Decoherence and Thermalization of a Pure Quantum State in Quantum Field Theory

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We study the real-time evolution of a self-interacting $O(N)$ scalar field initially prepared in a pure, coherent quantum state. We present a complete solution of the nonequilibrium quantum dynamics from a $1/N$ expansion of the two-particle-irreducible effective action at next-to-leading order, which includes scattering and memory effects. We demonstrate that, restricting one's attention (or ability to measure) to a subset of the infinite hierarchy of correlation functions, one observes an effective loss of purity or coherence and, on longer time scales, thermalization. We point out that the physics of decoherence is well described by classical statistical field theory.

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Quantum decoherence is a fundamental process whose understanding is a central issue in many areas of physics. Topical examples include measurement theory in quantum mechanics [1], the physics of Bose-Einstein condensates [2], or of quantum computers [3], neutrino physics [4], high-energy nuclear collisions [5], black hole physics [6], or the description of primordial fluctuations in inflationary cosmology [7,8]. It is a genuine nonequilibrium process, which requires the real-time description of quantum dynamics. Analytic descriptions can be obtained for exactly solvable models and/or simple enough approximations, e.g., assuming a linear coupling between the system and its environment, neglecting backreaction, etc. A complete microscopic description in realistic quantum field theories (QFT) is a notoriously difficult task [9], which requires first-principles calculations of the nonequilibrium quantum dynamics.

Recent years have witnessed substantial progress concerning the description of quantum fields out of equilibrium [10]. Two-particle-irreducible (2PI) functional techniques provide a powerful tool to devise systematic, practicable approximation schemes, valid for arbitrarily far-from-equilibrium situations [9,10]. It has been demonstrated that a coupling or $1/N$ expansion of the 2PI effective action at lowest nontrivial order can describe far-from-equilibrium dynamics and subsequent (quantum) thermalization without further assumption [11–13]. In this Letter, we use 2PI techniques to compute the dynamics of decoherence from first principles in QFT [14].

There are various uses of the concept of (de)coherence [16], the most widely discussed being the so-called environment-induced decoherence, which results from the interaction of the system under study with a (thermal) bath of unobserved degrees of freedom (d.o.f.) [1]. Even in the absence of an environment, decoherence of a subset of d.o.f. may result from some kind of coarse graining [17,18]. Here, we adopt a different point of view, also advocated, e.g., in [8,9,15,19]. Even if one keeps all the dynamical d.o.f., reconstructing the actual state of a given (closed) system requires a precise knowledge of its independent correlation functions. In practice, however, such information is often not experimentally accessible and one has to infer the state of the system from the subset of measured correlation functions. This "incomplete description" picture actually underlies the very concept of thermalization [9,19]. Similarly, a system prepared in a pure quantum state may appear as a statistical mixture to the observer who has only partial information.

In this Letter, we show that, starting from a pure, coherent quantum (Gaussian) state, an observer who only measures the subset of equal-time two-point functions observes an effective loss of purity or coherence and, eventually, (apparent) thermalization. We study a relativistic self-interacting $O(N)$ scalar field and present a complete numerical solution of the nonequilibrium dynamics from a $1/N$ expansion of the 2PI effective action at next-to-leading order [13]. The approach allows us to study the strong coupling regime and is a valid description for states with a high degree of quantum coherence which, as explained below, are characterized by strong—possibly nonperturbative—field fluctuations.

A pure quantum state remains such under a unitary evolution. Here, although the complete information about the initial Gaussian state is contained in the set of two-point functions, nontrivial higher correlators develop in time due to the non-Gaussian dynamics: The information about the initial state spreads in the space of correlation functions and gets lost to our observer, resulting in the effective loss of purity or coherence and, at late times, the thermalization of the effective density matrix. We stress that no environment of incoherent d.o.f. is needed. We illustrate this point by preparing a completely pure initial state. Finally, we show that the regime of decoherence, characterized by strong field fluctuations, is well described by classical (statistical) field theory.

We consider a relativistic real scalar field φ_a ($a = 1, \ldots, N$) with classical action

$$S[\varphi] = -\int d^4x \left\{ \frac{1}{2} \varphi_a (\Box + m^2) \varphi_a + \frac{\lambda}{4!N} (\varphi_a \varphi_a)^2 \right\}, \quad (1)$$

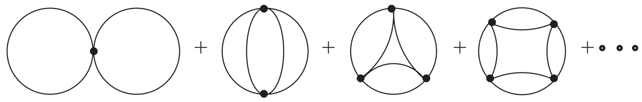

FIG. 1. The dots indicate that each diagram of the series is obtained from the previous one by adding another bubble.

where summation over repeated indices is implied. For vanishing field expectation value, $\langle\varphi_a(x)\rangle = 0$, the correlation functions of the quantum theory can be obtained from the 2PI effective action $\Gamma[G]$, parametrized by the time-ordered connected propagator $\langle T\varphi_a(x)\varphi_b(y)\rangle = \delta_{ab}G(x,y)$ [20]. The $1/N$ expansion of $\Gamma[G]$ at next-to-leading order includes the infinite series of diagrams shown in Fig. 1, where the lines represent the propagator G [13].

To set up the initial-value problem, it is useful to decompose the two-point function G into a statistical (F) and a spectral (ρ) component, both real functions:

$$G(x,y) = F(x,y) - \tfrac{i}{2}\mathrm{sgn}_{\mathcal{C}}(x^0 - y^0)\rho(x,y). \quad (2)$$

Notice that $F(x,y) = F(y,x)$ and $\rho(x,y) = -\rho(y,x)$. For Gaussian initial conditions, the equations of motion, obtained as $\delta\Gamma[G]/\delta G(x,y) = 0$, read

$$[\Box_x + M^2(x)]F(x,y) = -\int_0^{x^0} d^4z\Sigma_\rho(x,z)F(z,y) + \int_0^{y^0} d^4z\Sigma_F(x,z)\rho(z,y), \quad (3)$$

$$[\Box_x + M^2(x)]\rho(x,y) = -\int_{y^0}^{x^0} d^4z\Sigma_\rho(x,z)\rho(z,y), \quad (4)$$

where $\int_0^{x^0} d^4z \equiv \int_0^{x^0} dz^0 \int d\mathbf{z}$. The effective mass term is given by

$$M^2(x) = m^2 + \lambda\frac{N+2}{6N}F(x,x), \quad (5)$$

and the self-energies by [13]

$$\Sigma_F(x,y) = \frac{\lambda}{3N}\left[F(x,y)I_F(x,y) - \frac{1}{4}\rho(x,y)I_\rho(x,y)\right], \quad (6)$$

$$\Sigma_\rho(x,y) = \frac{\lambda}{3N}[\rho(x,y)I_F(x,y) + F(x,y)I_\rho(x,y)]. \quad (7)$$

The functions I_F and I_ρ resum the infinite series of bubble diagrams in Fig. 1:

$$I_F(x,y) = \Pi_F(x,y) - \int_0^{x^0} d^4z I_\rho(x,z)\Pi_F(z,y) + \int_0^{y^0} d^4z I_F(x,z)\Pi_\rho(z,y), \quad (8)$$

$$I_\rho(x,y) = \Pi_\rho(x,y) - \int_{y^0}^{x^0} d^4z I_\rho(x,z)\Pi_\rho(z,y), \quad (9)$$

with the elementary bubble

$$\Pi_F(x,y) = -\frac{\lambda}{6}\left[F^2(x,y) - \frac{1}{4}\rho^2(x,y)\right], \quad (10)$$

$$\Pi_\rho(x,y) = -\frac{\lambda}{3}F(x,y)\rho(x,y). \quad (11)$$

The self-energy kernels Σ_F and Σ_ρ describe scattering and memory effects and are responsible for non-Gaussian correlations to develop in time, a key ingredient in the present discussion. Gaussian—collisionless—evolution equations, such as leading-order large-N, or Hartree approximations, where the right-hand sides of Eqs. (3) and (4) vanish identically, are known to fail to describe phenomena such as damping of unequal-time correlators or thermalization [10]. We show below that they also fail to capture the physics of decoherence in the present approach.

We consider spatially homogeneous and isotropic states, for which $F(x,y) \equiv F(x^0, y^0, |\mathbf{x}-\mathbf{y}|)$. Accordingly, we introduce the Fourier decomposition ($p \equiv |\mathbf{p}|$)

$$F(t,t',|\mathbf{r}|) = \int\frac{d\mathbf{p}}{(2\pi)^3}e^{i\mathbf{p}\cdot\mathbf{r}}F_p(t,t'), \quad (12)$$

and similarly for $\rho(x,y)$. We consider an observer who only has access to the subset of equal-time two-point functions: $F_p(t) = \langle\varphi_\mathbf{p}^\dagger(t)\varphi_\mathbf{p}(t)\rangle$, $R_p(t) = \frac{1}{2}\langle\varphi_\mathbf{p}^\dagger(t)\pi_\mathbf{p}(t) + \pi_\mathbf{p}^\dagger(t)\varphi_\mathbf{p}(t)\rangle$, and $K_p(t) = \langle\pi_\mathbf{p}^\dagger(t)\pi_\mathbf{p}(t)\rangle$. The minimum-bias state compatible with these measured observables is described by an effective Gaussian density matrix [19] $D_{\mathrm{eff}}(t) = \prod_\mathbf{p} D_\mathbf{p}(t)$, where the product runs over independent d.o.f. in momentum space with, up to a normalization,

$$D_\mathbf{p}(t) \propto \exp\{\kappa_p(t)[F_p(t)\pi_\mathbf{p}^\dagger(t)\pi_\mathbf{p}(t) + K_p(t)\varphi_\mathbf{p}^\dagger(t)\varphi_\mathbf{p}(t) - R_p(t)(\pi_\mathbf{p}^\dagger(t)\varphi_\mathbf{p}(t) + \varphi_\mathbf{p}^\dagger(t)\pi_\mathbf{p}(t))]\}, \quad (13)$$

where $\kappa_p(t) = -\ln[1 + 1/n_p(t)]/[2n_p(t) + 1]$, with

$$n_p(t) + \frac{1}{2} = \sqrt{F_p(t)K_p(t) - R_p^2(t)} \equiv a_p(t). \quad (14)$$

Contrarily to the correlators $F_p(t)$, $R_p(t)$, and $K_p(t)$, which can be modified by a canonical redefinition of the field variables (φ, π), $n_p(t)$ is a canonical invariant and, actually, the only truly intrinsic property of the density matrix (13) [8]. It provides an absolute measure of the quantum purity of the system's state through [21]

$$\mathrm{tr}[D_\mathbf{p}^2(t)] = [2n_p(t) + 1]^{-1} \le 1, \quad (15)$$

which equals 1 for a pure state. Note also that, whenever the system is well described by a thermal ensemble of weakly interacting quasiparticle (QP), $n_p(t)$ defines a QP occupation number and follows a Bose-Einstein distribution as a function of the QP energy [13]. We shall make use of this property to characterize the degree of thermalization of the system, although we stress that none of our results rely on such a QP interpretation.

Note finally that $n_p(t)$ is time independent for Gaussian approximations [22]. Therefore, no loss of quantum purity, in the sense discussed here, occurs for such approximations. We stress that this is not in conflict with existing studies of decoherence in free-field [7] or mean-field approximations [18], which typically consider an effective coarse-grained Gaussian density matrix where one averages out some rapidly varying d.o.f. This results in an effective loss of information and hence of quantum purity or coherence, due, e.g., to dephasing [18], already at the Gaussian level. In the present incomplete description approach, decoherence is due to the non-Gaussian dynamics, i.e., direct scattering and memory effects [23].

We now come to the discussion of quantum coherence which, unlike purity, is a basis-dependent notion. The equal-time two-point correlators can be parametrized as

$$\epsilon_p(t)F_p(t) = \bar{a}_p(t)[1 - \gamma_p(t)\cos\phi_p(t)], \qquad (16)$$

$$R_p(t) = -\bar{a}_p(t)\gamma_p(t)\sin\phi_p(t), \qquad (17)$$

$$K_p(t)/\epsilon_p(t) = \bar{a}_p(t)[1 + \gamma_p(t)\cos\phi_p(t)], \qquad (18)$$

where

$$\bar{a}_p(t) = \frac{K_p(t) + \epsilon_p^2(t)F_p(t)}{2\epsilon_p(t)} \equiv \bar{n}_p(t) + \frac{1}{2} \qquad (19)$$

provides an alternative definition of a QP occupation number $\bar{n}_p(t)$. Note that $0 \leq n_p(t) \leq \bar{n}_p(t)$. Here, the energy scale $\epsilon_p(t)$ defines the QP basis in which to discuss decoherence. We use $\epsilon_p(t) = \sqrt{p^2 + M^2(t)}$, which we found gives a good description of the oscillation frequency of two-point correlators. The basis-dependent occupation number $\bar{n}_p(t)$ is related to the canonical invariant $n_p(t)$ through the coherence parameter [24]

$$\gamma_p(t) = \sqrt{1 - a_p^2(t)/\bar{a}_p^2(t)}. \qquad (20)$$

The case $\gamma_p(t) = 0$ or, equivalently, $n_p(t) = \bar{n}_p(t)$, corresponds to the thermal-like density matrix $D_{\mathbf{p}}(t) \propto \exp\{\kappa_p(t)F_p(t)[\pi_{\mathbf{p}}^\dagger(t)\pi_{\mathbf{p}}(t) + \epsilon_p^2(t)\varphi_{\mathbf{p}}^\dagger(t)\varphi_{\mathbf{p}}(t)]\}$. This includes the vacuumlike state: $n_p(t) = \gamma_p(t) = 0$. Moreover, $\gamma_p(t)$ controls the size of off-diagonal matrix elements of the density matrix in the so-called two-mode coherent state basis [25]: The latter exhibits nontrivial correlations (i.e., quantum coherence) between macroscopically distant semiclassical states for $\gamma_p(t) \to 1$. Note that this limit is also characterized by strong field fluctuations since the correlators $F_p(t)$, $R_p(t)$, and $K_p(t)$ are $\propto 1/\sqrt{1 - \gamma_p^2(t)} \gg 1$.

At time $t = 0$, we prepare modes with $p \leq p_c$ in a pure, highly coherent quantum state characterized by $n_p(0) \ll 1$, $\gamma_p(0) = \gamma_0 \sim 1$, and $\phi_p(0) = \pi/2$, while modes with $p_c < p \leq \Lambda$, with Λ the ultraviolet cutoff, are prepared in a vacuumlike state: $n_p(0) \ll 1$ and $\gamma_p(0) = 0$ [26]. We emphasize that there are no incoherent d.o.f.: The initial state is a completely pure quantum state. Equations (3)–(11) are solved numerically without further approximation (except for discretization of time or momentum integrals and truncation of memory integrals). We show results for $p_c/M_0 = 3.6$ and $\Lambda/M_0 = 10$, where $M_0 = M(0)$ is the initial effective mass.

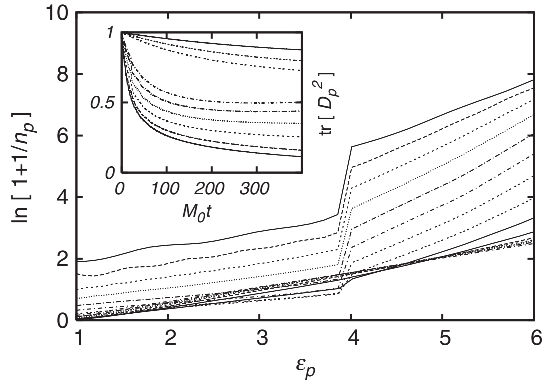

FIG. 2. The function $\ln[1 + 1/n_p(t)]$ as a function of $\epsilon_p(t)$ for times $M_0 t = 2.5 \times 2^n$ for $n = 0, \ldots, 14$. A straight line at late times corresponds to a Bose-Einstein distribution. The inset shows the rapid decrease of $\mathrm{tr}[D_p^2(t)]$ as a function of time for modes (from bottom to top) $p/a = 1, 5, 10, 15, 20, 24$, where $a/M_0 = 0.15$. Higher momentum modes, $p/a = 25, 27, 30$, are also shown for comparison.

Figure 2 presents an overview of the time evolution. It shows snapshots of the function $\ln[1 + 1/n_p(t)]$ as a function of $\epsilon_p(t)$ at various times. One observes a substantial growth of $n_p(t)$ for all modes, signaling the effective loss of quantum purity at early times, followed by a slow approach to an effective quantum thermal equilibrium, characterized by a Bose-Einstein distribution. The loss of quantum purity is further illustrated in the inset, which shows the rapid decay of $\mathrm{tr}[D_p^2(t)]$ for modes $p \leq p_c$.

After the loss of quantum purity, we find that $\bar{n}_p(t) \approx n_p(t)$, signaling a corresponding loss of quantum coherence according to Eq. (20). Figure 3 shows the time evolution of the coherence parameter $\gamma_p(t)$ for the mode $p/M_0 = 0.15$, for various sets of parameters. In all cases we find that decoherence is well described by an exponential law. The inset shows the corresponding decoherence rates for the modes $p \leq p_c$.

Classical scaling.—In the highly coherent limit, $\gamma_0 \to 1$, one has, roughly speaking $F \sim 1/\sqrt{1 - \gamma_0^2} \gg \rho \sim 1$, which signals the enhancement of classical versus quantum fluctuations [12]. In this regime one can neglect the second term in brackets on the left-hand sides of Eqs. (10) and (6). It is then easy to check that under the simultaneous rescaling of the correlators and the coupling constant $F \to \eta F$, $\rho \to \rho$, and $\lambda \to \lambda/\eta$, with η an arbitrary constant, the F and ρ- components of Π, I, and Σ scale just as F and ρ, respectively, and that Eqs. (3) and (4) are left invariant. This is characteristic of the regime of strong field fluctuations, where a classical (statistical) field theory description is appropriate. Indeed, in classical field theory, the action being defined up to a multiplicative constant, a rescaling of the field (i.e., of the initial conditions) can be entirely absorbed in a change of coupling. Therefore, as long as the system is highly coherent [$\gamma_p(t) \sim 1$], we expect the dynamics not to depend separately on γ_0 and λ, but instead

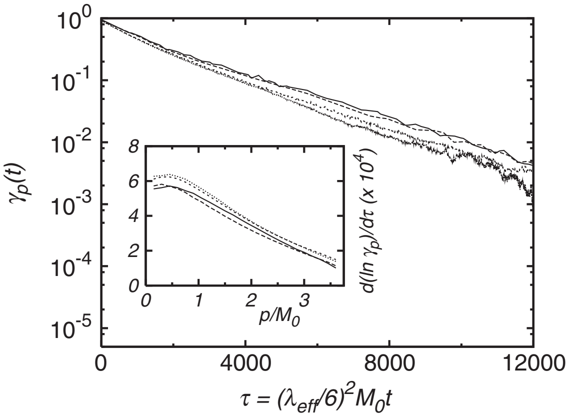

FIG. 3. Exponential decay of the coherence parameter $\gamma_p(t)$ as a function of rescaled time $\tau = (\lambda_{\rm eff}/6)^2(M_0 t)$ (see text), for the mode $p/M_0 = 0.15$, for four couples of parameters (γ_0, λ): (0.99, 3.05) (solid line) and (0.95, 6.62) (long-dashed line), for which $\lambda_{\rm eff} = 21.7$; (0.95, 2.2) (dashed line), for which $\lambda_{\rm eff} = 7.215$; and (0.95, 0.915) (dotted line), for which $\lambda_{\rm eff} = 3.0$. The inset shows the corresponding decay rates, obtained from exponential fits, for modes $p \leq p_c$. The agreement of the first two runs illustrates the $\lambda_{\rm eff}$ scaling of early-time decoherence. The overall agreement shows the approximate $\lambda_{\rm eff}^2$ dependence of the decoherence rate.

on the combination $\lambda_{\rm eff} = \lambda/\eta$ where $\eta = \sqrt{1-\gamma_0^2}$. We checked, from our numerical simulation of the full quantum dynamics, that this is indeed the case during the early-time decoherence regime, as illustrated in Fig. 3: Runs with different values of γ_0 and λ but the same $\lambda_{\rm eff}$ are essentially indistinguishable. Furthermore, we observe that, despite the rather strong (effective) couplings employed in some simulations, the decoherence rates approximately follow a perturbativelike $\lambda_{\rm eff}^2$ scaling.

As a final remark, we mention that fixing the value of the initial mass M_0 absorbs a large Λ^2 dependence. This simple, though approximate, renormalization turns out to be numerically sufficient for the results presented here. We find that if the late time thermalization is cutoff dependent, a known artifact of Gaussian initial conditions [27], the regime of effective loss of quantum purity or coherence is largely cutoff insensitive.

To the best of our knowledge, this work provides the first complete microscopic description of the process of decoherence in a realistic QFT. It is an exciting observation that the relevant dynamics is well described by classical statistical field theory, which can be solved exactly by means of standard Monte Carlo techniques. A particularly interesting question is to investigate how the present results are modified as one includes higher order equal-time correlation functions in the set of measured observables.

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[22] Gaussian dynamics is equivalent to a time-dependent canonical transformation; $n_p(t)$ is a canonical invariant.
[23] The loss of information from the subset of Gaussian correlators is measured by the so-called correlation entropy [8,9,15,19]: $S(t) = -\mathrm{tr}[D_{\rm eff}(t)\ln D_{\rm eff}(t)] = \sum_{\mathbf{p}}\{[n_p(t)+1]\ln[n_p(t)+1] - n_p(t)\ln n_p(t)\}$.
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