Crossover from coherent to incoherent dynamics in damped quantum systems

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The destruction of quantum coherence by environmental influences is investigated by taking the damped harmonic oscillator and the dissipative two-state system as prototypical examples. It is shown that the location of the coherent-incoherent transition depends to a large degree on the dynamical quantity under consideration. [S1063-651X(97)50704-5]

The destruction of quantum coherence by dissipative influences continues to be a problem of central interest in atomic physics, condensed matter physics, and chemical physics. It is relevant to phenomena as diverse as wave packet dynamics in atoms [1], defect tunneling in solids [2], electron transfer in chemical and biological reactions [3], or quantum computers [4]. Important insight into the effects of an environment on quantum coherence was obtained in the last decade based on studies of simple quantum systems in contact with a heat bath [5,6]. Very recently, focusing on the archetypical two-state system, two groups [7,8] arrived at a result that, at first glance, seems to invalidate earlier studies. They found that quantum coherence is destroyed at significantly smaller damping strengths than thought previously, typically differing by a factor 2/3.

In this paper, we show that the coherent-incoherent transition depends on the particular dynamical quantity under consideration (e.g., correlation function, occupation probability, etc.). Since different dynamical quantities may be associated with different initial preparations of the system, quantum coherence may be more or less sensitive to dissipation. The resulting critical value of the damping strength then changes to a surprisingly large degree with the respective coherence criterion. This will be explicitly demonstrated for the two fundamental dissipative quantum systems, namely, the damped harmonic oscillator and the dissipative two-state system. As the differences are most pronounced at zero temperature, we confine ourselves to this limit.

We start with the exactly solvable case of a *harmonic oscillator* subject to Ohmic damping [6]. The respective classical equation of motion for the position $q(t)$ is

$$\ddot{q}(t) + \gamma \dot{q}(t) + \omega_0^2 q(t) = F(t)/M, \qquad (1)$$

where γ is the usual Ohmic damping rate, ω_0 the frequency of the bare oscillator, and M the mass of the particle. The response to the external force $F(t)$ is described by

$$\langle q(t) \rangle = \frac{1}{M\omega_0} \int_{-\infty}^{t} dt' \chi_{\text{osc}}(t-t') F(t'), \qquad (2)$$

where $\langle q(t) \rangle$ denotes the expectation value, and $\chi_{\text{osc}}(t)$ is the linear response function, which for the harmonic oscillator coincides with the classical response function.

One dynamical quantity of interest is the *equilibrium* correlation function

$$C_{\text{osc}}(t) = \text{Re}\langle q(t)q(0) \rangle, \qquad (3)$$

where the brackets denote a ground-state average. Consider now the associated spectral function [7]

$$S_{\text{osc}}(\omega) = C_{\text{osc}}(\omega)/|\omega|,$$

which at $T=0$ is related to the absorptive part of the dynamical susceptibility by (we set $\hbar = 1$)

$$S_{\text{osc}}(\omega) = \text{Im}\chi_{\text{osc}}(\omega)/\omega.$$

It is an even function of ω, and the second form follows from the fluctuation-dissipation theorem. From Eq. (1), we have the dynamical susceptibility

$$\chi_{\text{osc}}(\omega) = \frac{\omega_0}{\omega_0^2 - \omega^2 - i\gamma\omega}, \qquad (4)$$

and hence the spectral function

$$S_{\text{osc}}(\omega) = \frac{\gamma\omega_0}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2}. \qquad (5)$$

Another problem of interest is the relaxation of the expectation value $\langle q(t) \rangle$ starting from a *nonequilibrium* initial state. Applying the force $F(t) = M\omega_0^2 q_0 \Theta(-t)$, the initial condition $\langle q(0) \rangle = q_0$ is prepared [cf. Eq. (2)], and the relevant dynamical quantity is

$$P_{\text{osc}}(t) = \langle q(t) \rangle / q_0. \qquad (6)$$

With the Fourier transform (4) of the response function, one obtains from Eq. (2)

$$P_{\text{osc}}(t) = \cos(\Omega t - \phi)\exp(-\gamma t/2)/\cos(\phi), \qquad (7)$$

where $\Omega = \sqrt{\omega_0^2 - \gamma^2/4}$ and $\phi = \arctan(\gamma/2\Omega)$.

Let us now discuss the coherent-incoherent transition as a function of the dimensionless damping strength

$$\alpha = \gamma/2\omega_0.$$

We first consider the appropriate coherence criterion based on the spectral function $S_{\text{osc}}(\omega)$. For weak damping, $\alpha < \alpha_c$, the function $S_{\text{osc}}(\omega)$ exhibits two inelastic peaks at finite frequency $\omega = \pm \omega_m(\alpha)$. At the critical damping strength α_c, one has $\omega_m(\alpha_c) = 0$, and the two peaks merge into a single quasielastic peak centered at $\omega = 0$. This quasielastic peak then persists for $\alpha > \alpha_c$. The value of α_c can be determined by inspecting the sign of the curvature of $S_{\text{osc}}(\omega)$ at zero frequency. From Eq. (5), we have the small-ω expansion

$$S_{\text{osc}}(\omega) = 2\alpha\chi_0^2[1 + (2 - 4\alpha^2)\chi_0^2\omega^2 + O(\omega^4)], \quad (8)$$

where $\chi_0 = 1/\omega_0$ is the static susceptibility. Thus the curvature of $S_{\text{osc}}(\omega)$ is positive (implying coherence) for $\alpha < 1/\sqrt{2}$, but changes sign at the critical value. Regarding the equilibrium correlations $C_{\text{osc}}(t)$, quantum coherence is suppressed for $\alpha > \alpha_c = 1/\sqrt{2}$.

A different coherence criterion can be developed based on the quantity $P_{\text{osc}}(t)$. For weak damping, one finds damped oscillations such that $P_{\text{osc}}(t)$ changes sign occasionally. As the damping strength α is increased, $P_{\text{osc}}(t)$ shows a transition from damped oscillatory to a purely incoherent behavior. The coherent-incoherent transition is reached at the critical value $\alpha = \alpha_c^*$. For $\alpha > \alpha_c^*$, one has $P_{\text{osc}}(t) \geq 0$ for all times t. This coherence criterion based on a nonequilibrium initial preparation has been used in most previous work [5,6]. For the damped harmonic oscillator, we see from Eq. (7) that $P_{\text{osc}}(t)$ becomes overdamped for $\alpha > 1$, while damped oscillations persist for $\alpha < 1$. Regarding the nonequilibrium quantity $P_{\text{osc}}(t)$, one has destruction of quantum coherence for $\alpha > \alpha_c^* = 1$. The ratio between the critical damping strengths for the two dynamical quantities $C_{\text{osc}}(t)$ and $P_{\text{osc}}(t)$ is then given by

$$\alpha_c/\alpha_c^* = 1/\sqrt{2}. \quad (9)$$

We now turn to the case of a symmetric *two-state system*. Coupling to an Ohmic heat bath is described in terms of the spin-boson Hamiltonian [5,6]

$$H = -(\Delta/2)\sigma_x + \sum_i \left(\frac{p_i^2}{2m_i} + \frac{m_i\omega_i^2 x_i^2}{2} - \frac{c_i x_i \sigma_z}{2} \right).$$

The two eigenstates of σ_z with eigenvalues ± 1 are coupled by the transfer matrix element Δ representing the tunnel splitting of the free system. The Ohmic bath of harmonic oscillators is fully characterized by the spectral density

$$J(\omega) = \frac{\pi}{2}\sum_i \frac{c_i^2}{m_i\omega_i}\delta(\omega - \omega_i) = 2\pi\alpha\omega\exp(-\omega/\omega_c),$$

where α is a dimensionless damping strength, and ω_c is a high-frequency cutoff.

An important aspect of this model is its correspondence with the Kondo effect. By writing the partition function in the Coulomb gas representation, a firm equivalence with the anisotropic Kondo model can be established [9]. This correspondence has been exploited by Costi and Kieffer [7], who applied a dynamical version of Wilson's numerical renormalization group to the anisotropic Kondo model. Further-

more, Lesage, Saleur, and Skorik [8] have employed integrability and form-factor techniques to study this model as well. Both groups have calculated the ground-state spin-spin correlation function of the Kondo model equivalent to the $T = 0$ equilibrium two-state correlation function

$$C(t) = \text{Re}\langle\sigma_z(t)\sigma_z(0)\rangle.$$

This quantity is the direct analog of the harmonic oscillator correlation function $C_{\text{osc}}(t)$ defined in Eq. (3).

Another useful quantity, particularly in the context of macroscopic quantum coherence [4,5], is the occupation probability

$$P(t) = \langle\sigma_z(t)\rangle,$$

corresponding to the harmonic oscillator quantity $P_{\text{osc}}(t)$ defined in Eq. (6). In contrast to $C(t)$, the function $P(t)$ is subject to the nonequilibrium initial preparation $\sigma_z(t = 0) = +1$. This preparation of the initial state may be realized by applying a large external bias. Thereby the spin is held fixed in the state $\sigma_z = +1$ with equilibrated environment. At time zero, the constraint is released, and the dynamics starts out from $P(0) = 1$ with this factorized system-environment initial state.

Let us now discuss the coherent-incoherent transition for the dissipative two-state system, starting with the equilibrium correlations. Similar to Eq. (8), the function $S(\omega) = C(\omega)/|\omega|$ has the low-frequency expansion

$$S(\omega) = 2\pi\alpha\chi_0^2[1 + \kappa(\alpha)\chi_0^2\omega^2 + O(\omega^4)], \quad (10)$$

where χ_0 is the static susceptibility and $\kappa(\alpha)$ is a dimensionless parameter. The zero-frequency limit of Eq. (10) is the generalized Shiba relation for the spin-boson problem [10]. As a result of this relation, spin-spin correlations decay asymptotically as $C(t) = -2\alpha\chi_0^2/t^2$. In Refs. [7,8], the function $\kappa(\alpha)$ has been computed and was found to change sign at the critical value $\alpha_c = 1/3$.

Next we analyze the transition from oscillations to incoherent relaxation in the quantity $P(t)$. Within the widely used noninteracting-blip approximation (NIBA), the critical value is $\alpha_c^* = 1/2$ [5]. This result can easily be seen by switching to the Laplace transform $P(\lambda)$ and defining a self-energy $\Sigma(\lambda)$,

$$P(\lambda) = 1/[\lambda + \Sigma(\lambda)]. \quad (11)$$

NIBA gives for the self-energy [5,6]

$$\Sigma(\lambda) = \Delta^2\cos(\pi\alpha)\int_0^\infty d\tau \frac{\exp(-\lambda\tau)}{(\omega_c\tau)^{2\alpha}} = \Delta_e(\Delta_e/\lambda)^{1-2\alpha}, \quad (12)$$

with the effective frequency scale

$$\Delta_e = \Delta[\cos(\pi\alpha)\Gamma(1 - 2\alpha)]^{1/2(1-\alpha)}(\Delta/\omega_c)^{\alpha/(1-\alpha)}.$$

In the limit $\alpha \to 1/2$, the frequency Δ_e approaches $\pi\Delta^2/2\omega_c$. For $\alpha > 0$, the function $P(\lambda)$ has a branch point at $\lambda = 0$. The complex λ plane is cut along the negative real axis, and in the cut plane $P(\lambda)$ is single valued. The cut leads to an incoherent contribution to $P(t)$. Moreover, for

$\alpha < 1/2$, the integrand has a conjugate pair of poles in the cut λ plane describing damped oscillations.

To study the coherent-incoherent transition, we consider the pole condition from Eq. (11),

$$(\lambda/\Delta_e)^{2-2\alpha} = -1, \tag{13}$$

and put

$$\alpha = 1/2 - \epsilon, \quad |\epsilon| \ll 1 . \tag{14}$$

For $\epsilon > 0$ ($\alpha < 1/2$), insertion of the ansatz

$$\lambda/\Delta_e = -1 + \epsilon u \pm i\epsilon v + O(\epsilon^2)$$

into Eq. (13) yields $u = 0$ and $v = 2\pi$. Hence, in the NIBA the damping rate Γ and the oscillation frequency Ω are up to corrections of order ϵ^2,

$$\Gamma/\Delta_e = 1, \quad \Omega/\Delta_e = 2\pi\epsilon. \tag{15}$$

This results in damped oscillations with frequency Ω. In contrast, for $\epsilon < 0$ ($\alpha > 1/2$), the poles are not in the cut plane and therefore give no contribution to $P(t)$. In that case, $P(t)$ is completely given by the incoherent branch-cut contribution. Thus the critical damping strength is indeed $\alpha_c^* = 1/2$.

Remarkably, exactly at the special value $\alpha = 1/2$, NIBA becomes exact [5], while it is only an approximation for $\alpha \neq 1/2$. One serious deficiency comes from the branch-cut contribution, which would imply the existence of an algebraic long-time tail. From Eq. (12), for $\alpha = 1/2 - \epsilon$ and $\lambda \to 0$, one finds $P(\lambda) \sim \lambda^{2\epsilon}$. The asymptotic branch-cut contribution is therefore

$$P(t) = -2\epsilon/(\Delta_e t)^{1+2\epsilon}. \tag{16}$$

This term, decaying slower than $1/t^2$, contradicts the fluctuation-dissipation theorem. Hence, the long-time tail (16) is an unphysical artifact of NIBA [5]. Such a failure raises the question of whether the NIBA value $\alpha_c^* = 1/2$ for the coherent-incoherent transition remains correct.

To investigate the coherent-incoherent transition beyond NIBA, we now systematically expand around the exactly solvable case $\alpha = 1/2$. In diagrammatic terms, the exact self-energy $\Sigma(\lambda)$ is the sum over all irreducible arrangements of ''blips'' and ''sojourns.'' A blip (sojourn) refers to the time spent in an off-diagonal (diagonal) state of the reduced density matrix [5,6]. For instance, the NIBA expression (12) is just given by the single-blip contribution, thereby effectively disregarding all interblip interactions in $P(\lambda)$. The fact that NIBA becomes exact for $\alpha = 1/2$ is explained simply by the concept of *collapsed blips* [6]. In view of Eq. (14), there is a factor $\cos(\pi\alpha) = \pi\epsilon$ in Eq. (12). This $O(\epsilon)$ factor must be canceled by a $1/\epsilon$ short-time contribution of the τ integral over the length of the blip such that a finite result can arise. Therefore, for $\alpha \to 1/2$, only blips of effectively vanishing length, that is, ''collapsed'' blips, contribute. Since interactions among different collapsed blips vanish, NIBA becomes exact [6].

For nonzero ϵ, the blip length is finite, and one has to take into account all sequences of *collapsed sojourns* within an extended blip of length τ. Their presence crucially modifies

the self-energy in the limit $\lambda \to 0$. Since collapsed sojourns do not interact with blips or other sojourns, a grand-canonical gas of collapsed sojourns merely gives a factor $\exp(-\Delta_e \tau/2)$, and the self-energy (12) is changed into

$$\Sigma(\lambda) = \Delta^2 \pi\epsilon \int_0^\infty d\tau \frac{\exp[-(\lambda + \Delta_e/2)\tau]}{(\omega_c \tau)^{1-2\epsilon}}$$

$$= \Delta_e(\lambda/\Delta_e + 1/2)^{-2\epsilon}. \tag{17}$$

With the regularized self-energy (17), the pole condition now reads

$$\lambda(1/2 + \lambda/\Delta_e)^{2\epsilon} = -\Delta_e .$$

This yields the exact decay rate and oscillation frequency up to corrections of order ϵ^2,

$$\Gamma/\Delta_e = 1 - 2\epsilon\ln 2, \quad \Omega/\Delta_e = 2\pi\epsilon.$$

Compared to the NIBA result (15), the rate acquires a correction in order ϵ. However, the oscillation frequency remains completely unchanged. Therefore, the NIBA value $\alpha_c^* = 1/2$ for the location of the coherent-incoherent transition turns out to be the *exact* result. This implies the critical ratio

$$\alpha_c/\alpha_c^* = 2/3,$$

which is slightly smaller than the respective ratio (9) for the damped harmonic oscillator.

The exact self-energy (17) shifts the branch point of $P(\lambda)$ and thereby removes the spurious algebraic long-time tails (16). For $\epsilon > 0$, the leading branch-cut contribution at long times is now given by

$$P(t) = -2\epsilon \frac{\exp(-\Delta_e t/2)}{(\Delta_e t)^{1+2\epsilon}},$$

while for $\epsilon < 0$, we obtain

$$P(t) = 8|\epsilon| \frac{\exp(-\Delta_e t/2)}{(\Delta_e t)^{1+2|\epsilon|}}.$$

Thus, the unphysical algebraic long-time tails are suppressed by an exponential decay factor. It is straightforward to see that for $\epsilon > 0$ ($\alpha < 1/2$), the full cut contribution is negative, while it becomes positive for $\epsilon < 0$ ($\alpha > 1/2$). Indeed, for $\alpha \geq 1/2$, the function $P(t)$ is positive and monotonically decaying; i.e., the dynamics is fully incoherent. In marked contrast to the NIBA result (16), the power of the algebraic decay factor does not depend on the sign of ϵ.

The remarkable success of NIBA in predicting the correct value of α_c^* provokes questions about the general quality of such a simple approximation for the full range of α. A convenient tool to investigate this issue is the real-time quantum Monte Carlo simulation method [11]. This technique permits a numerically exact calculation of both dynamical quantities $C(t)$ and $P(t)$ by stochastic evaluation of the respective real-time path-integral representations. The dynamical sign problem arising from the interference between different real-time paths can be largely circumvented by a partial summation scheme, and stable simulations can be carried out for rather
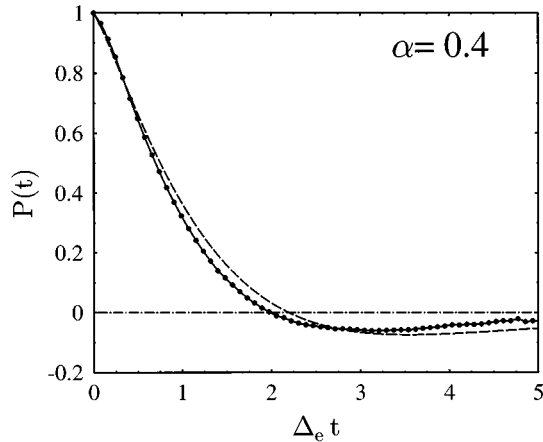
FIG. 1. Monte Carlo data for $P(t)$ at $\alpha = 0.4$ and $T = 0$. Circles are data points for $\Delta/\omega_c = 1/6$, the solid curve connecting them is a guide for the eye only. Statistical errors are well below 5%. The dashed curve is the NIBA result.

long times. The simulation code permits a computation of $P(t)$ directly at zero temperature, where the case $\alpha = 1/2$ serves as a convenient benchmark that is indeed passed accurately [11].

Numerical results for $P(t)$ at $\alpha = 0.4$ are shown in Fig. 1, and data for $\alpha \geq 1/2$ can be found in Ref. [11]. These data represent universal scaling curves in the sense that they can be obtained from different ω_c and/or Δ by employing the effective frequency scale Δ_e. Apparently, on short-to-intermediate time scales, NIBA yields a very accurate prediction for $P(t)$. However, the prediction $C(t) = P(t)$ as well as the long-time tails (16) are clear deficiencies of this approximation [11].

In conclusion, we have demonstrated that the initial preparation of a dissipative quantum system leads to drastic changes regarding the transition from coherence to incoherence as the damping strength is increased. Both the damped harmonic oscillator and the dissipative two-state system show that the two coherence criteria previously employed in the literature lead to a factor $1/\sqrt{2}$ and 2/3 difference in the critical damping strengths, respectively. Any investigation of the environmental destruction of quantum coherence thus necessitates a clear specification of the physical quantities under study.

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