Quantum Aging in Mean-Field Models

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We study the real-time dynamics of quantum models with long-range interactions coupled to a heat bath within the closed-time path-integral formalism. We show that quantum fluctuations depress the transition temperature. In the subcritical region there are two asymptotic time regimes with (i) stationary and (ii) slow aging dynamics. We extend the quantum fluctuation-dissipation theorem to the nonequilibrium case in a consistent way with the notion of an effective temperature that drives the system in the aging regime. The classical results are recovered for $\hbar \to 0$. [S0031-9007(98)06264-4]

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The dynamics of nonequilibrium systems is being intensively studied now. Notably, glassy systems below their critical temperature have a very slow evolution with nonstationary dynamics [1]. Several theoretical ideas [2] are used to describe it, namely, scaling arguments, phase space models, analytical solutions to mean-field models, and numerical simulations. The analysis of simple mean-field models (with long-range interactions) has provided a general scenario [3,4] that is now being verified numerically for more realistic models [5,6]. All these studies concern classical systems.

Recent experiments [7] have motivated a renewed interest on the effect of quantum fluctuations (QF) on glassy systems. Up to the present, theoretical studies have focused on how QF affect their *equilibrium* properties [8–12].

Since glasses below T_g are not expected to reach equilibrium in experimentally accessible times, it is important to devise a method to understand the influence of QF on the truly nonequilibrium *real-time* dynamics of this type of systems. Intuitively, one expects QF to affect only the short-time dynamics; however, they are also expected to act as thermal fluctuations. It is then not clear whether QF would destroy glassiness or modify it drastically.

Our aims are (i) to present a formalism suited to study the real-time dynamics of a nonlinear, possibly disordered, model in contact with a bath; (ii) to propose a framework to study its dynamics that could also be applicable to more realistic, finite dimensional, models; (iii) to show that below a critical line QF do not destroy the nonequilibrium effects of the glassy phase and that QF have the side effect of adding up to an effective temperature T_{EFF}; and (iv) to prove that T_{EFF} is nonzero even at zero bath temperature, that it drives the dynamics at late epochs, and that it makes the dynamics appear classical in that time regime. A longer account of our results will appear elsewhere.

The real-time dynamics of a quantum system is described with a closed-time path-integral generating functional (CTP-GF) [13]. We choose a set of noninteracting harmonic oscillators with an adequate distribution of frequencies as a bath, and a linear interaction between bath and system [14]. The bath variables are next integrated out, and the effect of the bath manifests in the effective action through two nonlocal kernels associated with dissipation (η) and noise (ν). If the model is disordered, one needs to compute averaged expectation values. However, the CTP-GF without sources is independent of the realization of disorder and one can hence avoid, as in the classical case [15], the introduction of replicas. In addition, when $\hbar \to 0$, the CTP-GF yields the classical Martin-Siggia-Rose one.

For the sake of concreteness, we study a generalization of the p spin glass (or the model of a quantum particle in an N-dimensional random potential):

$$H_J[\boldsymbol{\phi}] = \frac{1}{2m} \sum_{i=1}^{N} \Pi_i^2 + \sum_{i_1,\dots,i_p} J_{i_1\dots i_p} \phi_{i_1} \cdots \phi_{i_p} \qquad (1)$$

with Π_i the canonical momenta, $[\Pi_i, \phi_j] = -i\hbar\delta_{ij}$. The multispin interactions $J_{i_1\dots i_p}$ are taken from a Gaussian distribution with zero mean and variance $\tilde{J}^2 p!/(2N^{p-1})$, and we impose $\sum_{i=1}^{N}[\langle \phi_i^2(t)\rangle]_J = N, \forall\ t$. Square brackets denote an average over disorder and $\langle \bullet \rangle$ the average over temporal histories. The quantum mean-field equations follow from a saddle-point approximation and involve the symmetrized autocorrelation $NC(t,t_w) \equiv [\langle \boldsymbol{\phi}(t)\boldsymbol{\phi}(t_w) + \boldsymbol{\phi}(t_w)\boldsymbol{\phi}(t)\rangle]_J$ and the response to an infinitesimal perturbation h applied at time t_w, $NR(t,t_w) \equiv \delta[\langle \boldsymbol{\phi}(t)\rangle / \delta \mathbf{h}(t_w)]_J|_{h=0}$. We define the vertex and self-energy as

$$D(t,t_w) = \tilde{D}(t,t_w) + 2\hbar\nu(t-t_w),$$
$$\Sigma(t,t_w) = \tilde{\Sigma}(t,t_w) - 4\eta(t-t_w).$$

$\tilde{\Sigma}$ and $\tilde{D}$ do not depend on the system-bath interactions. Their explicit form for the p-spin model and $t \geq t_w$ after averaging over disorder and a saddle-point evaluation is

$$\tilde{D}(t,t_w) + \frac{i\hbar}{2}\tilde{\Sigma}(t,t_w) = \frac{p\tilde{J}^2}{2}\left(C(t,t_w) + \frac{i\hbar}{2}R(t,t_w)\right)^{p-1}.$$

The terms associated with the bath are

$$\nu(t-t_w) = \int_0^\infty d\omega\, I(\omega)\coth(\beta\hbar\omega/2)\cos[\omega(t-t_w)],$$

$$\eta(t-t_w) = \theta(t-t_w)\int_0^\infty d\omega\, I(\omega)\sin[\omega(t-t_w)].$$

We chose an Ohmic distribution of oscillator frequencies $I(\omega) = (M\gamma_o/\pi)\omega\exp(-|\omega|/\Lambda)$ with Λ a cutoff and $M\gamma_o$ a constant that plays the role of a friction coefficient [16]. Their particular form depends on the choice of bath. The equations, for a random initial condition, are

$$R(t,t_w) = G_o(t,t_w) + \int_0^t \int_0^t du\, dv\, G_o(t,u)\Sigma(u,v)R(v,t_w),$$
$$C(t,t_w) = \int_0^t du \int_0^{t_w} dv\, R(t,u)D(u,v)R(t_w,v), \tag{2}$$

with $G_o^{-1}(t,u) = \delta(t-u)[m\partial_t^2 + \mu(t)]$ the propagator. $\mu(t)$ is a Lagrange multiplier enforcing a spherical constraint. It is determined by the gap equation: $\mu(t) = \int_0^t du\Sigma(t,u)C(t,u) + D(t,u)R(t,u) - m\partial_{t^2}C(t,t_w)|_{t_w\to t^-}$. Causality implies $R(t,t_w) = \Sigma(t,t_w) = 0$ if $t_w > t$. The inertia imposes continuity on the equal-times correlator $\lim_{t_w\to t^-}\partial_t C(t,t_w) = \lim_{t_w\to t^+}\partial_t C(t,t_w) = 0$, and $R(t,t) = 0$, $\lim_{t_w\to t^-}\partial_t R(t,t_w) = 1/m$. In what follows we set $t \geq t_w$. The coupling to the bath implies dissipation; if $M\gamma_o \neq 0$ the energy density $\mathcal{E}$ of the system decreases. One can then envisage to switch off the coupling (set $M\gamma_o = 0$) when $\mathcal{E}$ reaches a desired value and follow the subsequent evolution at constant $\mathcal{E}$. This would be useful to further understand the energy landscape. Here, we keep $M\gamma_o \neq 0$ for all times, reparametrize time according to $t \to M\gamma_o t$, and transform $\hbar$ in a free parameter $\hbar \to M\gamma_o\hbar$. Consistently, $C \to C$, $R \to R/(M\gamma_o)$, $m \to (M\gamma_o)^2 m$, $\tilde{J} \to \tilde{J}$, $\beta \to \beta$, $\Lambda \to \Lambda/(M\gamma_o)$, and the units are $[C] = [R] = [\hbar] = 1$, $[m] = [\beta] = [1/\tilde{J}] = [1/\Lambda] = [t]$.

We focus on $p > 2$, since $p = 2$ needs a special treatment [17]. Since Eqs. (2) are causal, we can construct the solution numerically, step by step in t, spanning $0 \leq t_w \leq t$. The numerical and analytical studies yield the following.

(i) *Quantum mode-coupling equations.*—For $\hbar$ and T above a critical line, there is a finite equilibration time $\tau_{\rm EQ}$ after which equilibrium dynamics sets in. The solution satisfies invariance under time translations (TTI) and the quantum fluctuation-dissipation theorem (QFDT). It is a "paramagnetic/liquid" phase. A TTI-QFDT ansatz yields

$$R(\omega) = \frac{1}{-m\omega^2 + \mu_\infty - \Sigma(\omega)}, \tag{3}$$

$$C(\omega) = D(\omega)\,|R(\omega)|^2, \tag{4}$$

with the couples R and C, and Σ and D, verifying QFDT:

$$R(\tau) = \frac{2i}{\hbar}\theta(\tau)\int \frac{d\omega}{2\pi} e^{-i\omega\tau}\tanh\left(\frac{\beta\hbar\omega}{2}\right)C(\omega) \tag{5}$$

($\tau = t - t_w$). Equations (3) and (4) are the quantum version of the mode-coupling equations used to describe supercooled liquids [18]. Away from the critical line, C and R decay to zero very fast, with oscillations. Approaching the critical line $T_d(\hbar_d)$, the decay slows down. If $T_d(\hbar_d) \neq 0$, a plateau develops in C. At the critical line, the length of the plateau tends to infinity. We discuss the quantum critical point ($T_d = 0, \hbar_d \neq 0$) below.

(ii) *Dynamics in the glassy phase.*—For $\hbar$ and T below the critical line, $\tau_{\rm EQ} \to \infty$ (as a function of N): times are always finite with respect to $\tau_{\rm EQ}$. The system does not reach equilibrium. This is a "spin-glass/glass" phase. There are two time regimes with different behaviors according to the relative value of $t - t_w$ and a characteristic (model-dependent) time $\mathcal{T}(t_w)$.

If $t - t_w \leq \mathcal{T}(t_w)$ $[C(t,t_w) \geq q]$ the dynamics is *stationary;* TTI and QFDT hold. In other words,

$$q + C_{\rm ST}(t-t_w) = \lim_{t_w\to\infty} C(t,t_w) \tag{6}$$

and $R_{\rm ST}(t-t_w) = \lim_{t_w\to\infty} R(t,t_w)$. The correlation approaches a plateau q since $\lim_{t-t_w\to\infty} C_{\rm ST}(t-t_w) = 0$. The response approaches zero, $\lim_{t-t_w\to\infty} R_{\rm ST}(t-t_w) = 0$. The equations for $C_{\rm ST}$ and $R_{\rm ST}$ are identical to Eqs. (3) and (4) apart from contributions to μ_∞ coming from the aging regime. $C_{\rm ST}$ and $R_{\rm ST}$ are linked through Eq. (5).

If $t - t_w > \mathcal{T}(t_w)$ $[C(t,t_w) < q]$ the dynamics is *nonstationary;* TTI and FDT do not hold, and there is quantum aging. The correlation decays from q to 0, and we call it $C_{\rm AG}(t,t_w)$. The decay of C becomes *monotonic* in the aging regime; the properties of monotonic two-time correlation functions derived in Ref. [4] imply

$$C_{\rm AG}(t,t_w) = q\jmath^{-1}\left(\frac{h(t_w)}{h(t)}\right). \tag{7}$$

$h(t)$ increases with t and can be determined only by solving the matching problem [2,3]. For the p-spin model, $\jmath^{-1}$ is the identity. The system has a weak long-term memory (WLTM) meaning that the response tends to zero, *but* its integral over a growing time interval is *finite*.

Guided by the classical limit and the notion of effective temperatures we generalize the QFDT [Eq. (5)] to

$$R(t,t_w) = \frac{2i}{\hbar}\theta(t-t_w)\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\exp[-i\omega(t-t_w)] \times \tanh\left(\frac{X(t,t_w)\beta\hbar\omega}{2}\right)C(t,\omega), \tag{8}$$

$$C(t,\omega) \equiv 2\,{\rm Re}\int_0^t ds\exp[i\omega(t-s)]C(t,s), \tag{9}$$

with $X(t, t_w)$ a function of t *and* t_w. If the evolution is TTI and $X(t, t_w) = 1$ for all times, Eq. (8) reduces to Eq. (5). Interestingly enough, $T_{\rm EFF} \equiv T/X(t, t_w)$ acts as an effective temperature in the system [19]. For a model with two two-time sectors like this one we propose

$$X(t, t_w) = \begin{cases} X_{\rm ST} = 1, & \text{if} \quad t - t_w \leq \mathcal{T}(t_w), \\ X_{\rm AG}(\hbar, T), & \text{if} \quad t - t_w > \mathcal{T}(t_w). \end{cases}$$

When t and t_w are widely separated, the integration over ω in Eq. (8) is dominated by $\omega \sim 0$ and $\tanh[X_{\rm AG}(t, t_w) \times \beta\hbar\omega/2]$ can be substituted by $X_{\rm AG}(\hbar, T)\beta\hbar\omega/2$. This holds *even at* $T = 0$ since $X_{\rm AG}(\hbar, T) = x(\hbar)T$ when $T \sim 0$ as we show below. Hence,

$$R_{\rm AG}(t, t_w) \sim \theta(t - t_w) X_{\rm AG} \beta \partial_{t_w} C_{\rm AG}(t, t_w), \qquad (10)$$

and one recovers, in the aging regime, the *classical* modified FDT [3,12]. Numerically (and experimentally), it is simpler to check it using the integrated response $\chi(t, t_w) = \int_{t_w}^{t} dt''\, R(t, t'')$ over a large time window [4,6]:

$$\chi(t, t_w) = \begin{cases} \int_0^{t - t_w} d\tau'\, R_{\rm ST}(\tau'), \\ \int_0^{\infty} d\tau'\, R_{\rm ST}(\tau') + \frac{X_{\rm AG}}{T}[q - C_{\rm AG}(t, t_w)], \end{cases}$$

the first line holds for $C(t, t_w) > q$, while the second holds for $C(t, t_w) < q$. Remarkably, the correlation *and* the violation of QFDT are given by similar expressions to the classical one—though the values of q and $X_{\rm AG}$ depend on $\hbar$. In this sense, we say that $\mathcal{T}(t_w)$ acts as a *waiting-time dependent* "decoherence time," beyond which the nonequilibrium regime is "classical."

An ansatz like Eqs. (7)–(10) and the assumption of WLTM that allows us to approximate $\Sigma_{\rm AG} \sim \tilde{J}^2 p(p - 1)/2 C_{\rm AG}^{p-2} R_{\rm AG}$ and $D_{\rm AG} \sim J^2 p/2 C_{\rm AG}^{p-1}$ solve the equations in the aging regime. One has

$$1 = (R_{\rm ST}(\omega = 0))^2 \tilde{J}^2 p(p - 1) q^{p-2}/2, \qquad (11)$$

$$X_{\rm AG}/T = R_{\rm ST}(\omega = 0)\,(p - 2)/q \qquad (12)$$

that become $\tilde{J}^2 p(p - 1)/2 q^{p-2}(1 - q)^2 = T^2$ and $X_{\rm AG} = (p - 2)(1 - q)/q$ when $\hbar \to 0$ [3].

QF depress the critical temperature. The transition line $T_d(\hbar_d)$ ends at a quantum critical point $(T_d = 0, \hbar_d \neq 0)$. Equations (11) and (12) indicate that when the transition occurs at $T_d(\hbar_d) \neq 0$, $X_{\rm AG} \to 1$, $q \to q_d \neq 0$, and there is a finite linear stationary susceptibility $R_{\rm ST}(\omega = 0) < +\infty$ (as in the classical limit). On this line, $q_d \propto T_d^{2/p}$ and $q_d \to 0$ for $T_d \to 0$. At the quantum critical point, q_d tends to zero, and if $q_d \sim (\hbar_d - \hbar)^{\alpha p/2}$ then $X_{\rm AG}/T \sim (\hbar_d - \hbar)^{-\alpha}$ and $R_{\rm ST}(\omega = 0) \sim (\hbar_d - \hbar)^{\alpha(1-p/2)}$ diverges when $p > 2$ (α is positive).

Let us now discuss some numerical checks. In all figures $p = 3$, $\Lambda = 5$, $\tilde{J} = 1$, and $m = 1$. We use $T = 0$ and $\hbar = 0.1$ to illustrate the dynamics in the glassy phase. We also discuss the dependence upon T and $\hbar$.

In Figs. 1 and 2 we show the correlation $C(\tau + t_w, t_w)$ (log-log plot) and the response $R(\tau + t_w, t_w)$ (linear plot) vs the subsequent time τ obtained from the numerical solution to Eqs. (2). These plots demonstrate the existence of the stationary and aging regimes. For $t - t_w < \mathcal{T}(t_w)$ [e.g., $\mathcal{T}(40) \sim 5$] TTI and FDT are established, while beyond $\mathcal{T}(t_w)$ they break down. For $\hbar = 0.1$ the plateau in C is at $q \sim 0.97$. C oscillates around q but is monotonic when it goes below it. In the inset we present the dependence of q on $\hbar$ for $T = 0$. QF generate a $q < 1$ such that the larger $\hbar$ the smaller q. The addition of thermal fluctuations has a similar effect, the larger T, the smaller q. In order to check FDT in the stationary regime, in the inset of Fig. 2 we compare $R(t, t_w)$ from the numerical algorithm for $t = 40$ fixed and $t_w \in [0, 40]$ with $R(t, t_w)$ from

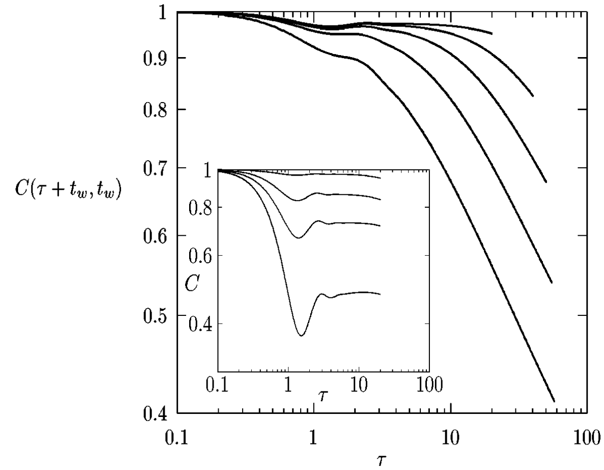

FIG. 1. The correlation function $C(\tau + t_w, t_w)$ vs τ for the $p = 3$ SG model, $\Lambda = 5$, $\tilde{J} = 1$, $m = 1$, $T = 0$, and $\hbar = 0.1$. The waiting times are, from bottom to top, $t_w = 2.5$, 5, 10, 20, and 40. $q \sim 0.97$. In the inset, the same curves for $t_w = 40$ and, from top to bottom, $\hbar = 0.1$, 0.5, 1, and 2.

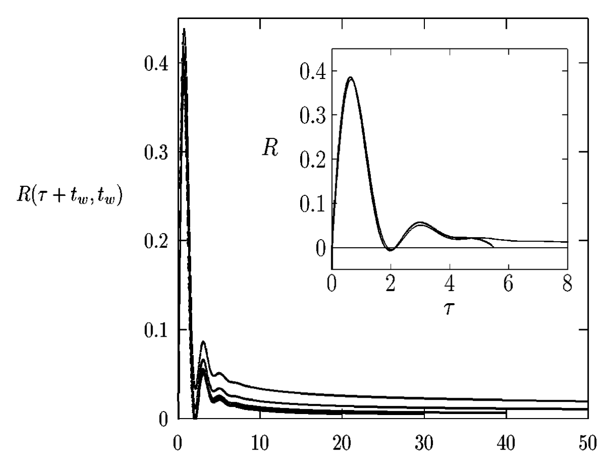

FIG. 2. The response function for the same model as above. The waiting times increase from top to bottom. In the inset, check of FDT in the stationary regime. The full line is $R(t, t_w)$ for $t = 40$ fixed and $t_w \in [0, 40]$. The thin line is obtained from Eq. (8) with $X = 1$, using the numerical data for $C_{\rm ST}(t - t_w) = C(t, t_w) - q$ ($q \sim 0.97$, see Fig. 1). In both cases the response is plotted against $\tau \equiv t - t_w$.

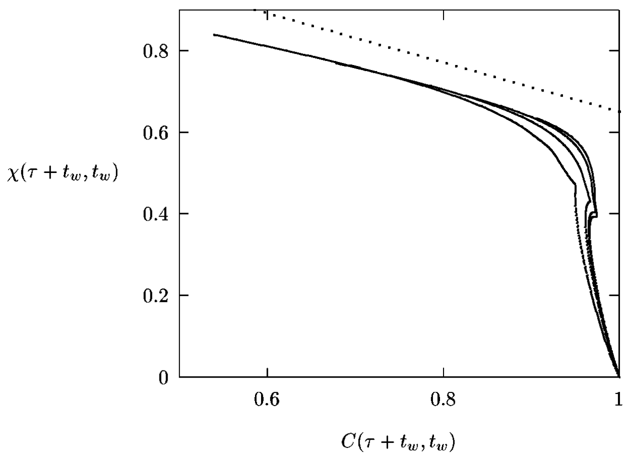

FIG. 3. The integrated response χ vs the correlation function C in a parametric plot. The curves correspond to $t_w = 10$, 20, 30, and 40. $T = 0$ and $\hbar = 0.1$. The dots are a guide to the eye and represent the analytic result $X_{\rm AG}/T \sim 0.60$.

Eq. (8), using $X = 1$ and $C_{\rm ST}(t - t_w) = C(t, t_w) - q$, $q \sim 0.97$, obtained from the algorithm. The accord is very good if $t - t_w \le \mathcal{T}(t_w) \sim 5$.

In Fig. 3 we plot the integrated response χ vs C in a parametric plot. When $C < q \sim 0.97$ the χ vs C curve approaches a straight line of *finite* slope $1/T_{\rm EFF} = X_{\rm AG}/T$ that we estimate from Eqs. (11) and (12) as $X_{\rm AG}/T \sim 0.60$. Note that this implies that the effective temperature is nonzero even at zero bath temperature. The dots follow from Eqs. (11) and (12).

To summarize, this formalism provides a clear framework to study the nonequilibrium regime and/or the eventual approach to equilibrium of quantum systems. It circumvents the difficulties of performing numerical simulations in real time and predicts the existence and the structure of a rich nonequilibrium regime for glassy systems even in the presence of QF. It is well-suited to analyze either disordered systems or nonlinear nondisordered models with some self-consistent approximation (mode coupling, direct interaction approximation, etc). Based on the success of mean-field-like classical glassy models to describe some aspects of the dynamics of realistic glassy systems (see, e.g., [2,18]) one can expect that quantum mean-field models of the type considered here do also capture important features of the real-time dynamics of real systems [7].

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