Dissipation and Decoherence in Mean Field Theory

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The time evolution of a closed system of mean fields and fluctuations is Hamiltonian, with the canonical variables parametrizing the general time-dependent Gaussian density matrix of the system. Yet, the evolution manifests both quantum decoherence and apparent irreversibility of energy flow from the coherent mean fields to fluctuating quantum modes. Using scalar QED as an example, we show how this collisionless damping and decoherence may be understood as the result of *dephasing* of the rapidly varying fluctuations and particle production in the time varying mean field. [S0031-9007(96)00360-2]

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Mean field methods have a long history in such diverse areas as atomic physics (Born-Oppenheimer), nuclear physics (Hartree-Fock), condensed matter (BCS) and statistical physics (Landau-Ginzburg), quantum optics (coherent or squeezed states), and semiclassical gravity. Because no higher than second moments of the fluctuations are incorporated, the mean field approximation is related to a Gaussian variational ansatz for the wave function of the system. The broad applicability of the approximation, as well as the variety of different approaches to it in the literature, makes it worthwhile to exhibit its general features unobscured by the particulars of specific applications. Accordingly, our first purpose in this Letter is to demonstrate the equivalence of the time-dependent mean field approximation to the general Gaussian ansatz for the mixed state density matrix ρ , and to underline its Hamiltonian structure.

The Hamiltonian nature of the evolution makes it clear from the outset that the mean field approximation does not introduce dissipation or time irreversibility at a fundamental level. Nevertheless, typical evolutions seemingly manifest an arrow of time, in the sense that energy flows from the mean field to the fluctuations without returning over times of physical interest [1] (Fig. 1). Closely connected to this effective dissipation is the phenomenon of quantum decoherence [2], i.e., the suppression with time of the overlap between wave functions corresponding to two different mean field evolutions (Fig. 2). Decoherence is the reason why quantum superpositions of different mean field states are difficult to observe in nature, and is crucial to understanding the quantum to classical transition in macroscopic systems. Our second aim in this Letter is to provide a clear physical explanation of both these behaviors in terms of dephasing of the fluctuations, i.e., the averaging to zero of their rapidly varying phases on time scales short compared to the collective motion of the mean field(s), and to present an explicit example of a quantum mean field theory (scalar QED) where these effects are observed.

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To expose the general structure of the time-dependent mean field (or Gaussian) approximation consider first a one-dimensional harmonic oscillator with Hamiltonian

$$H_{\rm osc}(q, p; t) = \frac{1}{2} [p^2 + \omega^2(t)q^2], \qquad (1)$$

where the frequency $\omega(t)$ is a smooth function of time, otherwise unspecified for the moment. The most general



FIG. 1. Evolution of the electric field, and the Boltzmann and effective entropies for $e^2 = 0.1$. The electric field is expressed in units of $E_c = m^2 c^3/e\hbar$. Pair creation is rapid when $|E| > E_c$.

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FIG. 2. Absolute values of the decoherence functional $|F_{12}|$ as a function of time. The two field values are E and $E - \Delta$. The top figure shows (for fixed Δ) the sharp dependence of decoherence on particle production when $|E| \ge 0.2E_c$. The second illustrates the relatively milder dependence on Δ .

Gaussian form for the mixed state normalized density matrix may be presented as

$$\langle x' | \rho(\overline{q}, \overline{p}; \xi, \eta; \sigma) | x \rangle = (2\pi\xi^2)^{-1/2}$$

$$\times \exp \left\{ i \frac{\overline{p}}{\hbar} (x' - x) - \frac{\sigma^2 + 1}{8\xi^2} [(x' - \overline{q})^2 + (x - \overline{q})^2] \right.$$

$$+ i \frac{\eta}{2\hbar\xi} [(x' - \overline{q})^2 - (x - \overline{q})^2]$$

$$+ \frac{\sigma^2 - 1}{4\xi^2} (x' - \overline{q}) (x - \overline{q}) \left. \right\}$$

$$(2)$$

in the coordinate representation. The five parameters $(\overline{q}, \overline{p}; \xi, \eta; \sigma)$ of this Gaussian may be identified with the two mean values, $\overline{q} = \langle q \rangle \equiv \text{Tr}(q\rho), \ \overline{p} = \langle p \rangle \equiv \text{Tr}(p\rho)$, and the three symmetrized variances via

$$\langle (q - \overline{q})^2 \rangle = \xi^2, \qquad \langle (pq + qp - 2\overline{q}\,\overline{p}\,) \rangle = 2\xi\eta, \langle (p - \overline{p}\,)^2 \rangle = \eta^2 + \hbar^2 \sigma^2 / 4\xi^2.$$
 (3)

The one antisymmetrized variance is fixed by the commutation relation, $[q, p] = i\hbar$. The parameter σ measures the degree to which the state is mixed: $\text{Tr}\rho^2 = \sigma^{-1} \leq 1$, the equality holding for pure states. If the state is pure, ρ decomposes into a product, $|\psi\rangle\langle\psi|$, and only two of the three symmetrized variances in (3) are independent.

The Gaussian form of the density matrix (2) is preserved under time evolution with H_{osc} . In the Schrödinger picture, ρ evolves according to the Liouville equation, $\dot{\rho} = -i[H, \rho]$. Substitution of the Gaussian form (2) into this equation with Hamiltonian (1) and equating coefficients of x, x', x², x'², and xx' gives five evolution equations for the five parameters specifying the Gaussian,

$$\begin{aligned} \dot{\overline{q}} &= \overline{p}, \qquad \dot{\overline{p}} &= -\omega^2(t)\overline{q}, \\ \dot{\overline{\xi}} &= \eta, \qquad \dot{\eta} &= -\omega^2(t)\overline{\xi} + \hbar^2\sigma^2/4\xi^3, \end{aligned}$$
(4)

and $\dot{\sigma} = 0$. Evolution equations for the diverse applications of the time-dependent mean field approximation reduce to (multiple copies of) equations of precisely the general form of (4), with $\omega^2(t)$ a different selfconsistently determined function of the coordinates and time, depending on the application. This establishes the equivalence between mean field methods and Gaussian density matrices for all evolutions of the form of Eqs. (4). We give explicit examples below.

An essential property of the evolution equations (4) is that they are Hamilton's equations (hence, time reversible) for an effective classical Hamiltonian [3], with η playing the role of the momentum conjugate to ξ ,

$$H_{\rm eff}(\overline{q},\overline{p};\xi,\eta;\sigma) = {\rm Tr}(\rho H) = \frac{1}{2}(\overline{p}^2 + \eta^2) + V_{\rm eff},$$
(5)

and $V_{\text{eff}}(\overline{q}, \xi; \sigma)$ depending on the particular form of $\omega^2(\overline{q}(t), \xi(t); t)$. For example, if the original system is an anharmonic double well with quantum Hamiltonian

$$H(q,p) = \frac{1}{2}p^2 + (\lambda/4)(q^2 - v^2)^2, \qquad (6)$$

then the (large N) mean field equations of motion are identical to Eqs. (4) with $\omega^2(t) = \lambda [\overline{q}^2(t) + \xi^2(t) - v^2]$. In this case,

$$V_{\rm eff}(\bar{q},\xi) = (\lambda/4)(\bar{q}^2 + \xi^2 - v^2)^2 + \hbar^2 \sigma^2/8\xi^2, \quad (7)$$

and the resulting Eqs. (4) are now quite nonlinear. The last "centrifugal" term in the effective potential (7) is a manifestation of the quantum uncertainty principle which prevents the Gaussian width ξ from vanishing.

The unitary operator U(t) which affects the time evolution of the Gaussian density matrix (2) is easily found, but we shall not need its explicit form here. It generates the time evolution of the Heisenberg operators,

$$q(t) = U^{\dagger}(t)q(0)U(t) = \overline{q}(t) + af(t) + a^{\dagger}f^{*}(t),$$

$$p(t) = U^{\dagger}(t)p(0)U(t) = \overline{p}(t) + a\dot{f}(t) + a^{\dagger}\dot{f}^{*}(t),$$
(8)

in the Fock representation where $[a, a^{\dagger}] = 1$, and the commutation relation requires the complex functions *f* to satisfy the Wronskian condition,

$$\dot{f}\dot{f}^* - \dot{f}f^* = i\hbar.$$
(9)

Actually, there is considerable latitude to redefine f by the Bogoliubov transformation $f \rightarrow \cosh \gamma e^{i(\theta + \phi)} f + \sinh \gamma e^{i(\theta - \phi)} f^*$ without affecting the Wronskian condition. Such Bogoliubov transformations form a noncompact Lie group, whose Lie algebra is generated by the three symmetric bilinears aa, $a^{\dagger}a^{\dagger}$, and $aa^{\dagger} + a^{\dagger}a$. If the *a* and a^{\dagger} operators are appended to these three, the algebra again closes upon itself, forming a five parameter

Lie group. The unitary evolution of the Gaussian density matrix (2) is an explicit representation of this group with Casimir invariant $\hbar^2 \sigma^2/4$.

The Lie group structure can be exploited to choose a basis in which all expectation values vanish, except

$$\langle a^{\dagger}a\rangle = \langle aa^{\dagger}\rangle - 1 \equiv N \ge 0.$$
 (10)

The Gaussian density matrix is diagonal in the corresponding $a^{\dagger}a$ time-independent number basis,

$$\langle n'|\rho|n\rangle = \frac{2\delta_{n'n}}{\sigma+1} \left(\frac{\sigma-1}{\sigma+1}\right)^n,\tag{11}$$

with

$$\sigma = 2N + 1, \qquad \xi^2(t) = \sigma |f(t)|^2, \qquad \eta = \dot{\xi}.$$
(12)

Upon identifying $\sigma = \operatorname{coth}(\hbar \omega/2k_BT)$, the diagonal form (11) will be recognized as a thermal density matrix at temperature *T*. The smoothness of the finite temperature classical limit $\hbar \sigma \rightarrow 2k_BT/\omega$ as $\hbar \rightarrow 0, \sigma \rightarrow \infty$ shows that quantum and thermal fluctuations are treated by the mean field approximation in a unified way.

By making another group transformation it is always possible to diagonalize (1) at any given time, bringing the quadratic Hamiltonian into the standard harmonic oscillator form, $H_{osc} = (\hbar \omega/2)(\tilde{a}\tilde{a}^{\dagger} + \tilde{a}^{\dagger}\tilde{a})$ with \tilde{a} time dependent. This time-dependent basis is defined by

$$q(t) = \tilde{a}f + \tilde{a}^{\mathsf{T}}f^{*}, \qquad p(t) = -i\omega\tilde{a} + i\omega\tilde{a}^{\mathsf{T}}f^{*},$$
$$\tilde{f}(t) = \sqrt{\frac{\hbar}{2\omega(t)}} \exp\left(-i\int_{0}^{t} dt'\omega(t')\right), \qquad (13)$$

in place of (8). In the $\tilde{a}^{\dagger}\tilde{a}$ number basis, ρ is no longer diagonal, $\langle \tilde{a} \rangle$, $\langle \tilde{a}\tilde{a} \rangle$, etc., are nonvanishing, and $\tilde{N} \equiv \langle \tilde{a}^{\dagger}\tilde{a} \rangle \neq N$ in general, becoming equal only in the static case of constant ω .

If $\omega(t)$ varies slowly in time, an adiabatic invariant *W* may be constructed from the Hamilton-Jacobi equation corresponding to the effective Hamiltonian (5), i.e.,

$$W/2\pi\hbar = H_{\rm eff}/\hbar\omega - \sigma/2 = \tilde{N} - N.$$
(14)

Since N is time independent, $\tilde{N}(t)$ is an adiabatic invariant of the evolution. On the other hand, the phase angle conjugate to the action variable W varies rapidly in time. Since the diagonal matrix elements of ρ in the \tilde{N} basis are independent of this phase angle, they are slowly varying, whereas the *off-diagonal* matrix elements of ρ in this basis (which depend on the phase angle) are *rapidly* varying functions of time. If we are interested only in the effects of the fluctuations on the more slowly varying mean fields, it is natural to define an *effective* density matrix $\rho_{\text{eff}}(t)$ by *time averaging* the density matrix (2), thereby truncating ρ to its diagonal elements only, in the adiabatic \tilde{N} basis [4]. Clearly, for this truncation to be justified there must be very efficient phase cancellation, i.e., *dephasing*, either by averaging the fluctuations over time or by summing over many independent fluctuating degrees of freedom at a fixed time, as in field theory.

Obtaining the general form of the diagonal matrix elements of ρ in the \tilde{N} basis is straightforward, but the result is rather unwieldy and will be presented elsewhere. Here we restrict our attention to the case of a pure state with vanishing \overline{q} mean field. Using the methods of Ref. [5], one finds simply

$$\langle \tilde{n} = 2l | \rho | \tilde{n} = 2l \rangle |_{\overline{q} = \overline{p} = 0}^{\sigma = 1} = \frac{(2l - 1)!!}{2^l l!} \operatorname{sech} \gamma \tanh^{2l} \gamma,$$
(15)

with $\rho_{\tilde{n}\tilde{n}} = 0$ for \tilde{n} odd and $\gamma(t)$ the parameter of the Bogoliubov transformation between the *a* and \tilde{a} bases, given explicitly by

$$\sinh^2 \gamma = \tilde{N} = |\dot{f} + i\omega f|^2 / 2\hbar\omega.$$
(16)

Decoherence is addressable within the same mean field framework. Consider the case where $\omega(t)$ is a function of one mean field degree of freedom A(t). If only the evolution of A is of interest, then the fluctuating modes described by f(t) may be treated as the "environment." To solve for the evolution of the reduced density matrix of A, one needs to compute the influence functional. This is a functional of two trajectories $A_1(t)$ and $A_2(t)$ [corresponding to two different evolution operators $U_1(t)$ and $U_2(t)$], and is defined by

$$F_{12}(t) \equiv \exp[i\Gamma_{12}(t)] \equiv \operatorname{Tr}[U_1(t)\rho(0)U_2^{\dagger}(t)].$$
(17)

Restricting again to pure states with vanishing \overline{q} mean fields, we find

$$\Gamma_{12}\Big|_{\substack{\sigma=1\\ \overline{q}=\overline{p}=0}} = -\frac{i}{2} \ln\left\{\frac{i\hbar}{|f_1f_2|}\left(\frac{f_1f_2^*}{f_1f_2^*-\dot{f}_1f_2^*}\right)\right\} \quad (18)$$

in terms of the two sets of mode functions $f_1(t)$ and $f_2(t)$. This Γ_{12} is precisely the closed time path (CTP) effective action functional which generates the connected real time *n*-point vertices in the quantum theory [6,7]. For a pure initial state, the absolute value of F_{12} measures the overlap of the two different evolutions at some time *t*, beginning with the same initial $|\psi(0)\rangle$. In mean field theory, instead of evaluating Γ_{12} for two arbitrary trajectories, the evaluation is over trajectories determined by the *self-consistent* evolution of the closed system, beginning with two different initial mean fields.

For an explicit field theoretic example, consider scalar QED with no scalar self-coupling. In the large *N* limit, the evolution of electric fields and charged matter field fluctuations may be described in the self-consistent mean field or Gaussian approximation. For a spatially homogeneous electric field in the \hat{z} direction, in the gauge $\vec{A} = A(t)\hat{z}$, the time evolution equations read [1,7]

$$\begin{bmatrix} \frac{d^2}{dt^2} + \omega_{\vec{k}}^2(t) \end{bmatrix} f_{\vec{k}}(t) = 0,$$

$$\omega_{\vec{k}}^2(t) \equiv [\vec{k} - e\vec{A}(t)]^2 + m^2,$$

$$\ddot{A}(t) = \langle j_z(t) \rangle$$

$$= \frac{2e}{V} \sum_{\vec{k}} [k_z - eA(t)] |f_{\vec{k}}(t)|^2 \sigma_{\vec{k}},$$
(19)

with (9) holding for every discrete wave number \vec{k} in the finite volume V. In field theory there are an infinite number of fluctuating plane wave modes $f_{\vec{k}}$ of the charged scalar field, each varying rapidly in time with its own characteristic frequency, $\omega_{\vec{k}}$. The Gaussian density matrix for the complex scalar field Φ is an infinite product of Gaussians each of the form (2) with zero mean values,

$$\prod_{\vec{k}} \rho(\overline{\phi} = 0, \dot{\overline{\phi}} = 0; \xi_{\vec{k}}, \eta_{\vec{k}}; \sigma_{\vec{k}})$$
(20)

and the parameters $(\xi_{\vec{k}}, \eta_{\vec{k}}, \sigma_{\vec{k}})$ having the same significance as in (12), for each plane wave \vec{k} independently. Likewise, there is a Bogoliubov parameter $\gamma(\vec{k}; t)$ for each \vec{k} given by an expression of the form (16).

The equations of motion (19) are again Hamiltonian in structure, and, in this example,

$$\frac{H_{\rm eff}}{V} = \frac{E^2}{2} + \frac{1}{V} \sum_{\vec{k}} \left(\eta_{\vec{k}}^2 + \omega_{\vec{k}}^2 \xi_{\vec{k}}^2 + \frac{\hbar^2 \sigma_{\vec{k}}^2}{4\xi_{\vec{k}}^2} \right) \quad (21)$$

describes charged particle production in the electric field $E = -\dot{A}$ by the Schwinger mechansm and the effects of the current $\langle j_z(t) \rangle$ generated by these charged particles back on the electric field, through the semiclassical Maxwell equation in (19) [1,7]. The mean value of the scalar field itself $\overline{\phi} = \langle \Phi \rangle = 0$ so that we may use the expressions (15) and (18) for the effective density matrix and decoherence functional of the charged field fluctuations. The values ρ_{2l} given by (15) are then the probabilities of observing *l* charged particle pairs in the adiabatic \tilde{N} basis. The diagonal matrix elements of ρ for odd \tilde{n} vanish because particles can only be created in pairs from the vacuum.

In this specific model we present numerical results (in 1 + 1 dimensions with vacuum initial conditions, $\sigma_{\vec{k}} =$ 1) on damping and decoherence of the mean electric field in Figs. 1 and 2. The nonlinear collective oscillations of the electric field observed in Fig. 1 are plasma oscillations with $\omega_{pl}^2 \approx e^2 \tilde{n}_{tot}/m$, where $\tilde{n}_{tot} = 2 \sum_{\vec{k}} \tilde{N}(\vec{k})/V$ is the total number density of created particles plus antiparticles. Since all the $\omega_{\vec{k}} \gg \omega_{pl}$, the phase cancellation between the fluctuations is very effective on the time scale of the plasma oscillations. A measure of the apparently irreversible flow of energy from the electric field towards the charged particle modes observed due to this dephasing is the von Neumann entropy of the *effective* density matrix. In Fig. 1 we plot this effective entropy and the Boltzmann entropy for comparison.

The two entropies are defined by

$$S_{B} = \sum_{\vec{k}} \{ [\tilde{N}(\vec{k}) + 1] \ln[\tilde{N}(\vec{k}) + 1] - \tilde{N}(\vec{k}) \ln\tilde{N}(\vec{k}) \},$$

$$S_{\text{eff}} \equiv -\text{Tr}\rho_{\text{eff}} \ln\rho_{\text{eff}} = -\sum_{\vec{k}} \sum_{l=0}^{\infty} \rho_{2l}(\vec{k}) \ln\rho_{2l}(\vec{k}),$$
(22)

respectively. Both display a general increase during intervals of particle creation [4,6], when the electric field is sufficiently strong for the Schwinger pair creation mechanism to be effective. Neither quantity is a strictly monotonic function of time (no H theorem). Since the charged particle modes $f_{\vec{k}}$ interact with the mean electric field but not directly with each other, the effective damping observed is certainly *collisionless*, and the dephasing here is similar to that responsible for Landau damping of collective modes in classical electromagnetic plasmas. The entropy $S_{\rm eff}$ of the effective density matrix provides a precise measure of the information lost by treating the phases as random. The Boltzmann "entropy" would be expected to equal $S_{\rm eff}$ only in true thermodynamic equilibrium, which is not achieved in the collisionless approximation of Eqs. (19). Otherwise, we see from Fig. 1 that S_B generally overestimates the amount of information lost by phase averaging. That decoherence is closely related to the same dephasing of the particle modes is seen most clearly by comparing the absolute value of F_{12} for different initial electric fields. Decoherence is very slow for electric fields less than the Schwinger pair production threshold but becomes very rapid above it [8]. This shows the strong dependence of the decoherence process on the particle production by the mean field.

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