)G^{1/2}(1-\xi_R)^{-1}G^{1/2}(\Pi-\xi_I)]_{ij}(\mathbf{r},\mathbf{r}') \ , \tag{5.9b}$$

$$\langle \Phi^i(\mathbf{r}) \Pi^j(\mathbf{r}') \rangle = \frac{i}{2}\delta_{ij}\delta(\mathbf{r}-\mathbf{r}') + 2[G^{1/2}(1-\xi_R)^{-1}G^{1/2}(\Pi-\xi_I)]_{ij}(\mathbf{r},\mathbf{r}') \ . \tag{5.9c}$$

In Appendix A we present a more general *Ansatz* that leads to nonvanishing averages for the coordinate and momentum.

To develop further understanding of the Gaussian *Ansatz*, let us simplify to one quantum-mechanical degree of freedom:

$$\rho(x_1,x_2) = e^{-\gamma} \exp\left[-\frac{1}{4G}(x_1^2 + x_2^2 - 2x_1 x_2 \xi) \right] \exp[i\Pi(x_1^2 - x_2^2)] \ . \tag{5.10}$$

This is equivalent to the operator *Ansatz*

$$\rho(x_1,x_2) = \langle x_1 | \hat{\rho} | x_2 \rangle, \quad \hat{\rho} = \left[\frac{2\pi}{w} \sinh bw \right]^{1/2} e^{-\gamma} \exp\left[-\frac{b}{2}[p^2 - 2\Pi(xp+px) + ax^2] \right] , \tag{5.11}$$

with the following identification:

$$G=\frac{1}{2w}\tanh bw \ , \tag{5.12a}$$

$$\xi^{-1}=\cosh bw \ , \tag{5.12b}$$

$$w=\sqrt{a-4\Pi^2} \ . \tag{5.12c}$$

Proper normalization is ensured when γ is taken from (5.4):

$$\hat{\rho}=2\sinh\frac{bw}{2}\exp\left[-\frac{b}{2}[p^2-2\Pi(xp+px)+ax^2]\right] , \tag{5.13a}$$

$$\begin{aligned}\rho(x_1,x_2)&=\left[\frac{1-\xi}{2\pi G}\right]^{1/2}\exp\left[-\frac{1}{4G}(x_1^2+x_2^2-2x_1x_2\xi)\right]\exp[i\Pi(x_1^2-x_2^2)]\\&=\left[\frac{w}{\pi}\tanh\frac{bw}{2}\right]^{1/2}\exp\left[-\frac{w}{2\sinh bw}[(x_1^2+x_2^2)\cosh bw-2x_1x_2]\right]\exp[i\Pi(x_1^2-x_2^2)] \ .\end{aligned} \tag{5.13b}$$

From (5.13) it is easy to evaluate the entropy (3.8):

$$S=-k\left\langle \ln\left[2\sinh\frac{bw}{2}\right]-\frac{b}{2}p^2+b\Pi(xp+px)-\frac{ba}{2}x^2\right\rangle . \tag{5.14a}$$

The averages are given in (5.6), and with (5.12) we get

$$\begin{aligned}S&=-k\ln\left[2\sinh\frac{bw}{2}\right]+k\frac{bw}{2}\coth\frac{bw}{2}\\&=kz^2\frac{d}{dz}\left[\frac{1}{z}\ln(2\sinh z)\right]\Bigg|_{z=bw/2} .\end{aligned} \tag{5.14b}$$

Since by (5.12b) bw is functionally related to ξ, constant entropy means that the degree of mixing ξ stays constant during the Liouville evolution, and only G and Π can vary in time.

Note further that (5.13) may be diagonalized as follows. Consider a Gaussian wave function with covariance $\Omega=\Omega_R+i\Omega_I$, which may be complex and time dependent:

$$\Psi_0=e^{i\varphi_0}\left[\frac{\Omega_R}{\pi}\right]^{1/2}e^{-x\Omega x/2} . \tag{5.15}$$

Here φ_0 is a position-independent phase. This state is annihilated by

$$a=\frac{1}{\sqrt{2\Omega_R}}(p-i\Omega x) \tag{5.16a}$$

whose conjugate

$$a^\dagger=\frac{1}{\sqrt{2\Omega_R}}(p+i\Omega^* x) \tag{5.16b}$$

satisfies the expected commutation relation

$$[a,a^\dagger]=1 \ . \tag{5.17}$$

We may therefore form the orthonormal states

$$\Psi_n=e^{i\varphi_n}\frac{(a^\dagger)^n}{\sqrt{n!}}\Psi_0 \tag{5.18}$$

which apart from x-independent phases are related to harmonic-oscillator wave functions given by Hermite polynomials H_n:

$$\Psi_n(x)=i^n e^{i\varphi_n}\left[\frac{\Omega_R}{\pi}\right]^{1/4}\left[\frac{1}{2^n n!}\right]^{1/2}\times H_n(\sqrt{\Omega_R}\,x)e^{-x\Omega x/2} . \tag{5.19}$$

Standard summation formulas[18] allow one to conclude that (5.13b) may be written as

$$\rho(x_1,x_2)=\frac{\sum_n e^{-bw(n+1/2)}\Psi_n(x_1)\Psi_n^*(x_2)}{\sum_n e^{-bw(n+1/2)}} \tag{5.20}$$

when Ω_R is chosen to be w, $\Omega_I=-2\Pi$, and bw is related to ξ by (5.12b). Therefore, the occupation probabilities

$$p_n=e^{-bwn}-e^{-bw(n+1)} \tag{5.21}$$

are solely determined by the degree of mixing.

Within the parametrizations (5.3) and (5.7) we can describe the classical limit as the situation when the next-to-last terms in (5.6b) and (5.9b) are dominated by the last terms, and when the next-to-last imaginary terms in (5.6c) and (5.9c) are dominated by the real last terms. The reason is that the next-to-last terms are $O(\hbar)$, while the last terms are ~ 1. (Remember that in our units $\hbar=1$ and, hence, is invisible in the above formulas.) Indeed the next-to-last imaginary terms in (5.6c) and (5.9c) give rise to the Heisenberg commutator. When the classical limit holds, then (for one quantum-mechanical degree of freedom)

$$\langle x^2\rangle=(\Delta x)^2=\frac{G}{1-\xi}\equiv\langle x^2\rangle_c\ , \tag{5.22a}$$

$$\langle p^2\rangle=(\Delta p)^2\approx\frac{4\Pi^2G}{1-\xi}\equiv\langle p^2\rangle_c=4\Pi^2\langle x^2\rangle_c\ , \tag{5.22b}$$

$$\langle xp\rangle\approx\frac{2\Pi G}{1-\xi}\equiv\langle xp\rangle_c=2\Pi\langle x^2\rangle_c\ , \tag{5.22c}$$

and $\Delta p\Delta x=\langle xp\rangle$. The imaginary contribution to $\langle xp\rangle$ that is ignored in the classical limit has magnitude $\frac{1}{2}$. Hence, the classical limit is alternatively characterized by $\Delta p\Delta x\gg\frac{1}{2}$, which expresses the fact that one is far from the minimal quantum uncertainty. Evidently Π must not vanish in the classical limit.

A classical distribution function $f(p,x)$ can be constructed to reproduce the classical expectations (5.22):

$$f(p,x)=\delta(p-2\Pi x)\rho(x,x)\ . \tag{5.23}$$

One easily verifies that $\langle x^2\rangle_c=\int dp\,dx\,x^2f(p,x)$, $\langle p^2\rangle_c=\int dp\,dx\,p^2f(p,x)$, $\langle xp\rangle_c=\int dp\,dx\,xpf(p,x)$. For another perspective on this matter we calculate the Wigner distribution function f_W:

$$f_W(p,x)=\int\frac{dy}{2\pi}e^{ipy}\rho(x-\tfrac{1}{2}y,x+\tfrac{1}{2}y)\ . \tag{5.24a}$$

With the Gaussian ρ in (5.13), this becomes

$$f_W(p,x)=\left[\frac{2G}{\pi(1+\xi)}\right]^{1/2}\times\exp\left[-\frac{2G}{1+\xi}(p-2\Pi x)^2\right]\rho(x,x). \tag{5.24b}$$

For large $2G(1+\xi)^{-1}$, this coincides with (5.23).

It still remains to choose an *Ansatz* for Λ, select a Hamiltonian, evaluate I in (4.8), and vary all the parameters to obtain equations for them. Before doing this we observe that the Gaussian density matrix exactly solves the Liouville equation for quadratic systems; hence, we discuss these first.

B. Quadratic Hamiltonians and linear dynamics

The Gaussian density matrix is an exact solution to Liouville's equation when the Hamiltonian is quadratic and dynamics is linear, without self-interaction. It is instructive to examine the solvable cases, but first we must assess their relevance to problems of equilibrium/non-equilibrium behavior.

When an external agent acts on a system and destroys its equilibrium, it is natural to believe that after the disturbance ceases equilibrium will be reestablished due to self-interactions. Conversely, in the absence of self-interactions, one would not expect a return to equilibrium. It would therefore appear that linear systems, without self-interaction, though solvable, never exhibit initial equilibrium, out-of-equilibrium evolution in the presence of a disturbance, return to equilibrium after the disturbance.

Our explicit calculations support the above observations in most, but not all, cases. We find for generic quadratic Hamiltonians that equilibrium indeed is not reestablished. However, for a class of very special models, which bear a mathematical relation to reflectionless potentials, the system does settle into thermal equilibrium again.

For a quantum-mechanical example, we chose a harmonic oscillator with time-dependent frequency:

$$H=\tfrac{1}{2}\mathbf{p}^2+\tfrac{1}{2}\omega^2(t)\mathbf{x}^2\ . \tag{5.25}$$

The frequency is constant, equal to ω_i in the past, and again constant, ω_f, in the future. (We consider first only real frequencies.) Substituting the Gaussian *Ansatz* for ρ into (3.12) shows that the Liouville equation is satisfied (the exact solution is Gaussian) when the following equations hold:

$$\frac{\dot N}{N}=\mathrm{tr}\,A_I\ , \tag{5.26a}$$

$$\dot A_R\pm\dot B_R\pm[B_I,A_R\pm B_R]=\{A_I,A_R\pm B_R\}\ , \tag{5.26b}$$

$$\dot B_I=\{A_I,B_I\}+[B_R,A_R]\ , \tag{5.26c}$$

$$\dot A_I=-A_R^2+B_R^2+A_I^2+B_I^2+\omega^2\ . \tag{5.26d}$$

The overdot signifies differentiation with respect to time, and we use the parametrization (5.1), with subscripts R and I denoting the real and imaginary parts, respectively, of the matrices. As a consequence of (5.26b), Eq. (5.26a) is satisfied by (5.4), where the argument of the logarithm is recognized as $\det\pi(A_R-B_R)^{-1}$. The equations simplify if B_I can be taken to vanish. Then (5.26c) requires B_R and A_R to be simultaneously diagonalizable, and (5.26b) shows that A_I can be taken diagonal with A_R and B_R. This complete diagonalization, which we shall henceforth assume, of course, holds in the one-dimensional case (no matrix structure) or in the $O(n)$-symmetric n-dimensional case, with all matrices proportional to the $n\times n$ unit matrix. The diagonal equations read

$$\dot\xi=0\ , \tag{5.27a}$$

$$\dot G=4\Pi G\ , \tag{5.27b}$$

$$\dot\Pi=\frac{1-\xi^2}{8G^2}-2\Pi^2-\frac{\omega^2}{2}\ . \tag{5.27c}$$

Thus we need to analyze only (5.27b) and (5.27c) with constant real ξ. Recalling that ξ is a measure of how much our state differs from a pure state, we see that the degree of mixing remains constant in time, as is expected since entropy does not change. Note that the classical limit, which requires $4G\Pi\gg1-\xi$, is eqivalently characterized by $\dot G/(1-\xi)\gg1$.

The two equations (5.27b) and (5.27c) may be presented in various ways. Π may be eliminated and a second-order equation for G results, which is conveniently expressed in terms of a new variable $Q\equiv(1-\xi)^{-1/2}G^{1/2}$, whose definition is motivated by the fact that $(1-\xi)^{-1}G$ is the expected value of x^2, and the classical limit sets in when $(d/dt)Q^2\gg1$. Q satisfies

$$\ddot{Q}-\frac{l^2}{Q^3}+\omega^2 Q=0\ , \tag{5.28a}$$

$$l^2=\frac{1}{4}\left[\frac{1+\xi}{1-\xi}\right]\ , \tag{5.28b}$$

which may be analyzed by a mechanical analogy to a "particle" moving in the "potential" $\frac{1}{2}l^2/Q^2+\frac{1}{2}\omega^2Q^2$. The "angular momentum" in the "centrifugal term" is determined by the degree of mixing. For constant ω, the static solution is at the minimum of the "potential." Upon introducing temperature through ξ,

$$\xi^{-1}=\cosh\beta\omega \tag{5.29}$$

we get

$$G=\frac{1}{2\omega}\tanh\beta\omega,\quad \Pi=0\ , \tag{5.30}$$

and regain the canonical density matrix for a harmonic oscillator in thermal equilibrium:

$$\rho(x_1,x_2)=\left[\frac{\omega}{\pi}\tanh\frac{\beta\omega}{2}\right]^{1/2}\exp\left[-\frac{\omega}{2\sinh\beta\omega}\right]((x_1^2+x_2^2)\cosh\beta\omega-2x_1x_2)\ . \tag{5.31}$$

With (5.31), the expectations are the familiar ones:

$$\langle x^2\rangle=\frac{1}{2\omega}\coth\frac{\beta\omega}{2}\ , \tag{5.32a}$$

$$\langle p^2\rangle=\frac{\omega}{2}\coth\frac{\beta\omega}{2}\ , \tag{5.32b}$$

$$\langle xp\rangle=\frac{i}{2}\ . \tag{5.32c}$$

A classical limit is never attained, because $\Pi=0$. At zero temperature $\beta=\infty$, ξ vanishes, and the state becomes pure.

The time-dependent problem may be analyzed with (5.28), but another rewriting is preferable. Upon defining

$$\Omega_\xi=\frac{\sqrt{1-\xi^2}}{2G}-2i\Pi \tag{5.33}$$

the two real equations (5.27b) and (5.27c) combine in a single Riccati equation for the complex quantity Ω_ξ,

$$i\dot{\Omega}_\xi=\Omega_\xi^2-\omega^2 \tag{5.34}$$

which is linearized by the definition

$$\Omega_\xi=-i\frac{d}{dt}\ln D\ , \tag{5.35}$$

$$\ddot{D}+\omega^2 D=0\ . \tag{5.36}$$

For static ω the general solution is

$$D=Ae^{i\omega t}+Be^{-i\omega t}\ . \tag{5.37}$$

This corresponds to the static density matrix $\rho_i(\beta)$ in (5.31) only if A or B is zero. Taking B to vanish we define $\Omega_\xi=\omega$, which reproduces (5.30) and (5.31) from (5.29), (5.33), and (5.35) (Ref. 19).

Equation (5.36) is especially suited for discussing the general case, because its structure is that of a familiar and well-studied equation: the time-independent, continuum Schrödinger equation for a unit-mass particle moving on a line t in a "potential" $v(t)$ and energy ϵ, with $\omega^2(t)=2[\epsilon-v(t)]$. In the past, for $t\le t_i$ where ω is equal to the static initial value ω_i and the density matrix is $\rho_i(\beta_i)$, $D=e^{i\omega_i t}$. In the future, $t\ge t_f$, ω becomes static again, ω_f, and D in general will be a superposition $Ae^{i\omega_f t}+Be^{-i\omega_f t}$, with the constants A and B determined by continuity, and satisfying

$$\frac{\omega_i}{w_f}=|A|^2-|B|^2 \tag{5.38}$$

by virtue of the time-independence of the Wronskian $(1/2i)(\dot{D}D^*-\dot{D}^*D)$. The temperature enters in the initial period through the definition of ξ:

$$\xi^{-1}=\cosh\beta_i\omega_i \tag{5.39}$$

and ξ remains constant throughout the time evolution.

In the general case, both A and B are nonvanishing and the final density matrix remains time dependent—equilibrium is not regained. Upon parametrizing A and B by

$$\begin{aligned}|A|&=\left[\frac{\omega_i}{\omega_f}\right]^{1/2}\cosh\frac{\Delta}{2}\ ,\\ |B|&=\left[\frac{\omega_i}{\omega_f}\right]^{1/2}\sinh\frac{\Delta}{2},\quad \arg AB^*=2\delta\ ,\end{aligned} \tag{5.40}$$

where Δ and δ depend on the details of the problem we find

$$G=\frac{1}{2\omega_f}\tanh\beta_i\omega_i[\cosh\Delta+\sinh\Delta\cos2(\omega_f t+\delta)]\ , \tag{5.41a}$$

$$\Pi=-\frac{\omega_f}{2}\frac{\sinh\Delta\sin2(\omega_f t+\delta)}{\cosh\Delta+\sinh\Delta\cos2(\omega_f t+\delta)}\ , \tag{5.41b}$$

which together with (5.39) determine the density matrix from (5.13). The various expectations, which become classical at high temperatures for limited periods of time [i.e., when Π is not close to zero) are

$$\langle x^2\rangle=\frac{1}{2\omega_f}\coth\frac{\beta_i\omega_i}{2}[\cosh\Delta+\sinh\Delta\cos2(\omega_f t+\delta)]\ , \tag{5.42a}$$

$$\langle p^2\rangle=\frac{\omega_f}{2}\coth\frac{\beta_i\omega_i}{2}\left[\frac{1+\sinh^2\Delta\sin^2 2(\omega_f t+\delta)}{\cosh\Delta+\sinh\Delta\cos2(\omega_f t+\delta)}\right]\ , \tag{5.42b}$$

$$\langle xp\rangle=\frac{i}{2}-\frac{1}{2}\coth\frac{\beta_i\omega_i}{2}[\sinh\Delta\sin2(\omega_f t+\delta)]\ . \tag{5.42c}$$

However, for very particular forms of $\omega^2(t)$, B and Δ can vanish, and the density matrix becomes static, corresponding to a Boltzmann distribution, whose temperature is determined from ξ, which remains time independent regardless of the form of $\omega^2(t)$: $\cosh\beta_i\omega_i=\xi^{-1}=\cosh\beta_f\omega_f$. For these very special disturbances, thermal equilibrium is reestablished at a shifted temperature: $\beta_f=(\omega_i/\omega_f)\beta_i$.

It is clear from the Schrödinger equation analogy that reestablishment of equilibrium is equivalent to reflectionless transmission in the corresponding Schrödinger problem. Reflectionless transmission can arise in two ways. For very special potentials, there is no reflection at any energy. Alternatively and less restrictively, for a wide class of potentials, the reflection coefficient can vanish at a particular energy (Ramsauer-Townsend effect).[20] Both mechanisms provide a construction of $\omega^2(t)$ that leads to restoration of thermal equilibrium.

For an example of the first mechanism, consider the reflectionless Pöschl-Teller potentials. For our problem, these give rise to a frequency profile

$$\omega^2(t)=\omega_0^2+\frac{n(n+1)\mu^2}{\cosh^2\mu t}\ , \tag{5.43}$$

where μ is a parameter and n any positive integer. The initial and final times are $-\infty$ and $+\infty$, respectively, and $\omega_i=\omega_f=\omega_0$. The results for $n=1$ are

$$G=\frac{1}{2\omega_0}\tanh\beta\omega_0\left[1-\frac{\mu^2}{(\omega_0^2+\mu^2)\cosh^2\mu t}\right]\ , \tag{5.44a}$$

$$\Pi=\frac{1}{2}\frac{\mu^3\tanh\mu t}{\omega_0^2\cosh^2\mu t+\mu^2\sinh^2\mu t}\ , \tag{5.44b}$$

and the expectations become

$$\langle x^2\rangle=\frac{1}{2\omega_0}\coth\frac{\beta\omega_0}{2}\left[1-\frac{\mu^2}{(\omega_0^2+\mu^2)\cosh^2\mu t}\right]\ , \tag{5.45a}$$

$$\langle p^2\rangle=\frac{1}{2\omega_0}\coth\frac{\beta\omega_0}{2}\left[\frac{\mu^6\sinh^2\mu t+\omega_0^2(\omega_0^2+\mu^2)^2\cosh^6\mu t}{(\omega_0^2+\mu^2)\cosh^4\mu t(\omega_0^2\cosh^2\mu t+\mu^2\sinh^2\mu t)}\right]\ , \tag{5.45b}$$

$$\langle xp\rangle=\frac{i}{2}+\frac{1}{2}\coth\frac{\beta\omega_0}{2}\left[\frac{\mu^3}{\omega_0(\omega_0^2+\mu^2)}\frac{\sinh\mu t}{\cosh^3\mu t}\right]\ . \tag{5.45c}$$

These can be classical for a limited time at high temperatures.

The second mechanism is exemplified by the profile

$$\omega^2(t)=\begin{cases}\omega_i^2, & t\le t_i\ ,\\ \omega_0^2, & t_i<t<t_f\ ,\\ \omega_f^2, & t\ge t_f\ .\end{cases} \tag{5.46}$$

When $\omega_0^2=\omega_i\omega_f$ and $(t_f-t_i)=(n+1/2)\pi/\omega_0$, the corresponding Schrödinger transmission problem is reflectionless at one value of the energy—the Ramsauer-Townsend effect ocurrs. For intermediate times $t_i<t<t_f$, we find

$$G=\frac{1}{4\omega_i}\tanh\beta_i\omega_i\left[\left[1+\frac{\omega_i}{\omega_f}\right]-(-1)^n\left[1-\frac{\omega_i}{\omega_f}\right]\sin\omega_0(2t-t_i-t_f)\right]\ , \tag{5.47a}$$

$$\Pi=-\frac{\omega_0}{2}\frac{(-1)^n\left[1-\frac{\omega_i}{\omega_f}\right]\cos\omega_0(2t-t_i-t_f)}{\left[1+\frac{\omega_i}{\omega_f}\right]-(-1)^n\left[1-\frac{\omega_i}{\omega_f}\right]\sin\omega_0(2t-t_i-t_f)}\ . \tag{5.47b}$$

For $t\le t_i$ and $t\ge t_f$, ρ is the Boltzmann distribution density matrix, at β_i and $\beta_f=(\omega_i/\omega_f)\beta_i$, respectively.

An example, where equilibrium is not restored, is given by a single sudden jump in frequency:

$$\omega^2(t)=\begin{cases}\omega_i^2, & t<0\ ,\\ \omega_f^2, & t>0\ .\end{cases} \tag{5.48}$$

The solution (5.37) for $t>0$ with $\omega=\omega_f$ is matched to $e^{i\omega_i t}$ for $t<0$. The continuity of D and $\dot{D}$ at the origin allows evaluating the parameters in (5.40): $\Delta=|\ln\omega_i/\omega_f|$, $\delta=0$.

It is interesting to follow the transition from ω_i when it occurs more gradually than in (5.48), and to examine the dependence of the final density matrix on the rate of transition. This we do numerically. Assuming that

$$\omega(t)=\begin{cases}w_i, & t\le t_i\ ,\\ \dfrac{(\omega_i-\omega_f)t+\omega_f t_i-\omega_i t_f}{t_i-t_f}, & t_i<t<t_f\ ,\\ \omega_f, & t\ge t_f\ ,\end{cases} \tag{5.49}$$

we solve for $G(t)$. Figures 1(a)–1(d) exhibit the behavior in time of

$$\Delta G(t)\equiv\frac{G(t)-G_{\rm eq}(t)}{G_{\rm eq}(t)}\ , \tag{5.50}$$

where $G_{\rm eq}(t)=\tanh\beta_i\omega_i/2\omega(t)$. At a given time t, $\Delta G(t)$ measures how far the state is out of thermal equilibrium. As can be seen from Fig. 1, for fixed ω_i and ω_f, the departure from thermal equilibrium diminishes as $t_f-t_i\equiv\tau$ increases. From the numerical results we can learn that the amplitude of oscillation of $\Delta G(t)$ (for $t>t_f$) is roughly proportional to $1/\tau$. We shall prove below that for an infinitely slow transition from ω_i to ω_f equilibrium is always regained.

When the time evolution carries an initial frequency into a final imaginary frequency $-\omega_f^2=\nu^2>0$, so that the harmonic oscillator becomes unstable, equilibrium is never restored because there are no static solutions to (5.27) with negative ω^2 and $\xi<1$; the latter being constrained to this domain because it is constant and initially equal to $\operatorname{sech}\beta_i\omega_i<1$. The final time-dependent density matrix is found from (5.33)–(5.37):

$$D=Ae^{\nu t}+Be^{-\nu t}\ . \tag{5.51}$$

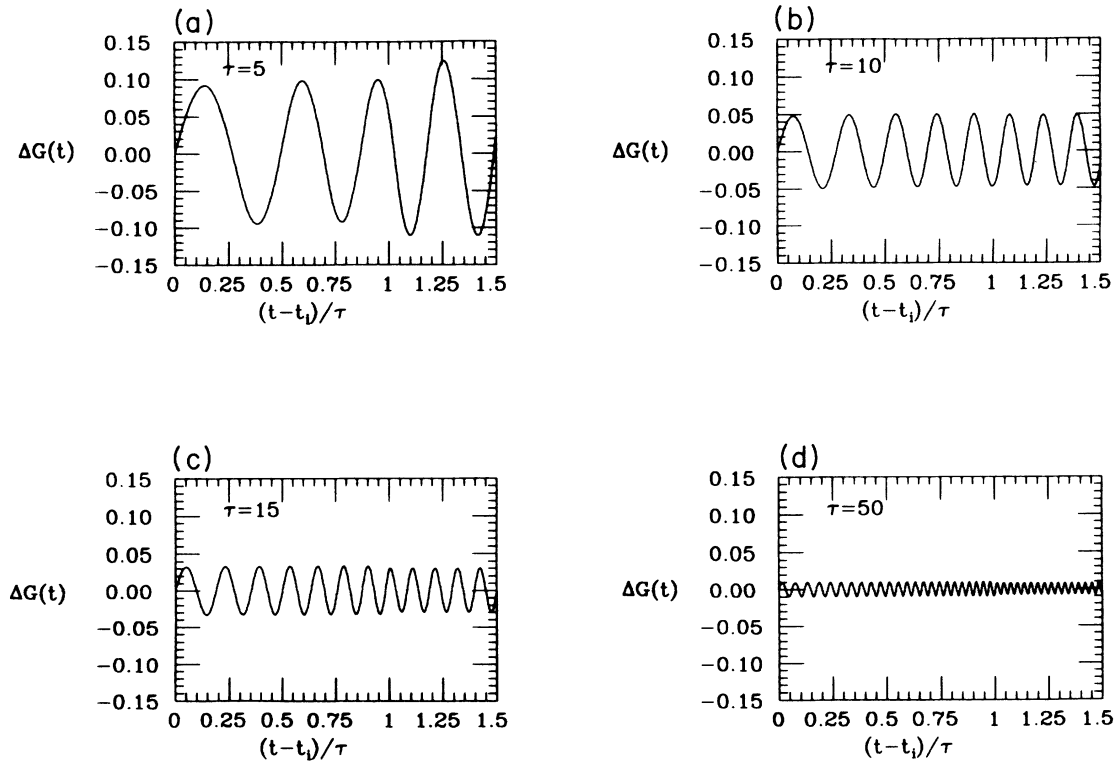

FIG. 1. $\Delta G(t)$ as a function of $(t-t_i)/\tau$ for different values of τ: (a) $\tau=5$; (b) $\tau=10$; (c) $\tau=15$; (d) $\tau=50$. In the numerical work we took $\omega_i=1$, $\omega_f=2$, and $\beta=1$.

The constancy of the Wronskian here fixes the imaginary part of AB^*:

$$\mathrm{Im}\, AB^* = \frac{1}{2}\frac{\omega_i}{\nu} \tag{5.52}$$

which ensures that the magnitudes $|A|$ and $|B|$ are nonvanishing; they are determined by continuity. Thus

$$G = \frac{1}{2\omega_i}\tanh\beta_i\omega_i(|A|^2 e^{2\nu t} + |B|^2 e^{-2\nu t} + 2\,\mathrm{Re}\, AB^*)\,, \tag{5.53a}$$

$$\Pi = \frac{\nu}{2}\left[\frac{|A|^2 e^{2\nu t} - |B|^2 e^{-2\nu t}}{|A|^2 e^{2\nu t} + |B|^2 e^{-2\nu t} + 2\,\mathrm{Re}\, AB^*}\right]. \tag{5.53b}$$

These give rise to the expectations

$$\langle x^2\rangle = \frac{1}{2\omega_i}\coth\frac{\beta_i\omega_i}{2}(|A|^2 e^{2\nu t} + |B|^2 e^{-2\nu t} + 2\,\mathrm{Re}\, AB^*)\,, \tag{5.54a}$$

$$\langle p^2\rangle = \frac{\omega_i}{2}\coth\frac{\beta_i\omega_i}{2}\left[\frac{1+\frac{\nu^2}{\omega_i^2}(|A|^2 e^{2\nu t} - |B|^2 e^{-2\nu t})^2}{|A|^2 e^{2\nu t} + |B|^2 e^{-2\nu t} + 2\,\mathrm{Re}\, AB^*}\right], \tag{5.54b}$$

$$\langle xp\rangle = \frac{i}{2} + \frac{\nu}{2\omega_i}\coth\frac{\beta_i\omega_i}{2}(|A|^2 e^{2\nu t} - |B|^2 e^{-2\nu t})\,. \tag{5.54c}$$

Owing to the growing exponential, the expectations become classical at late time, where they can be approximated by

$$\langle x^2\rangle \approx \frac{1}{2\omega_i}\coth\frac{\beta_i\omega_i}{2}|A|^2 e^{2\nu t} \equiv \langle x^2\rangle_c\,, \tag{5.55a}$$

$$\langle p^2\rangle \approx \nu^2\langle x^2\rangle_c\,, \tag{5.55b}$$

$$\langle xp\rangle \approx \nu\langle x^2\rangle_c\,. \tag{5.55c}$$

This is equivalently described by a classical distribution function

$$f(x,p) = \delta(p-\nu x)\left[\frac{\omega_i}{\pi}\tanh\frac{\beta_i\omega_i}{2}\right]^{1/2}\frac{1}{|A|e^{\nu t}}\exp\left[-\left[\omega_i\tanh\frac{\beta_i\omega_i}{2}\right]\frac{x^2}{|A|^2 e^{2\nu t}}\right]. \tag{5.56}$$

An example is given by the sudden jump

$$\omega^2(t) = \begin{cases}\omega_i^2, & t<0\,,\\ -\nu^2, & t>0\,,\end{cases} \tag{5.57}$$

for which

$$A = B^* = \frac{1}{2}\left[1 + i\frac{\omega_i}{\nu}\right]. \tag{5.58}$$

A more gradual evolution,

$$\omega^2(t) = \begin{cases}\omega_i^2, & t\le 0\,,\\ e^{-\chi t}(\omega_i^2+\nu^2)-\nu^2, & t\ge 0\,,\end{cases} \tag{5.59}$$

leads to equations that may be integrated in terms of known functions. The analysis of this problem is the same as for free field theory in de Sitter space, which we now examine.

Consider a scalar free-field theory in de Sitter space-time, with d spatial dimensions, described by the metric[21]

$$ds^2 = dt^2 - e^{2\chi t}d\mathbf{x}^2\,. \tag{5.60}$$

The Universe is expanding at a constant rate χ. The dynamics of the scalar field Φ is governed by the Lagrange density $\mathcal{L}$:

$$\mathcal{L} = e^{d\chi t}[\tfrac{1}{2}\dot\Phi^2 - \tfrac{1}{2}e^{-2\chi T}(\nabla\Phi)^2 - \tfrac{1}{2}(m^2+gR)\Phi^2]\,, \tag{5.61}$$

where g controls a nonminimal coupling to the Ricci scalar R, given by $R = d(d+1)\chi^2$ in de Sitter space. [The scalar field is conformally coupled when $g = \frac{1}{4}(1-1/d)$.]

It is convenient to introduce a new field by $\tilde\Phi = e^{d\chi t/2}\Phi$. Apart from a total time derivative, which we drop, the Lagrange density, expressed in terms of $\tilde\Phi$, reads

$$\mathcal{L} = \tfrac{1}{2}\dot\Phi^2 - \tfrac{1}{2}e^{-2\chi t}(\nabla\Phi)^2 + \frac{1}{2}\left[\frac{d^2\chi^2}{4} - m^2 - gR\right]\Phi^2\,. \tag{5.62}$$

(The tilde has been suppressed.) The Hamiltonian density corresponding to (5.62) is quadratic:

$$\mathcal{H} = \tfrac{1}{2}\Pi^2 + \tfrac{1}{2}e^{-2\chi t}(\nabla\Phi)^2 + \frac{1}{2}\left[-\frac{d^2\chi^2}{4} + m^2 + gR\right]\Phi^2\,, \tag{5.63}$$

so the Gaussian *Ansatz* (5.7) for the density matrix is a solution to Liouville's equation, provided that the kernels ξ, G, and Π satisfy appropriate equations. Translation invariance of the dynamics allows diagonalizing all kernels by Fourier transformation as in (5.8); thus the relevant equations become

$$\dot{\xi}(\mathbf{p})=0 , \tag{5.64a}$$

$$\dot{G}(\mathbf{p})=4\Pi(\mathbf{p})G(\mathbf{p}) , \tag{5.64b}$$

$$\dot{\Pi}(\mathbf{p})=\frac{1-\xi^2(\mathbf{p})}{8G^2(\mathbf{p})}-2\Pi^2(\mathbf{p}) -\frac{1}{2}\left[e^{-2\chi t}\mathbf{p}^2-\frac{d^2\chi^2}{4}+m^2+gR\right] , \tag{5.64c}$$

and $\xi_I(\mathbf{p})$ vanishes. For each momentum mode, these are identical to (5.27), with $\omega(t)$ given by an effective de Sitter frequency $\omega_s(t)$:

$$\omega_s^2(t)=e^{-2\chi t}\mathbf{p}^2-\nu^2\chi^2 , \qquad \nu^2=\frac{d^2}{4}-\frac{m^2}{\chi^2}-\frac{g}{\chi^2}R . \tag{5.65}$$

As in (5.59), ω_s^2 becomes negative in late times because ν^2 is assumed positive. To analyze the system we solve

$$\ddot{D}(\mathbf{p})+\left[e^{-2\chi t}\mathbf{p}^2-\frac{d^2\chi^2}{4}+m^2+gR\right]D(\mathbf{p})=0 \tag{5.66}$$

and obtain

$$D(\mathbf{p})=A(\mathbf{p})H_\nu^{(1)}(\tau\,|\,\mathbf{p}\,|\,)+B(\mathbf{p})H_\nu^{2}(\tau\,|\,\mathbf{p}\,|\,) , \tag{5.67}$$

where $\tau\equiv(1/\chi)e^{-\chi t}$ is called the *conformal time* and $H_\nu^{(1,2)}$ are the two Hankel functions of order ν. The coefficients A and B are specified by imposing an initial condition. In keeping with our procedures thus far, we could cut off the effective de Sitter frequency $\omega_s(t)$ at some initial time t_i, replace it by a constant $\omega_i=\omega_s(t_i)$ for $t\le t_i$, and chose a Boltzmann distribution, $D=e^{i\omega_i t}$, for the early epoch before the expansion begins, compare (5.59). Then A and B are determined by continuity. Alternatively we can let $t_i=-\infty$ and impose physically plausible conditions at the beginning of time on the de Sitter solution (5.67). At $t\to-\infty$, $\tau\to\infty$, and

$$D(\mathbf{p})\xrightarrow[t\to-\infty]{r\to\infty}\left[\frac{2}{\pi\,|\,\mathbf{p}\,|\,\tau}\right]^{1/2}\left\{A(\mathbf{p})\exp\left[i\left[|\,\mathbf{p}\,|\,\tau-\frac{\pi}{2}\nu-\frac{\pi}{4}\right]\right]+B(\mathbf{p})\exp\left[-i\left[|\,\mathbf{p}\,|\,\tau-\frac{\pi}{2}\nu-\frac{\pi}{4}\right]\right]\right\} , \tag{5.68}$$

D approaches the form (5.37), but in conformal time τ rather than real time t. It is therefore plausible to insist that only one exponential is present, so that $\Omega_\xi\equiv-i\partial_t\ln D$ is dominantly real; hence, G^{-1} (determined by $\Omega_{\xi R}$) dominates Π (determined by $\Omega_{\xi I}$). With this point of view, one would set $A(\mathbf{p})=0$—a choice that is the density matrix analog of the pure "Bunch-Davies" vacuum, which is the unique de Sitter-invariant solution to the time-dependent (functional) Schrödinger equation.[22]

To retain generality we remain with arbitrary coefficients in (5.67) and reparametrize as follows. First define the modulus and phase of the Hankel function:

$$e^{i\nu\pi/2}H_\nu^{(1)}=M_\nu e^{i\Theta_\nu} , \tag{5.69a}$$

$$M_\nu^2(z)\Theta_\nu'(z)=\frac{2}{\pi z} . \tag{5.69b}$$

[The formula (5.69a) differs from convention by the additional factor $e^{i\nu\pi/2}$. With our definition, Θ_ν remains real as ν becomes imaginary. The second formula is the Wronskian relation, where the prime signifies differentiation with respect to the argument.] Apart from an irrelevant multiplicative constant, (5.67) is

$$D(\mathbf{p})=M_\nu\cos(\Theta_\nu+\alpha) , \tag{5.70}$$

where α is a τ-independent, complex integration constant. This then leads to

$$G(\mathbf{p})=\frac{\pi}{4\chi r}M_\nu^2\sqrt{1-\xi^2}[1-(1-r^2)\sin^2(\Theta_\nu-\theta)] , \tag{5.71a}$$

$$\Pi(\mathbf{p})=-\frac{1}{2}\tau\,|\,\mathbf{p}\,|\,\chi\frac{M_\nu'}{M_\nu}+\frac{1}{2}\tau\,|\,\mathbf{p}\,|\,\chi\Theta_\nu'\frac{(1-r^2)\tan(\Theta_\nu-\theta)}{1+r^2\tan^2(\Theta_\nu-\theta)} . \tag{5.71b}$$

We have defined $\theta=-\mathrm{Re}\alpha$, $r=\tanh \mathrm{Im}\alpha>0$, and $r=1$ corresponds to $A=0$ in (5.67). The argument of M_ν and Θ_ν is $\tau|\mathbf{p}|$.

If the frequency is time independent before an initial time $t_i, \omega_i=\omega_s(t_i)$, then as usual the constant degree of mixing ξ may be related to an initial temperature by

$$\sqrt{1-\xi^2}=\tanh\beta\omega \ . \tag{5.72}$$

(The subscript i is suppressed.) On the other hand, if expansion extended from $t=-\infty$, there is no well-defined concept of temperature, although a plausible strategy is the following. For large negative time $\omega_s(t) \approx e^{-\chi t}|\mathbf{p}| \equiv \omega$. Hence allowing a time dependence in the temperature so that $\beta\omega$ is time independent, $Te^{-\chi t}\equiv 1/k\beta$, we can still remain with (5.72).

For late times $\tau\to 0$, and in this limit

$$M_\nu \to \frac{1}{\pi}\left[\frac{\tau|\mathbf{p}|}{2}\right]^{-\nu}\Gamma(\nu), \quad \Theta_\nu \to \frac{\pi}{2}(\nu-1) \ .$$

Therefore

$$G(\mathbf{p})\to \frac{1}{4\pi\chi r}\left[\frac{\tau|\mathbf{p}|}{2}\right]^{-\nu}\sqrt{1-\xi^2}(1-\epsilon) \ , \tag{5.73a}$$

$$\Pi(\mathbf{p})\to \frac{\nu}{2}\chi \ , \tag{5.73b}$$

where ϵ is $(1-r^2)\sin^2[(\pi/2)\nu-\pi/2-\theta]$. For $\epsilon<1$, $G\Pi/(1-\xi)$ dominates $\frac{1}{2}$ at nonvanishing β, so that the classical limit holds, a result obtained previously for $r=1$ (Ref. 21).

To conclude this discussion of quadratic systems, note that the Riccati equation (5.34) is also obeyed by the covariance of Ω of a Gaussian wave function Ψ_0 that solves the time-dependent Schrödinger equation, with the quadratic Hamiltonian (5.25). This Gaussian is annihilated by the annihilation operator (5.16a), which also satisfies (we write formulas for 1 degree of freedom)

$$i[H,a]+\frac{\partial a}{\partial t}=-i\Omega_R a \ . \tag{5.74}$$

Therefore, the states (5.18) and (5.19) with

$$\varphi_n=-n\int_0^t \Omega_R(t')dt' \tag{5.75}$$

solve the time-dependent Schrödinger equation as well. Hence the density matrix constructed as (5.19) and (5.20), with bw identified with $\beta_i\omega_i$, satisfies the Liouville equation. This provides an alternative derivation of our results for quadratic systems.

C. *Ansatz* for Λ

Choice of a variational expression for Λ is dictated by several considerations. Because the action to be varied is linear in Λ and ρ, variation of the former produces equations determining the latter. Consequently, there should be as many parameters in the trial expression for Λ as in ρ, so that a sufficient number of equations determining the parameters of ρ is obtained. From the boundary condition (4.11) $\Lambda|_{t=t_f}=\mathbb{1}$, we know that the solution for Λ is $\Lambda=\mathbb{1}$. Therefore the trial form for Λ must accommodate this possibility. Λ should be parametrized in such a way that $\dot{\xi}=0$ emerges as a variational equation; this expression of constant entropy should characterize the approximation. Finally note that while the exact variational equations for Λ and ρ decouple, this need not be the case for the approximate equations. But it would be most convenient to preserve decoupling, and this also influences the selection of Λ.

To motivate the choice we make for Λ, let us first consider a static variational principle that determines the Boltzmann distribution density matrix in the case of time-independent Hamiltonians. As is well known, one minimizes the expected value of $\ln\rho$, proportional to the entropy, subject to the subsidiary condition of constant average energy $U\equiv \mathrm{tr}\rho H$. Thus, one varies the Helmholtz free energy $F\equiv U-TS$:

$$\beta F=\mathrm{tr}\rho\ln\rho+\beta\,\mathrm{tr}\rho H=\langle\ln\rho\rangle+\beta\langle H\rangle \ . \tag{5.76}$$

Here β serves as a Lagrange multiplier enforcing constant average energy; an arbitrary additive constant in the Hamiltonian is adjusted to absorb a further multiplier, which ensures $\mathrm{tr}\rho=1$. Setting the variation of ρ in (5.76) to zero gives

$$\hat{\rho}=\frac{e^{-\beta H}}{\mathrm{tr}e^{-\beta H}} \tag{5.77}$$

which maximizes the entropy at constant energy. Clearly $\hat{\rho}=e^{-\beta\Theta}/\mathrm{tr}e^{-\beta\Theta}$ maximizes the entropy when the average of an arbitrary operator Θ is kept fixed.

We now recognize, with the help of (5.10)–(5.12), that the Gaussian density matrix (5.3) is of the maximum entropy form, where the constrained operator Θ is a linear superposition of $x^ix^j, p^ip^j, x^ip^j+p^jx^i$, and the identity operator $\mathbb{1}$, with time-dependent coefficients related to γ, G, Π, and ξ. Therefore, it is natural to take Λ in the same space of operators. A choice advocated by Balian and Vénéroni[11] is

$$\Lambda(\mathbf{x}_1,\mathbf{x}_2)=\Lambda^{(1)}\delta(\mathbf{x}_1-\mathbf{x}_2)-\Lambda_{ij}^{(p^2)}\frac{\partial}{\partial x_1^i}\frac{\partial}{\partial x_1^j}\delta(\mathbf{x}_1-\mathbf{x}_2)+\Lambda_{ij}^{(xp)}i(x_1^i+x_2^i)\frac{\partial}{\partial x_1^j}\delta(\mathbf{x}_1-\mathbf{x}_2)+\Lambda_{ij}^{(x^2)}x_1^ix_1^j\delta(\mathbf{x}_1-\mathbf{x}_2) \tag{5.78a}$$

or, in operator notation $\Lambda(\mathbf{x}_1,\mathbf{x}_2)=\langle \mathbf{x}_1 \mid \hat{\Lambda} \mid \mathbf{x}_2 \rangle$,

$$\hat{\Lambda}=\Lambda^{(1)}\mathbb{1}+\Lambda_{ij}^{(p^2)}p^i p^j-\Lambda_{ij}^{(xp)}(x^i p^j+p^j x^i)+\Lambda_{ij}^{(x^2)}x^i x^j \ . \tag{5.78b}$$

Here, $\Lambda^{(a)}$ are variational parameters. They all depend on time, and satisfy the condition at final time $t=t_f$ that $\Lambda^{(1)}$ becomes 1, and the others vanish. The advantage of (5.78) is that the action (4.8) to be varied is linear in the $\Lambda^{(a)}$, so the equations for the parameters in ρ do not involve $\Lambda^{(a)}$. The equations for $\Lambda^{(a)}$ remain coupled to the parameters of ρ, but we need not solve them.

D. Interactions and nonlinear dynamics

We evaluate the action with ρ as in (5.3), Λ as in (5.78), and H describing an n-component anharmonic oscillator, with a time-dependent frequency:

$$H=\tfrac{1}{2}\mathbf{p}^2+\tfrac{1}{2}\omega^2(t)\mathbf{x}^2+\frac{\lambda(\mathbf{x}^2)^2}{2(n+2)} \ . \tag{5.79}$$

Upon setting the $\Lambda^{(a)}$ variations to zero, the resulting equations determine ρ. The equations are the same as in (5.26) except that (5.26d) acquires a further term arising from the self-interaction:

$$\omega^2\to\omega^2+\frac{\lambda}{n+2}[\mathrm{tr}(A_R-B_R)^{-1}+2(A_R-B_R)^{-1}] \ .$$

As before, we take the matrix structure to be trivial, and find

$$\dot{\xi}=0 \ , \tag{5.80a}$$

$$\dot{G}=4\Pi G \ , \tag{5.80b}$$

$$\dot{\Pi}=\frac{1-\xi^2}{8G^2}-2\Pi-\frac{\omega^2}{2}-\frac{\lambda G}{1-\xi} \ . \tag{5.80c}$$

Before analyzing (5.80) we mention another natural *Ansatz* for Λ. Since ρ and Λ satisfy the same equation, one could take a Gaussian for Λ as well:

$$\Lambda(\mathbf{x}_1,\mathbf{x}_2)=e^{-\gamma_\Lambda}\exp\left\{-\frac{1}{2}\left[x_1^i\left[\frac{G_\Lambda^{-1}}{2}-2i\Pi_\Lambda\right]_{ij}x_1^j+x_2^i\left[\frac{G_\Lambda^{-1}}{2}+2i\Pi_\Lambda\right]_{ij}x_2^j-x_1^i(G_\Lambda^{-1/2}\xi_\Lambda G_\Lambda^{-1/2})_{ij}x_2^j\right]\right\} \ . \tag{5.81}$$

However, with this form the equations for the parameters in the density matrix involve the parameters of Λ. Also it is difficult to incorporate the final boundary condition $\Lambda(\mathbf{x}_1,\mathbf{x}_2)\mid_{t=t_f}=\delta(\mathbf{x}_1-\mathbf{x}_2)$ in the expression (5.81). Both problems can be overcome by the following trick. We introduce a formal expansion parameter ϵ and expand the variational parameters in ρ and Λ in an ϵ series. All the parameters in ρ as well as Π_Λ and ξ_Λ begin with $O(\epsilon^0)$. The first term in G_Λ is $O(\epsilon)$ while γ_Λ begins with $\ln\epsilon$. The relevant equations are derived, and ϵ is set to zero. In this limit ρ continues to be a Gaussian described by its $O(\epsilon^0)$ parameters, while $\Lambda(\mathbf{x}_1,\mathbf{x}_2)$ tends to $\delta(\mathbf{x}_1-\mathbf{x}_2)$. We omit details, because the equations obtained in this fashion coincide with (5.80).

Our variational equations (5.80) exhibit several desirable and expected properties. The degree of mixing ξ remains constant, while in the absence of mixing, $\xi=0$, the equations reduce to the time-dependent Hartree-Fock equations that have been studied previously.[23] For the static problem, when ω^2 is time independent, a static solution to (5.80) is found by setting the left-hand sides of (5.80) as well as Π to zero. The resulting equation for G coincides with that obtained from the static variational principle (5.76) with a Gaussian *Ansatz* for ρ; see Appendix B.

When ω is time independent we define $G\equiv(\sqrt{1-\xi^2}/2\omega)g$, and g satisfies

$$2\frac{\lambda}{\omega^3}lg^3+g^2-1=0 \ , \tag{5.82}$$

where l is given by (5.28b). The cubic equation for g may be solved; for weak coupling it gives[24]

$$g\approx 1-\frac{\lambda}{\omega^3}l \tag{5.83a}$$

for strong coupling,

$$g\approx\frac{\omega}{(2\lambda l)^{1/3}}-\frac{\omega^3}{6\lambda l} \tag{5.83b}$$

while in the absence of the harmonic term, $\omega=0$, we find

$$G=\frac{(1-\xi)^{2/3}(1+\xi)^{1/3}}{2\lambda^{1/3}} \ . \tag{5.83c}$$

The density matrix is static and, hence, describes equilibrium, but it is not the canonical Boltzmann distribution for the anharmonic oscillator. Although ρ may be written in the form (5.20), the static Ψ_n's are not exact energy eigenfunctions nor are the energy eigenvalues equally spaced in units of some w. (The Ψ_n's even are not variational approximations; see Ref. 26 below.) Presumably though, the static Gaussian density matrix with G given by (5.83) is a good approximation to the true canonical density matrix. That b occurring in (5.20) should, in fact, be identified with β, proportional to the inverse temperature, is not obvious from the formal development presented here, but is justified by the static variational principle; see Appendix B.

For the time-dependent problem, we remain with (5.80). Equations (5.80b) and (5.80c) cannot be combined into a single equation for a complex quantity as in (5.33) and (5.34), but one may still get a second-order equation for $Q=(1-\xi)^{-1/2}G^{1/2}$.[25,26]

$$\ddot{Q}-\frac{l^2}{Q^3}+\omega^2 Q+2\lambda Q^3=0 . \tag{5.84}$$

This equation may alternatively be derived as follows. Upon differentiating the defining equation $Q^2=\langle x^2\rangle$ we get

$$\dot{Q}=\frac{1}{2Q}\mathrm{tr}\dot{\rho}x^2=\frac{1}{2Q}\mathrm{tr}i[\rho,H]x^2$$
$$=\frac{1}{2Q}\mathrm{tr}\rho i[H,x^2] . \tag{5.85a}$$

For a Hamiltonian of the form $H=p^2/2+V(x)$, the above becomes

$$\dot{Q}=\frac{1}{2Q}\langle px+xp\rangle . \tag{5.85b}$$

Differentiating once more and evaluating the relevant commutators with H gives

$$\ddot{Q}=-\frac{1}{4Q^3}\langle px+xp\rangle^2+\frac{1}{Q}\langle p^2\rangle$$
$$-\frac{1}{Q}\left\langle x\frac{d}{dx}V(x)\right\rangle . \tag{5.85c}$$

The first two terms on the right-hand side are evaluated with our Gaussian density matrix from (5.6), and they combine into l^2/Q^3. The last term, of course, depends on the form of the potential, for an even monomial $V(x)=\lambda_n x^{2n}$, we need the expected value of $2n\lambda_n x^{2n}$; in the Gaussian approximation this is $\lambda_n[(2n)!/2^{n-1}(n-1)!]Q^{2n}$, and with this result (5.84) is regained.[27]

The classical limit, $4G\Pi\gg 1-\xi$, continues to be characterized by $\dot{G}/(1-\xi)\gg 1$ by virtue of (5.80b), which does not see the interaction. Equivalently, the classical limit sets in when $(d/dt)Q^2\gg 1$.

The intricacy of the nonlinear problem renders analytic solution unfeasible. [Elliptic functions solve (5.84).] A mechanical analogy for (5.84) aids understanding. In particular note that at late times, when ω^2 becomes constant, the motion of $Q\sim\langle x^2\rangle^{1/2}$ is governed by an effective "potential," with "centrifugal" repulsion whose strength depends on the degree of mixing:

$$V_{\mathrm{eff}}(Q)=\frac{l^2}{2Q^2}+\frac{1}{2}\omega_f^2 Q^2+\frac{\lambda}{2}Q^4 . \tag{5.86}$$

Generically Q will oscillate about the minimum of (5.86) and static equilibrium is not regained. Presumably there exists specific time profiles for $\omega^2(t)$ such that Q settles at the minimum of V_{eff}. With such generalizations for the reflectionless potentials of the noninteracting case, equilibrium is regained, but we have no explicit examples.

It is expected that increasing the strength of the interaction dampens the oscillation, suppressing departures from equilibrium. This is confirmed by numerical analysis. Consider $\omega^2(t)$ given by

$$\omega^2(t)=\begin{cases}\nu^2, & t\le t_i ,\\ \dfrac{2t-t_i-t_f}{t_i-t_f}\nu^2, & t_i<t<t_f ,\\ -\nu^2, & t\ge t_f\end{cases} \tag{5.87}$$

and equilibrium at initial times, i.e., (5.82) and (5.83) hold for $t\le t_i$ with $\omega^2=\nu^2$. The profile (5.87) describes transition from a stable potential with minimum at the origin, to a bistable potential with two minima and instability at the origin. The numerical evaluation of subsequent evolution is shown in Figs. 2(a)–2(d) and Figs. 3(a)–3(d). The following conclusions are drawn. While equilibrium is not attained, increasing $t_f-t_i\equiv\tau$ at fixed λ decreases the oscillation about equilibrium. Similarly, at fixed τ, increasing the strength of the self-interaction decreases the excursions from equilibrium.

The return to equilibrium with increasing τ, anticipated from the analysis of the linear problem, can be also established on general principles, with the help of the quantum adiabatic theorem. Consider the defining expression for the Boltzmann distributed density matrix at the early times:

$$\rho_i(\mathbf{x},\mathbf{y})=\sum_n p_n\Psi_n(\mathbf{x};\omega_i)\Psi_n^*(\mathbf{y};\omega_i) , \tag{5.88a}$$

$$p_n=e^{-\beta_i E_n(\omega_i)}/\sum_{n'}e^{-\beta_i E_{n'}(\omega_i)} . \tag{5.88b}$$

Dependence on the parameter that will vary with time for $t_i<t<t_f$ is explicitly indicated. If the variation is sufficiently slow, the quantum adiabatic theorem states that apart from position-independent phases, the wave functions evolve into $\Psi_n(\mathbf{x};\omega(t))$; hence, at intermediate times the density matrix is

$$\rho(\mathbf{x},\mathbf{y};t)=\sum_n p_n\Psi_n(\mathbf{x};\omega(t))\Psi_n^*(\mathbf{y};\omega(t)) \tag{5.88c}$$

and in late times attains equilibrium:

$$\rho_f(\mathbf{x},\mathbf{y})=\sum_n p_n\Psi_n(\mathbf{x};\omega_f)\Psi_n^*(\mathbf{y};\omega_f) . \tag{5.88d}$$

But this need not be thermal equilibrium. The occupation probabilities remain given by (5.88b), and involve $\beta_i E_n(\omega_i)$ which in general cannot be written as $\beta_f E_n(\omega_f)$. Only for energy eigenvalues of the form $E_n(\omega)=f(\omega)e_n$, as in the harmonic oscillator, can a final temperature be defined by $\beta_f=[f(\omega_i)/f(\omega_f)]/\beta_i$. (Of course the argument holds for arbitrary slowly varying parameters in the Hamiltonian, not just frequency.)

Next consider the de Sitter field theory (5.61) with an additional quartic self-coupling. Extracting the factor $e^{d\chi t/2}$ from the field as before, we obtain the Hamiltonian density

$$\mathcal{H}=\tfrac{1}{2}\Pi^2+\tfrac{1}{2}e^{-2\chi t}(\nabla\Phi)^2$$
$$+\frac{1}{2}\left[-\frac{d^2\chi^2}{4}+m^2+gR\right]\Phi^2+\frac{\lambda}{6}e^{-d\chi t}\Phi^4 . \tag{5.89}$$

After diagonalization, the variational equations with the interaction term become

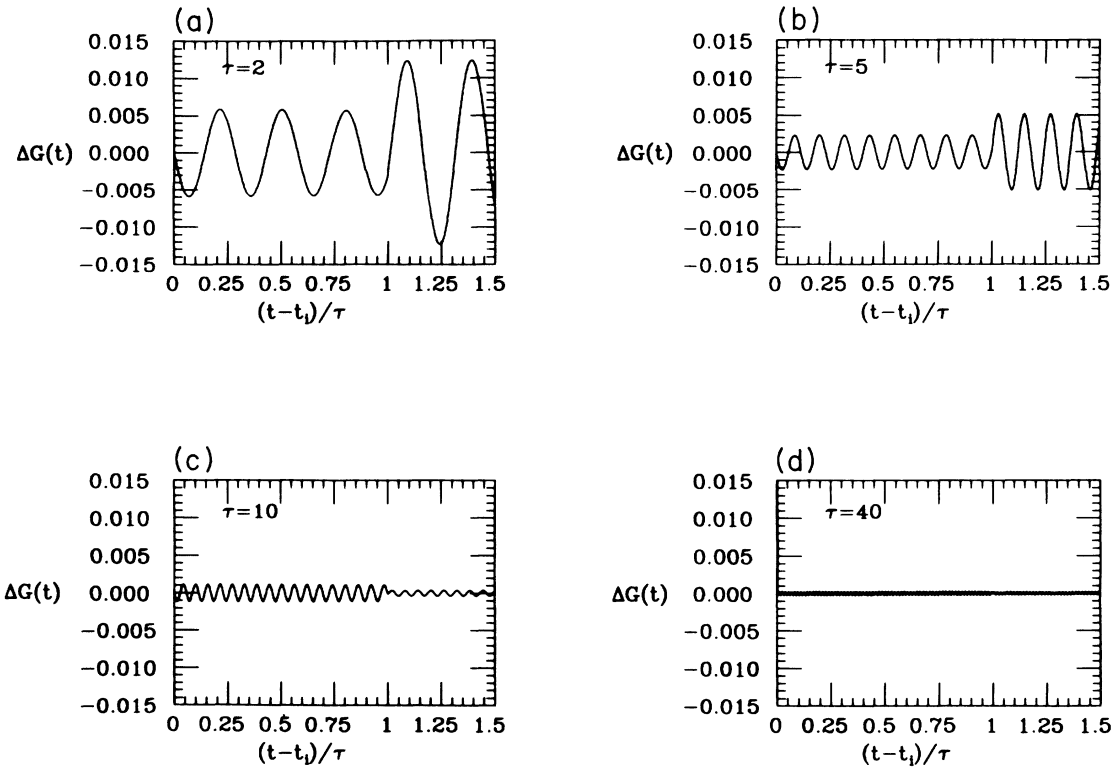

FIG. 2. $\Delta G(t)$ as a function of $(t-t_i)/\tau$ for different values of τ: (a) $\tau=2$; (b) $\tau=5$; (c) $\tau=10$; (d) $\tau=40$. In the numerical work we took $\xi=0.5$, $\nu^2=1$, and $\lambda=1$.

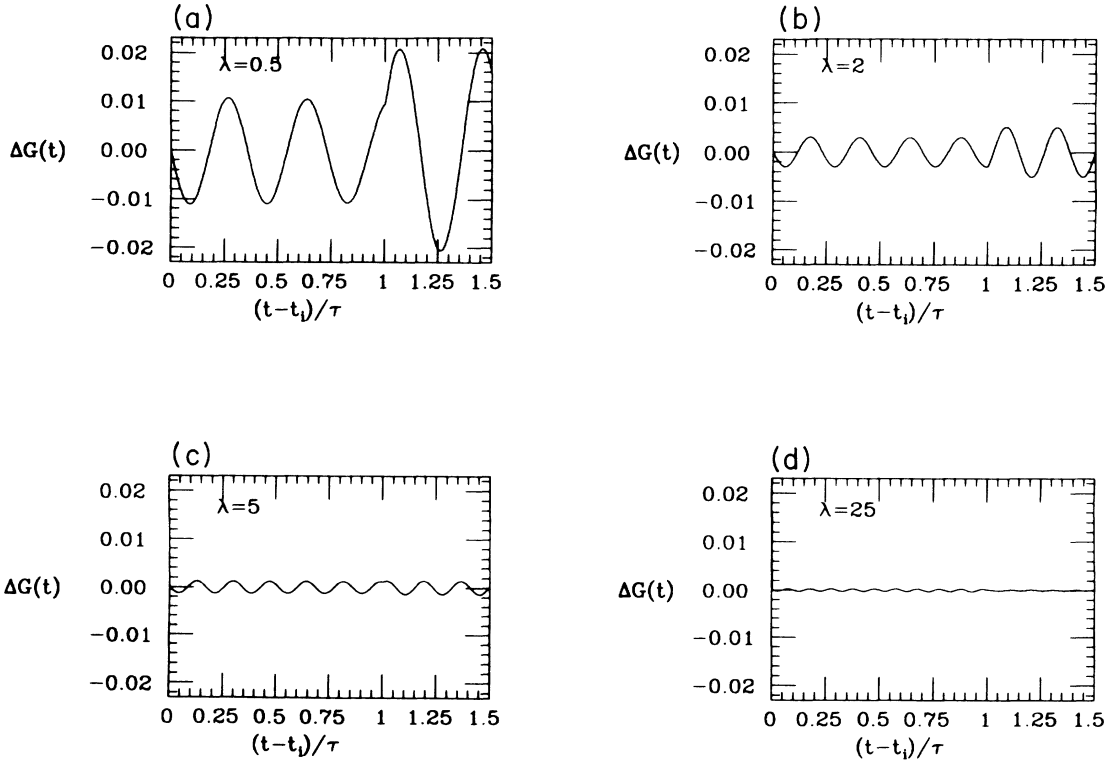

FIG. 3. $\Delta G(t)$ as a function of $(t-t_i)/\tau$ for different values of λ: (a) $\lambda=0.5$; (b) $\lambda=2$; (c) $\lambda=5$; (d) $\lambda=25$. We took $\tau=2$, $\nu^2=1$, and $\xi=0.5$.

$$\dot{G}(\mathbf{p})=4\Pi(\mathbf{p})G(\mathbf{p}) , \tag{5.90a}$$

$$\dot{\Pi}(\mathbf{p})=\frac{1-\xi^2(\mathbf{p})}{8G^2(\mathbf{p})}-2\Pi^2(\mathbf{p}) -\frac{1}{2}\left[e^{-2\chi t}\mathbf{p}^2-\frac{d^2\chi^2}{4}+m^2+gR +2\lambda e^{-d\chi t}\int_{\mathbf{k}}\frac{G(\mathbf{k})}{1-\xi(\mathbf{k})}\right] , \tag{5.90b}$$

and ξ is constant ($\xi_I=0$). Of course, these reduce to already studied examples in various limits.[21,23]

The equations must be renormalized to remove an ultraviolet divergence in the $\mathbf{k}$ integral. This is achieved more easily by passing to the second-order equation, which results when (5.90) are combined to

$$\ddot{G}(\mathbf{p})=\frac{1-\xi^2(\mathbf{p})}{2G(\mathbf{p})}+\frac{1}{2}\frac{\dot{G}^2(\mathbf{p})}{G(\mathbf{p})} -2[e^{-2\chi t}\mathbf{p}^2+\mu^2(t)]G(\mathbf{p}) , \tag{5.91}$$

where we have defined the time-dependent mass $\mu(t)$:

$$\mu^2(t)=-\frac{d^2\chi^2}{4}+m^2+gR+2\lambda e^{-d\chi t}\int_{\mathbf{k}}\frac{G(\mathbf{k})}{1-\xi(\mathbf{k})} . \tag{5.92}$$

In order to analyze the divergence in the above $\mathbf{k}$ integral, we obtain the high-p behavior of $G(\mathbf{p})$:

$$G(\mathbf{p})\underset{p\to\infty}{=}\frac{1}{2[e^{-2\chi t}\mathbf{p}^2+\sigma^2(t)]^{1/2}} , \tag{5.93a}$$

$$\sigma^2(t)=m^2+\left[g-\frac{1}{4}\left[1-\frac{1}{d}\right]\right]R +2\lambda e^{-d\chi t}\int_{\mathbf{k}}\frac{G(\mathbf{k})}{1-\xi(\mathbf{k})} . \tag{5.93b}$$

We have assumed that for large $\mathbf{p}$, the time-independent $\xi(\mathbf{p})$ goes to zero sufficiently fast to be neglected. (For example, we take $1/\xi(\mathbf{p})=\cosh[e^{-2\chi t_i}\mathbf{p}^2+\mu_i^2(t)]^{1/2}$.) Therefore, the ultraviolet behavior of the k integral is

$$I=2\lambda e^{-d\chi t}\int_{\mathbf{k}}\frac{1}{2[(e^{-\chi t}\mathbf{k})^2+\sigma^2(t)]^{1/2}} . \tag{5.94a}$$

It is convenient to integrate over the variable $\mathbf{q}\equiv e^{-\chi t}\mathbf{k}$, which is the physical momentum. This leaves a particularly simple form for the divergent integral:

$$I=2\lambda\int_{\mathbf{q}}\frac{1}{2[\mathbf{q}^2+\sigma^2(t)]^{1/2}} . \tag{5.94b}$$

In order to render (5.92) finite we use the same renormalization procedure[8] that renormalizes the Hartree-Fock approximation for pure states. In the case of (3 + 1)-dimensional spacetime, this prescription is

$$\frac{m^2}{\lambda}=\frac{m_R^2}{\lambda_R}-2I_1 , \tag{5.95a}$$

$$\frac{1}{\lambda}=\frac{1}{\lambda_R}-2I_2(M) , \tag{5.95b}$$

$$g_R=g[1-2\lambda_R I_2(M)]+\tfrac{1}{3}\lambda_R I_2(M) , \tag{5.95c}$$

where M is an arbitrary renormalization mass, and I_1, I_2 are defined by

$$I_1=\int_{\mathbf{q}}\frac{1}{2|\mathbf{q}|} , \tag{5.95d}$$

$$I_2(M)=\frac{1}{M^2}\int_{\mathbf{q}}\left[\frac{1}{2|\mathbf{q}|}-\frac{1}{2(\mathbf{q}^2+M^2)^{1/2}}\right] . \tag{5.95e}$$

Using (5.95), one can show that $\mu^2(t)$ satisfying

$$\mu^2(t)=m_R^2+\chi^2\left[-\frac{9}{4}+12g_R+\frac{\lambda_R}{2}I_2(M)\right] -2\lambda_R\left[I_1-\mu^2(t)I_2(M)-e^{-3\chi t}\int_{\mathbf{k}}\frac{G(\mathbf{k})}{1-\xi(\mathbf{k})}\right] \tag{5.96}$$

is finite.

For the cases $d=2$ or $d=1$ it is sufficient to perform a subtraction only in the mass:

$$m_R^2=m^2+2\lambda\int_{\mathbf{q}}\frac{1}{2(\mathbf{q}^2+M^2)^{1/2}} . \tag{5.97}$$

The solutions of (5.91) and (5.92), renormalized as in (5.96) or (5.97), can be achieved only numerically. However, we have not succeeded in the numerical analysis, because the exponentials in those equations give rise to large numbers, which overwhelmed our computational resources and rendered our results unreliable.

An interacting field-theoretic problem that is still tractable can be obtained from the above by working in flat space ($\chi=R=0$), but allowing a time variation in m^2: positive for early times, negative for late times. We take $m_R^2(t)$ to be

$$m_R^2(t)=\begin{cases} m_0^2, & t\le t_i , \\ \dfrac{2t-t_i-t_f}{t_i-t_f}m_0^2, & t_i<t<t_f , \\ -m_0^2, & t\ge t_f \end{cases} \tag{5.98}$$

and assume that, at t_i,

$$G(\mathbf{p},t_i)=\frac{[1-\xi^2(\mathbf{p})]^{1/2}}{2(\mathbf{p}^2+M^2)^{1/2}} , \tag{5.99a}$$

$$\frac{1}{\xi(\mathbf{p})}=\cosh(\beta_i\sqrt{\mathbf{p}^2+M^2}) , \tag{5.99b}$$

and that $\Pi(\mathbf{p},t_i)$ vanishes. Figures 4 and 5 present the results of our calculation for $m_0^2=M^2=10^{-2}$, $t_i=0$, $t_f=80$, $\beta_i=1$, $d=2$, and $\lambda=10^{-6}$. From these figures we see that the low-momentum modes behave as upside-down harmonic oscillators for $t\ge t_f$ until the time when their growth makes the last term in (5.92) compensate the fact that $m_R^2(t\ge t_f)$ is negative. The high-momentum modes (i.e., those with $p^2\gg m_0^2$) remain approximately

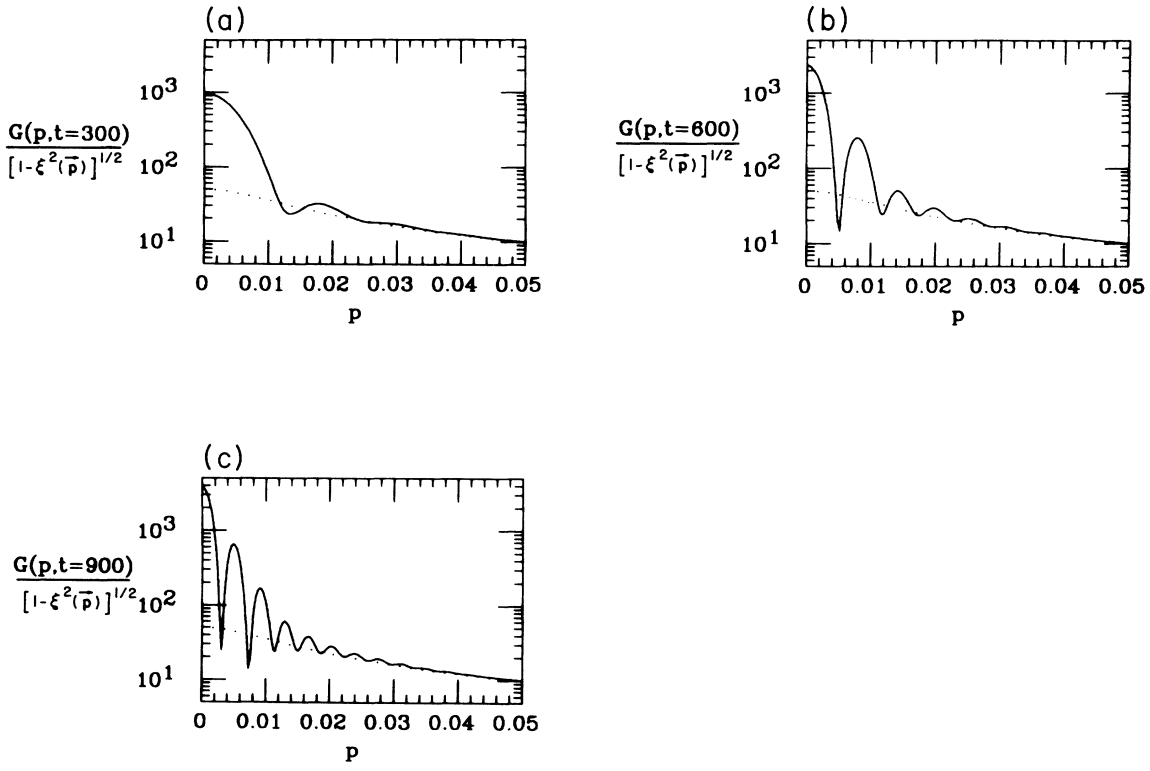

FIG. 4. $G(\mathbf{p},t)$ as a function of $|\mathbf{p}|$ for different values of t: dotted lines in (a)–(c) stand for $G(\mathbf{p},t=0)$, while the solid line stands for (a) $t=300$; (b) $t=600$; (c) $t=900$.

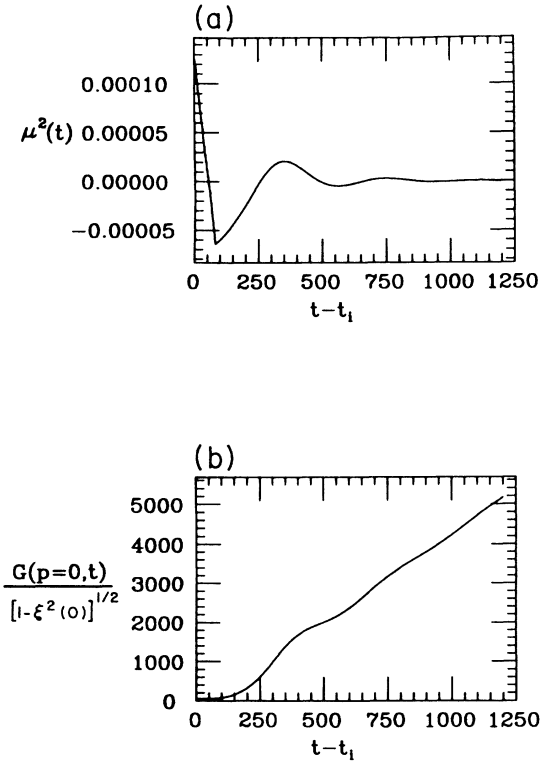

FIG. 5. (a) $\mu^2(t)$; (b) $G(\mathbf{p}=0;t)$.

constant, as is anticipated form (5.94). We expect these features to characterize the de Sitter problem; however we were not able to show this numerically. (This model, with our Gaussian *Ansatz*, does not permit a vacuum expectation value for Φ, even when the effective mass squared is negative.)

VI. CONCLUSION

The Schrödinger picture variational principle for the density matrix provides us in the Gaussian approximation with tractable variational equations that determine the time evolution of interesting physical quantities. Within this formalism one can study how a system in equilibrium loses and perhaps regains equilibrium when the Hamiltonian acquires a transient, time-dependent disturbance. The equations that we deal with are the analogs in the present context of time-dependent Hartree-Fock equations or large-n approximations. As such, they suffer from well-known shortcomings, especially in higher-dimensional field theory. Nevertheless, the field-theoretic equations are mathematically consistent, because they can be renormalized.

Improvement in our method should be looked for in two areas. First, one may wish to improve our calculational method by going beyond the Gaussian approximation. This may be achieved by choosing more elaborate trial density matrices, or one may develop a systematic

expansion, based on the nonequilibrium effective action. Second, improvement in the conceptual basis of our approach is also desirable; specifically one should relax the isoentropic restriction, by considering a more general equation than the Liouville–von Neumann one, which forms the basis of our work. In other words, one wants to allow time dependence in the occupation probabilities, as discussed in Sec. III. While this can be done in a variety of ways,[28] a dynamical model is required for the evolution of the environment and for the interaction of the environment with our system. When the Universe itself is our system, it is unclear what one should take for the environment. When attention is focused on one aspect of our system, for example, the inflation-driving axion field,[29] the environment can be the other elementary particle and radiation fields. Yet a question still remains on how the influence of one on the other should be parametrized. Alternatively, one may compute the isoentropic density matrix, as we have done, and then divide its variables into "environmental" and "systematic." Integrating over the former, coarse graining, produces a density matrix for the "system" with time-dependent occupation probabilities.

ACKNOWLEDGMENTS

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APPENDIX A

For completeness we record in this appendix the equations relevant to the most general Gaussian *Ansatz* for a density matrix of an O(n) quantum field theory in ($d+1$)-dimensional Robertson-Walker space time, described by the metric

$$ds^2=dt^2-a^2(t)d\mathbf{x}^2 , \tag{A1}$$

which leads to the curvature $R=2d\ddot{a}/a+d(d-1)\dot{a}^2/a^2$. The dynamics of the fields Φ^i is taken to be governed by the Lagrange density

$$\mathcal{L}=a^d\left[\frac{1}{2}\dot{\Phi}^i\dot{\Phi}^i-\frac{1}{2}a^{-2}\nabla\Phi^i\nabla\Phi^i-\frac{1}{2}(m^2+gR)\Phi^i\Phi^i-\frac{\lambda}{2(n+2)}(\Phi^i\Phi^i)^2\right] \tag{A2}$$

whose canonical momentum is

$$\Pi^i\equiv\frac{\partial\mathcal{L}}{\partial\dot{\Phi}^i}=a^d\dot{\Phi}^i . \tag{A3}$$

The special case of de Sitter space-time, dealt with in the text, corresponds to $a(t)=e^{\chi t}$. This factor, raised to the power $d/2$, was scaled from the field Φ to obtain simpler equations. Here we shall postpone the rescaling until the variational equations are derived. At that stage we shall rescale the variational parameters. This alternate procedure is entirely equivalent to what is done in the text, and is offered here merely for variety.

The Hamiltonian density corresponding to $\mathcal{L}$ is

$$\mathcal{H}=\tfrac{1}{2}a^{-d}\Pi^i\Pi^i+a^d\left[\frac{1}{2}a^{-2}\nabla\Phi^i\nabla\Phi^i+\frac{1}{2}(m^2+gR)\Phi^i\Phi^i+\frac{\lambda}{2(n+2)}(\Phi^i\Phi^i)^2\right] . \tag{A4}$$

In order to implement the variational principle (4.8) we make the following *Ansätze* for ρ and Λ:

$$\rho(\varphi_1,\varphi_2)=e^{-\gamma}e^{iP(\varphi_1-\varphi_2)}\exp\{-\tfrac{1}{2}[(\varphi_1-\bar{\varphi})A(\varphi_1-\bar{\varphi})+(\varphi_2-\bar{\varphi})A^*(\varphi_2-\bar{\varphi})-2(\varphi_1-\bar{\varphi})B(\varphi_2-\bar{\varphi})]\} , \tag{A5a}$$

$$\hat{\Lambda}=\Lambda^{(1)}\mathbb{1}+\Lambda^{(\Phi)}\Phi+\Lambda^{(\Pi)}\Pi+\Pi\Lambda^{(\Pi^2)}\Pi-(\Phi\Lambda^{(\Phi\Pi)}\Pi+\Pi\Lambda^{(\Phi\Pi)}\Phi)+\Phi\Lambda^{(\Phi\Phi)}\Phi . \tag{A5b}$$

The factor γ in ρ is given by $\frac{1}{2}\ln\det\pi(A_R-B_R)^{-1}$. With the above density matrix, linear averages no longer vanish,

$$\langle\Phi\rangle=\bar{\varphi} , \tag{A6a}$$

$$\langle\Pi\rangle=P , \tag{A6b}$$

and bilinears become

$$\langle\Phi_i(\mathbf{x})\Phi_j(\mathbf{y})\rangle=\bar{\varphi}_i(\mathbf{x})\bar{\varphi}_j(\mathbf{y})+\Xi_{ij}(\mathbf{x},\mathbf{y}) , \tag{A6c}$$

$$\langle\Pi_i(\mathbf{x})\Pi_j(\mathbf{y})\rangle=P_i(\mathbf{x})P_j(\mathbf{y})+\tfrac{1}{2}(A_R+B_R)_{ij}(\mathbf{x},\mathbf{y})-[(B_I-A_i)\Xi(B_I+A_I)]_{ij}(\mathbf{x},\mathbf{y}) , \tag{A6d}$$

$$\langle\Phi_i(\mathbf{x})\Pi_j(\mathbf{y})\rangle=\frac{i}{2}\delta_{ij}\delta(\mathbf{x}-\mathbf{y})+\bar{\varphi}_i(\mathbf{x})P_j(\mathbf{y})-[\Xi(B_I+A_I)]_{ij}(\mathbf{x},\mathbf{y}) , \tag{A6e}$$

where

$$\Xi^{-1}\equiv 2(A_R-B_R) . \tag{A7}$$

Upon demanding that the variations of the action with respect to the $\Lambda^{(a)}$ vanish, the following equations result:

$$\dot{\bar{\varphi}}_i(\mathbf{x})=a^{-d}P_i(\mathbf{x}) , \tag{A8a}$$

$$\dot{P}_i(\mathbf{x})=-a^d\left[a^{-2}\nabla^2\bar{\varphi}_i(\mathbf{x})+(m^2+gR)\bar{\varphi}_i(\mathbf{x})+\frac{2\lambda}{n+2}\bar{\varphi}_i(\mathbf{x})\bar{\varphi}_k(\mathbf{x})\bar{\varphi}_k(\mathbf{x})+\frac{2\lambda}{n+2}\bar{\varphi}_i(\mathbf{x})\Xi_{kk}(\mathbf{x},\mathbf{x})+\frac{4\lambda}{n+2}\Xi_{ik}(\mathbf{x},\mathbf{x})\varphi_k(\mathbf{x})\right] , \tag{A8b}$$

$$\dot{A}_R\pm\dot{B}_R\pm a^{-d}[B_I,A_R\pm B_R]=a^{-d}\{A_I,A_R\pm B_R\} , \tag{A8c}$$

$$\dot{B}_I=a^{-d}(\{A_I,B_I\}+[B_R,A_R]) , \tag{A8d}$$

$$\dot{A}_{I_{ij}}(\mathbf{x},\mathbf{y})=a^{-d}(-A_R^2+B_R^2+A_I^2+B_I^2)_{ij}(\mathbf{x},\mathbf{y})+a^d(-a^{-2}\nabla^2+m^2+gR)\delta_{ij}\delta(\mathbf{x}-\mathbf{y})$$
$$+\frac{2\lambda a^d}{n+2}[\delta_{ij}\bar{\varphi}_k(\mathbf{x})\bar{\varphi}_k(\mathbf{x})+2\bar{\varphi}_i(\mathbf{x})\bar{\varphi}_j(\mathbf{x})+\delta_{ij}\Xi_{kk}(\mathbf{x},\mathbf{x})+2\Xi_{ij}(\mathbf{x},\mathbf{x})]\delta(\mathbf{x}-\mathbf{y}) . \tag{A8e}$$

Translation invariance allows us to diagonalize the kernels through the use of (5.8) and also we assume that the matrix structure is trivial; thus $B_I=0$. In order to make contact with the notation of Sec. V we define

$$G(\mathbf{p})=\frac{1}{2A_R(\mathbf{p})} , \tag{A9a}$$

$$\Pi(\mathbf{p})=-\tfrac{1}{2}A_I(\mathbf{p}) , \tag{A9b}$$

$$\xi(\mathbf{p})=\frac{B_R(\mathbf{p})}{A_R(\mathbf{p})} . \tag{A9c}$$

In terms of $\bar{\varphi}$, P, ξ, G, and Π the equations of motion read

$$\dot{\bar{\varphi}}=a^{-d}P , \tag{A10a}$$

$$\dot{P}=-a^d\left[m^2+gR+\frac{2n\lambda}{n+2}\bar{\varphi}^2+2\lambda\int_{\mathbf{k}}\frac{G(\mathbf{k})}{1-\xi(\mathbf{k})}\right]\bar{\varphi} , \tag{A10b}$$

$$\dot{G}(\mathbf{p})=a^{-d}4\Pi(\mathbf{p})G(\mathbf{p}) , \tag{A10c}$$

$$\dot{\Pi}(\mathbf{p})=a^{-d}\left[\frac{1-\xi^2(\mathbf{p})}{8G^2(\mathbf{p})}-2\Pi^2(\mathbf{p})\right]-\frac{a^d}{2}\left[a^{-2}\mathbf{p}^2+m^2+gR+2\lambda\bar{\varphi}^2+2\lambda\int_{\mathbf{k}}\frac{G(\mathbf{k})}{1-\xi(\mathbf{k})}\right] , \tag{A10d}$$

and ξ is constant.[30] Next we change variables

$$\bar{\varphi}=a^{-d/2}\tilde{\varphi} , \tag{A11a}$$

$$P=a^{d/2}\left[\tilde{P}-\frac{d}{2}\frac{\dot{a}}{a}\tilde{\varphi}\right] , \tag{A11b}$$

$$G=a^{-d}\tilde{G} , \tag{A11c}$$

$$\Pi=a^d\left[\tilde{\Pi}-\frac{d}{4}\frac{\dot{a}}{a}\right] . \tag{A11d}$$

In terms of these variables Eqs. (A10) read

$$\dot{\varphi}=P , \tag{A12a}$$

$$\dot{P}=-\left[\left[-\frac{1}{4}+g\right]R+\frac{d}{4}\frac{\dot{a}^2}{a^2}+m^2+\frac{2n}{n+2}\lambda a^{-d}\varphi^2+2\lambda a^{-d}\int_{\mathbf{k}}\frac{G(\mathbf{k})}{1-\xi(\mathbf{k})}\right]\varphi , \tag{A12b}$$

$$\dot{G}(\mathbf{p})=4\Pi(\mathbf{p})G(\mathbf{p}) , \tag{A12c}$$

$$\dot{\Pi}=\frac{1-\xi^2(\mathbf{p})}{8G^2(\mathbf{p})}-2\Pi^2(\mathbf{p})=\frac{1}{2}\left[a^{-2}\mathbf{p}^2+\left[-\frac{1}{4}+g\right]R+\frac{d}{4}\frac{\dot{a}^2}{a^2}+m^2+2\lambda a^{-d}\varphi^2+2\lambda a^{-d}\int_{\mathbf{k}}\frac{G(\mathbf{k})}{1-\xi(\mathbf{k})}\right] , \tag{A12d}$$

with the tilde suppressed.

Equations (A12b) and (A12d) are potentially ultraviolet divergent. In order to analyze better the divergence let us eliminate Π from (A12d) using (A12c):

$$\ddot{G}(\mathbf{p})=\frac{1-\xi^2(\mathbf{p})}{2G(\mathbf{p})}+\frac{1}{2}\frac{\dot{G}^2(\mathbf{p})}{G(\mathbf{p})}-2[a^{-2}\mathbf{p}^2+\mu^2(t)]G(\mathbf{p}) . \tag{A13}$$

The time-dependent mass $\mu^2(t)$ has been introduced:

$$\mu^2(t)=(-\tfrac{1}{4}+g)R+\frac{d}{4}\frac{\dot{a}^2}{a^2}+m^2+2\lambda a^{-d}\varphi^2 +2\lambda a^{-d}\int_k \frac{G(\mathbf{k})}{1-\xi(\mathbf{k})} . \tag{A14}$$

The asymptotic (large-p) behavior of G can be obtained from (A13):

$$G(\mathbf{p})\underset{\mathbf{p}\to\infty}{=}\frac{1}{2[a^{-2}\mathbf{p}^2+\sigma^2(t)]^{1/2}}[1+O(|\mathbf{p}|^{-5})] \tag{A15a}$$

with

$$\sigma^2(t)=m^2+\left[g-\frac{1}{4}\left[1-\frac{1}{d}\right]\right]R+2\lambda a^{-d}\varphi^2 +2\lambda a^{-d}\int_{\mathbf{k}}\frac{G(\mathbf{k})}{1-\xi(\mathbf{k})} , \tag{A15b}$$

where we assumed that $\xi(\mathbf{k})$ goes to zero sufficiently fast to be neglected. Therefore, the ultraviolet behavior of the k integral in (A12) and (A14) is

$$I=2\lambda a^{-d}\int_{\mathbf{k}}\frac{1}{2[(a^{-1}\mathbf{k})^2+\sigma^2(t)]^{1/2}} . \tag{A16}$$

It is convenient to change the integration variable to $\mathbf{q}=\mathbf{k}/a$ ($\mathbf{q}$=physical momentum), which leaves the ultraviolet divergence in a form identical to (5.94):

$$I=2\lambda\int_{\mathbf{q}}\frac{1}{2[\mathbf{q}^2+\sigma^2(t)]^{1/2}} . \tag{A17}$$

As expected, the ultraviolet divergence is the same as in Sec. V and consequently we can obtain finite equations by using the renormalization prescription presented there.

APPENDIX B

In this appendix we use the static variational principle (5.76) to obtain the same static density matrix as in (5.82) for an anharmonic oscillation whose Hamiltonian is

$$H=\frac{p^2}{2}+\frac{\omega^2}{2}x^2+\frac{\lambda}{6}x^4 . \tag{B1}$$

We need to evaluate the Helmholtz free energy (5.76) with the Gaussian trial density matrix (5.13). The first term, the entropy, was already found in (5.14). The remainder is straightforwardly computed. The result is

$$\begin{aligned}\beta F&=\langle \ln\rho+\beta H\rangle \\ &=\ln\left[2\sinh\frac{bw}{2}\right] \\ &\quad+\left[\frac{\beta}{4}w+\frac{\beta}{4}\frac{\omega^2}{w}-\frac{1}{2}bw+\beta\frac{\Pi^2}{w}\right]\coth\frac{bw}{2} \\ &\quad+\frac{\beta\lambda}{8w^2}\coth^2\frac{bw}{2} .\end{aligned} \tag{B2}$$

[We have used the normalized trial density matrix (5.13). Alternatively one may use the *Ansatz* (5.10) with an arbitrary normalization parametrized by γ, and vary $\beta F+N(\mathrm{tr}\rho-1)$, where N enforces the normalization. Upon stationarizing with respect to γ and N, and eliminating these variables (B2) is regained.] Rather than expressing (B2) in terms of G and ξ, via (5.12), it is simpler to view w, bw, and Π as the variational parameters. Varying Π shows that it vanishes in the static case. Setting to zero the variation with respect to w, at fixed bw, and using (5.12), produces an equation that coincides with the static limit of (5.80), viz., (5.82) is obtained. Variation with respect to bw shows that

$$b=\beta , \tag{B3}$$

as a consequence of (5.80). This relates the variational parameter b to the temperature, which enters in the definition of the Helmholtz free energy.

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[16]The role of Λ in the formalism is not merely to provide a Lagrange multiplier for the Liouville equation. It is also needed to give our action a canonical structure, which requires a pair of variables; i.e., in a sense ρ and Λ are as a canonically conjugate pair. Analogy can also be drawn to the pair of states $|\Psi_{\pm};t\rangle$ that occur in the zero-temperature variation principle (4.5). Indeed, initial and final conditions (4.6) are specified for $|\Psi_{+};t\rangle$ and $|\Psi_{-};t\rangle$, respectively, just as for ρ and Λ. Both ρ and Λ satisfy the same Liouville equation, but in our formalism Λ cannot be viewed as a density matrix, because Λ retains for all times its final form (4.11), $\Lambda=1$. However, the analogy to the pure-state variational principle and effective action (4.5)–(4.7) is not complete. The former resides in Hilbert space, deals with transition amplitudes, and the quantum action is complex. The latter concerns probabilities and the action is real. The introduction of the additional quantity Λ is reminiscent of the doubling that occurs in thermo-field dynamics; see, for instance, H. Umezawa, H. Matsumoto, and M. Tachiki, *Thermo-Field Dynamics and Condensed States* (North-Holland, Amsterdam, 1982); and, also, G. Semenoff and N. Weiss, Phys. Rev. D **31**, 689 (1985). In the Balian-Vénéroni work (Ref. 11) the Lagrange multiplier Λ has a more central role in the formalism, which we do not use here; see, however, Sec. V C.

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[18]The relevant Hermite polynomial summation formula is

$$\sum_n \frac{1}{n!}\left[\frac{z}{2}\right]^n H_n(x)H_n(y) = \frac{1}{\sqrt{1-z^2}}\exp\left[-\frac{z}{1-z^2}[(x^2+y^2)z-2xy]\right].$$

[19]There is a connection between (5.28) and (5.33), (5.35), (5.36): write $D=Qe^{i\varphi}$. From (5.36) we learn that $\ddot{Q}+\omega^2 Q - Q\dot{\varphi}^2=0$ and $(d/dt)(Q^2\dot{\varphi})=0$. Setting $\dot{\varphi}=l/Q^2$, we see that Q satisfies (5.28a). Moreover (5.33) and (5.35) imply $\dot{Q}/Q=2\Pi$ and $\dot{\varphi}=\sqrt{1-\xi^2}/2G$. This reproduces the equations of the text with $Q=(1-\xi)^{-1/2}G^{1/2}$ and $l=\frac{1}{2}[(1+\xi)/(1-\xi)]^{1/2}$; see also Ref. 25 below.

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[24]The density matrix evaluated in perturbation theory to $O(\lambda)$ does not bear any simple relation to our variationally determined weak-coupling result.

[25]Our system of equations may also be presented in the following way. Equation (5.84) is equivalent to

$$\ddot{D}+\omega^2 D+2\lambda D\,|\,D\,|^2=0\,,$$

where D is the complex quantity $Qe^{i\varphi}$. As with $\lambda=0$, $Q^2\dot{\varphi}$ is constant, taken to equal l; see Ref. 19. In this form, the equations also hold in the time-dependent Hartree-Fock variational approximation for a quantum state $\Psi_0(x)\propto\exp(-\frac{1}{2}x\Omega x)$, $\Omega=G^{-1}/2-2i\Pi$, with $Q=G^{1/2}$, $\dot{Q}/Q=2\Pi$, and $l=\frac{1}{2}$, i.e., $\Omega=-i(d/dt)\ln D$; see Ref. 23.

[26]There is an alternative route to a Gaussian density matrix. One may solve the time-dependent variational equation for a time-dependent Gaussian wave function Ψ_0, construct Ψ_n as in (5.19), and then sum the density matrix as in (5.20). While this indeed leads to a Gaussian the result does not agree with the variationally determined Gaussian density matrix in the presence of nonlinear interactions. Specifically, the parameters in the alternative Gaussian density matrix do not satisfy the variational equations (5.80). [Only the interaction, the last term in (5.80c), spoils agreement.]

[27]This derivation is similar to the one used by G. Mazenko, in his large-n studies, Phys. Rev. Lett. **54**, 2163 (1985), Phys. Rev. D **34**, 2223 (1986).

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[30]The above equations (with vanishing linear averages) have also been derived by Mazenko (Ref. 27) in the large-n approximation, which, as is well known from equilibrium investigations, is also a Gaussian approximation. Mazenko presents three equations, while we have only two nontrivial ones: (A10c) and (A10d). Apparently, one linear combination of his three merely expresses the constancy of our ξ.