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 $\hbar \to 0$.

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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 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 that is now being verified numerically for more realistic models [2, 3]. All these studies concern classical systems.

Recent experiments have motivated a renewed interest on the effect of quantum fluctuations (QF) on glassy systems. Up to present, theoretical studies have focused on how QF affect their equilibrium properties [3, 4]. 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 trully nonequilibrium real-time dynamics of this type of systems. Intuitively, one expects QF to only affect 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 be also 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 add up to an effective temperature $T_{eff}$; (iv) to prove that $T_{eff}$ is non-zero 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) [2, 3]. 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 [3]. The bath variables are next integrated out and the effect of the bath manifests in the effective action through two non-local kernels associated to dissipation ($\eta$) and noise ($\nu$). 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, in a quantum dynamical calculation, 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 the $p$ spin-glass

$$H_J[\phi] = \frac{1}{2m_N} \sum_{i=1}^{N} \Pi_i^2 + \sum_{i_1,...,i_p} J_{i_1,...,i_p} \phi_{i_1} \ldots \phi_{i_p}$$

(1)

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

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

respectively. $\Sigma$ and $\bar{D}$ are functions of $C$ and $R$ that follow either from the average over disorder or from approximations of the nonlinear interactions in the model (e.g. mode-couling approximations). For the $p$-spin model and $t \geq t_w$ they read

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

The terms associated to 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 \( I(\omega) = (M\gamma_0/\pi) \omega \exp(-\omega\bar{\Lambda}/\hbar) \) with \( \Lambda \) a cut-off and \( M\gamma_0 \) a constant that plays the rôles of a friction coefficient. Their particular form depends on the choice of bath. The equations, for a random initial condition, are

\[ R(t, t_w) = G_\gamma(t, t_w) + \int_0^t dt \int_0^t du G_\gamma(t, u) \Sigma(u, v) R(v, t_w) \]
\[ C(t, t_w) = \int_0^t dt \int_0^t dw R(t, u) D(u, v) R(t_w, v) \]

(2)

with \( G_\gamma^{-1}(t, u) = \delta(t - u) (m\partial_u^2 + \mu(t)) \) the propagator and \( \mu(t) \) either a Lagrange multiplier enforcing a spherical constraint or the strength of a quadratic term. In the first case it is determined by the ‘gap’ equation:

\[ \mu(t) = \int_0^t dt \Sigma(t, u) C(t, u) + D(t, u) R(t, u) - m \partial_t C(t, t_w) \delta(t - t_w) \]

Causality implies \( R(t, t_w) = \Sigma(t, t_w) = 0 \) if \( t_w > t \). The inertial term 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 \( R(t, t) = 0, \lim_{t \to t_w} \partial_t R(t, t_w) = 1/m \). In what follows we set \( t \geq t_w \). The coupling to the bath implies dissipation: if \( M\gamma_0 \neq 0 \) the energy density \( \mathcal{E} \) of the system decreases. One can then envisage to switch-off the coupling (set \( M\gamma_0 = 0 \)) 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 \( M\gamma_0 \neq 0 \) for all times, reparametrize time according to \( t \to M\gamma_0 t \) and transform \( h \) in a free parameter \( h \to M\gamma_0 \hbar \). Consistently, \( C \to C, R \to R/(M\gamma_0), m \to (M\gamma_0)^2 m, J \to J, \beta \to \beta M\gamma_0 \) and the units are \( [C] = [R] = [h] = 1, [m] = [\beta] = [1/J] = [1/\Lambda] = [t] \).

We focus on \( p > 2 \), since \( p = 2 \) needs a special treatment [13]. Since Eqs. (2) are causal, we contruct its solution numerically, step by step in \( t \), spanning \( 0 \leq t_w \leq t \). The numerical and analytical studies yield:

(i) Quantum mode-coupling equations. For a \( \hbar \) and \( T \) above a critical line, there is a finite equilibration time \( \tau_{eq} \) 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

\[ R(\omega) = \frac{1}{-\mu - \omega - \Sigma(\omega)}, \]

(3)

\[ C(\omega) = D(\omega)|R(\omega)|^2. \]

(4)

with the couples \( R \) and \( C \), and \( \Sigma \) and \( D \), verifying QFDT:

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

(5)

\( \tau = \tau_{eq} \). Equations (3)-(4) are the quantum version of the mode-coupling equations used to describe supercooled-liquids [14]. 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 and, if \( T_d(\hbar_d) \neq 0 \), a plateau develops in \( C \). At the critical line, the length of the plateau tends to infinity. The quantum critical point \( (T_d = 0, \hbar_d \neq 0) \) is discussed below.

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

\[ q + C_{st}(t - t_w) = \lim_{t_w \to \infty} C(t, t_w) \]

(6)

and \( C_{st}(t - t_w) = \lim_{t_w \to \infty} R(t, t_w) \). The correlation approaches a plateau since \( \lim_{t_w \to \infty} C_{st}(t - t_w) = 0 \). The response approaches zero, \( \lim_{t - t_w \to \infty} R(t - t_w) = 0 \). The equations for \( C_{st} \) and \( R_{st} \) are identical to Eqs. (3)-(4) apart from contributions to \( \mu_{\infty} \) coming from the aging regime. \( C_{st} \) and \( R_{st} \) are linked through Eq. (6).

If \( t - t_w > T(t_w)(C(t, t_w) \geq q) \) the dynamics is stationary. TTI and QFDT hold. In other words,

\[ q + C_{st}(t - t_w) = \lim_{t_w \to \infty} C(t, t_w) \]

and \( C_{st}(t - t_w) = \lim_{t_w \to \infty} R(t, t_w) \). The correlation approaches zero, \( \lim_{t - t_w \to \infty} R(t - t_w) = 0 \). The equations for \( C_{st} \) and \( R_{st} \) are identical to Eqs. (3)-(4) apart from contributions to \( \mu_{\infty} \) coming from the aging regime. \( C_{st} \) and \( R_{st} \) are linked through Eq. (6).

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

\[ C_{ag}(t, t_w) = j^{-1}\left(\frac{\mu(t_w)}{\mu(t)}\right), \]

(7)

with \( \mu(t) \) a growing function of time. For the \( p \)-spin model, \( j^{-1} \) is the identity.

The system has a weak long-term memory, meaning that the response tends to zero but its integral over a growing time-interval is finite. The QFDT is more involved than the classical one since it is non-local (Eq. (6)). In the nonequilibrium case, we generalize it to

\[ R(t, t_w) = \frac{2i}{\hbar} \theta(t - t_w) \int \frac{d\omega}{2\pi} \exp(-i\omega(t - t_w)) \]

\[ \times \tanh\left(\frac{X(t, t_w)\beta\hbar\omega}{2}\right) C(t, \omega) \]

(8)

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

(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. (6). Interestingly enough, \( \tau_{ff} \equiv T/X(t, t_w) \) acts as an effective temperature in the system [17]. For a model with two two-time sectors we propose
\[
X(t, t_w) = \begin{cases} 
X_{ST} = 1 & \text{if } t - t_w \leq T(t_w) \\
X_{AG}(h, T) & \text{if } t - t_w > T(t_w)
\end{cases}
\]

with \(X_{AG}\) a non-trivial function of \(h\) and \(T\). When \(t\) and \(t_w\) are widely separated, the integration over \(\omega\) in Eq. (8) is dominated by \(\Omega \sim 0\). Therefore, the factor \(\tan h X_{AG}(t, t_w) / 2\) can be substituted by \(X_{AG} h / 2\) (even at \(T = 0\) if \(X_{AG}(h, T) = x(h) T\) when \(T \sim 0\)). Hence,

\[
R_{AG}(t, t_w) \sim \theta(t - t_w) X_{AG} h C_{AG}(t, t_w)
\]

and one recovers, in the aging regime, the classical modified FDT Eq. (9). Numerically (and experimentally), it is simpler to check it using the integrated response \(\chi(t, t_w) = \int_{t_w}^{t} d\tau R(t, \tau)\) over a large time window, that reads

\[
\chi(t, t_w) = \int_{t_w}^{t} d\tau' R_{ST}(\tau') + \frac{X}{\tau}(q - C_{AG}(t, t_w))
\]

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 — though the values of \(q\) and \(X_{AG}\) depend on \(h\). In this sense, we say that \(T(t_w)\) acts a time-dependent ‘decoherence time’, beyond which the nonequilibrium regime is ‘classical’.

An ansatz like Eq. (6) for \(C_{AG}\) combined with Eq. (10) for the FDT violation solves the equations in the aging regime. It yields

\[
1 = (R_{ST}(\omega = 0))^2 \frac{J^2}{2} p(p - 1) q^{p-2} / 2
\]

\[
X_{AG} / T = R_{ST}(\omega = 0) (p - 2) / q
\]

that become \(J^2 (p - 1) / 2 p^2 - 2 (1 - q)^2 = 2 T^2\) and \(X_{AG} = (p - 2) (1 - q) / q\) when \(h \rightarrow 0\).

QF depress the critical temperature. The transition line \(T_d(h_d)\) ends at a quantum critical point \((T_d = 0, h_d \neq 0)\). Equations (11)-(12) indicate that when the transition occurs at \(T_d(h_d) \neq 0\) it is first-order with \(X_{AG} \rightarrow 40\), \(q \rightarrow 0\) and a finite linear stationary susceptibility \(R_{ST}(\omega = 0) = 0\) (as in the classical limit). On this line, \(q_d \propto T_d^{2/3}\) and \(q_d \rightarrow 0\) for \(T_d \rightarrow 0\). At the quantum critical point, Eqs. (11)-(12) suggest a second-order transition; if \(q_d\) tends to zero as \(q_d \sim (h_d - h)^{40/2}\), then \(X_{AG} / T \sim (h_d - h)^{-2}\) and \(R_{ST}(\omega = 0) \sim (h_d - h)^{40 (1 - p/2)}\) diverges when \(p > 2\) (\(\alpha\) is positive).

Let us now discuss the numerical results. In all figures \(p = 3\), \(A = 5\), \(J = 1\) and \(m = 1\). We use \(T = 0\) and \(h = 0.1\) to illustrate the dynamics in the glassy phase. We also discuss the dependence upon \(T\) and \(h\).

In Figs. (3) and (4) we show the correlation \(C(t, t_w)\) (log-log plot) and the response \(R(t, t_w)\) (linear plot) vs the subsequent time \(t\). These plots demonstrate the existence of the stationary and aging regimes. For \(t - t_w < T(t_w)\) (e.g. \(T(40) \sim 5\)) TTI and FDT are established while beyond \(T(t_w)\) they break down. For \(h = 0.1\) the plateau in \(C\) is at \(q \sim 0.97\). \(C\) oscillates around \(q\) but is monotonous when it goes below it. In the inset we present the dependence of \(q\) on \(h\) for \(T = 0\). QF generate a \(q < 1\) such that the larger \(h\) 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. (3) we compare \(R(t, t_w)\) from the numerical algorithm for \(t = 40\)
fixed and \( t_w \in [0, 40] \) (full line) with \( R(t, t_w) \) from Eq.\[8] with \( X = 1 \) using \( C_{\text{st}}(t-t_w) = C(t, t_{\text{w}}) - q, \ q \sim 0.97 \) obtained from the algorithm (dots). The accord is very good if \( t - t_w \leq T(t_w) \sim 5 \).

In Fig.3 we plot the integrated response \( \chi \) vs. \( C \) in a parametric plot. When \( C < q \sim 0.97 \) the \( \chi \) vs \( C \) curve approaches a straight line of finite slope \( 1/T_{\text{eff}} = X_{\text{ag}}/T \) that we estimate from Eqs.\([11]\) and \([2]\) as \( X_{\text{ag}}/T \sim 0.60 \). The dots are a guide to the eye representing it.

![Integrated response](image)

FIG. 3. The integrated response \( \chi(t + t_w, t_w) \) vs. the symmetrized auto-correlation function \( C(t + t_w, t_w) \) in a parametric plot. The curves correspond to \( t_w = 10, 20, 30, 40 \). \( T = 0 \) and \( h = 0.1 \). The dots are a guide to the eye and represent the analytic result \( X_{\text{ag}}/T \sim 0.60 \) for the slope of the asymptotic curve in the aging regime \( C < q \sim 0.97 \).

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. Based on the success of mean-field like classical glassy models to describe some aspects of the dynamics of realistic glassy systems (see \([2,14]\) and references therein) 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.

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