Decoherent Dynamics of a Two-Level System Coupled to a Sea of Spins

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The dynamics of a two-level system which is coupled to an environmental sea of infinitely many spin-1/2 particles is investigated by use of the resolvent operator approach. Only at zero temperature does this spin-spin-bath model exhibit identical behavior as the more familiar spin-boson model. It is found that increasing temperature favors coherent dynamics. At high temperatures, the spin-spin-bath model for an Ohmic spectral density sustains a coherent dynamics if the dissipation coefficient α is sufficiently small, i.e., $\alpha < 1/2$; while the decoherence exhibits pure exponential decay if $\alpha > 1/2$. [S0031-9007(98)08029-6]

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In order to explore macroscopic quantum phenomena the influence of dissipation on quantum coherence has been extensively investigated over the past eighteen years. These efforts culminated in the systematic study of the spin-boson model [1–3]. The spin-boson system has witnessed many applications in physics and chemistry [1–7]. To take into account the effect of dissipation in a microscopic model a central task comprises the formulation of the environment. For weak couplings, Caldeira and Leggett [8] suggested that a bosonic heat bath consisting of an infinite number of harmonic oscillators constitutes a *universal* realization for any environment that occurs generically in the real physical world. In fact, when the couplings between the system and the heat bath are sufficiently weak, interactions between the excitations of the heat bath are negligibly small. Consequently, every excitation can be regarded as a quantum transition taking place in an individual two-level (sub)system. Based on such a reasoning, one may put forward the hypothesis that a spin bath composed of an infinite number of two-level systems may equally well provide a physically realistic environment [9]. Of course, such a spin-bath modeling is not merely of academic interest. Realistic physical situations are (i) a spin that interacts with the surrounding, effectively independent spin modes [10]; (ii) the magnetic relaxation of molecular crystals of Mn_{12} and Fe_8 [11] or coupled nanomagnets [12]. Moreover, this model is relevant for decoherence studies of stylized quantum measurement setups [13,14], and predominantly also for physical quantum computers [15] for which the ubiquitous phenomenon of spin decoherence within quantum information processors operating in terms of coupled two-level units (qubits) is limiting the performance [16,17].

A prominent question is whether (or to what extent) the two types of reservoirs exert identical effects on quantum coherence. In this Letter we shall answer this challenge by studying the dynamics of a two-level system, a spin or a qubit, immersed in a thermal sea of two-level systems composed of *independent modes* of weakly interacting spins or qubits. The model Hamiltonian $H \equiv H_s + H_b + H_{\text{int}}$ reads [18]

$$H = -\frac{1}{2}\hbar\Delta_0\sigma^x - \frac{1}{2}\sum_k \hbar\omega_k\sigma_k^z + \frac{1}{2}\sigma^z \otimes \sum_k \hbar C_k\sigma_k^x,$$
(1)

where H_s is the Hamiltonian of the central two-level system (written in the basis of *localized* states), H_b constitutes the spin bath, while H_{int} denotes the couplings. The zero-temperature thermostatics of this Hamiltonian for the idealized case that the spectral density is Einstein-like, i.e., $\omega_k = \omega/N$ and $C_k = \lambda/N$ for all k ($k = 1, 2, ..., N$), was studied by Mermin [18]. Within this mean-field version he was able to explain the physics of a phase transition (at $T = 0$) in quantum mechanics. Here, we shall reveal the characteristic features of the *dynamics* of the generic spin-spin-bath model. In order to compare the finding with the known results for the spin-boson model, we assume an Ohmic dissipation mechanism, i.e., $J(\omega) \equiv \pi\sum_k C_k^2\delta(\omega - \omega_k) = 2\pi\alpha\omega e^{-\omega/\omega_c}$, where α is the dissipation coefficient and ω_c denotes the cutoff frequency $\omega_c/\Delta_0 \gg 1$.

Use of a transformation.—Suppose that the system evolves from a localized initial state while the spin bath is initially at thermal equilibrium. This uncoupled initial density matrix is $\rho_0 = \rho_s \otimes \rho_b$, where $\rho_s = (\mathbf{1} + \sigma^z)/2$ and $\rho_b = \prod_k \otimes \{\exp(-\beta\hbar\omega_k\sigma_k^z/2)/\text{Tr}_k[\exp(-\beta\hbar\omega_k\sigma_k^z/2)]\}$. A diagnostic quantity related to quantum coherence is the probability difference between the two localized states, i.e., $P(t) = \text{Tr}[\rho(t)\sigma^z]$. We apply to the Hamiltonian (1) a transformation $\mathcal{U} = \prod_k \mathcal{U}_k$, where

$$\mathcal{U}_k = \frac{1}{\sqrt{2}}\mathbf{1}\otimes\mathbf{1}\cdots\begin{pmatrix}1 & \sigma^z \\ 1 & -\sigma^z\end{pmatrix}_k\otimes\mathbf{1}\cdots\otimes\mathbf{1}.$$

Note that each individual transformation acts on the composite Hilbert space of the central two-level system and the kth spin of the bath. The transformed Hamiltonian, which is feasibly diagonalized in the central spin manifold [19],

reads

$$\bar{H} = \mathcal{U} H \mathcal{U}^{-1} = \bar{H}_b + \bar{H}_{\text{int}}$$

$$= \sum_k \left(-\frac{1}{2} \hbar \omega_k \sigma_k^x + \frac{1}{2} \hbar C_k \sigma_k^z \right)$$

$$- \frac{1}{2} \hbar \Delta_0 \sigma^x \otimes \prod_k \otimes \sigma_k^x . \qquad (2)$$

This transformation is similar to the polaron transformation frequently used in the spin-boson model [20]; it allows us to diagonalize $\bar{H}$ if $\Delta_0 = 0$. Upon comparing Eqs. (1) and (2) we find——as the two-level system becomes dressed by the spin bath—that the couplings between them are now *converted* into interactions within each two-level system of the bath. Moreover, the initial density matrix changes to $\bar{\rho}_0 \equiv \mathcal{U} \rho_0 \mathcal{U}^{-1} = \rho_s \otimes \bar{\rho}_b$, with $\bar{\rho}_b = \prod_k \otimes \{[\mathbf{1} - \tanh(\beta \hbar \omega_k/2)\sigma_k^x]/2\}$; thus, the transformed spin bath remains formally no longer at initial equilibrium.

Given the Hamiltonian $\bar{H}$, it is convenient to use the resolvent operator approach to elucidate the behavior of the probability difference $P(t)$. Solving formally the Liouville equation, we obtain $P(t) = \text{Tr}[\sigma^z Q(t)\bar{\rho}(0)]$, where the superoperator $Q(t) \equiv \exp(iLt)$ is the propagator related to the Liouvillian L, being defined by $LA = [\bar{H}, A]/\hbar$ for any operator A. Let us denote the Laplace transform of $Q(t)$ by $\hat{Q}(z)$, i.e., $\hat{Q}(z) = \mathcal{L}\{Q(t)\}$. The thermodynamic average of $\hat{Q}(z)$ with respect to the *nonequilibrium* bath $\bar{\rho}_b$ reads $\langle \hat{Q}(z) \rangle_b = [z - \langle \hat{M}^c(z) \rangle_b]^{-1}$, where $\langle M^c(z) \rangle_b$ is termed the relaxation (self-energy) matrix [21,22]. Resorting to the perturbation expansion method, we obtain

$$\langle \hat{M}^c(z) \rangle_b = z \sum_{m=1}^{\infty} (-1)^{m+1} \left\langle \left(\sum_{n=1}^{\infty} (iL_{\text{int}}G)^n \right)^m \right\rangle_b, \quad (3)$$

where $G = 1/(z - iL_b)$ and L_b, L_{int} are the Liouvillians corresponding to $\bar{H}_b$ and $\bar{H}_{\text{int}}$, respectively. Note that Liouvillians act on the linear operators (of the Hilbert space) which themselves form the four-dimensional Liouville space. Thus, the superoperators $\langle \hat{Q}(z) \rangle_b$ and $\langle \hat{M}^c(z) \rangle_b$ can be represented by 4×4 matrices. Let $|\uparrow\rangle$ and $|\downarrow\rangle$ denote the two localized states of the two-level system. The four independent operators $|\mu\rangle\langle\nu| \equiv |\mu\nu)$ ($\mu, \nu = \uparrow$ or $\downarrow$) are used as the basis of the Liouville space. One can show that $\hat{P}(z) = \mathcal{L}\{P(t)\}$ is only related to two elements of $\langle \hat{Q}(z) \rangle_b$, i.e., $\hat{P}(z) = (\uparrow\uparrow |\langle \hat{Q}(z) \rangle_b| \uparrow\uparrow) - (\downarrow\downarrow |\langle \hat{Q}(z) \rangle_b| \uparrow\uparrow)$.

Second-order perturbation theory.—In applying second-order perturbation theory in L_{int} the self-energy matrix becomes

$$\langle \hat{M}^c(z) \rangle_b = z[i\langle L_{\text{int}}G \rangle_b - \langle (L_{\text{int}}G)^2 \rangle_b + \langle L_{\text{int}}G \rangle_b^2]. \qquad (4)$$

We use $\hat{M}_1^c(z)$, $\hat{M}_{2,c}^c(z)$, and $\hat{M}_{2,u}^c(z)$ to denote the three terms on the right-hand side (rhs) in Eq. (4), respectively. For instance, the first-order term can be cast as

$$(\mu\nu|\hat{M}_1^c(z)|\mu'\nu') = \frac{1}{2} iz\Delta_0(\delta_{\mu\mu'} - \delta_{\nu\nu'})$$

$$\times \mathcal{L}\left\{ \text{Tr}\left[\prod_k \sigma_k^x \tilde{\rho}_b(t) \right] \right\},$$

where $|m\rangle$ and ϵ_m are the mth eigenvectors and eigenenergies of $\bar{H}_b$ and the tilde represents the interaction representation, i.e., $\tilde{\rho}_b(t) = e^{i\bar{H}_b t/\hbar} \bar{\rho}_b e^{-i\bar{H}_b t/\hbar}$. Defining $g(z) = iz\Delta_0 \mathcal{L}\{A(t)\}/2$, where $A(t) = \text{Tr}[\prod_k \sigma_k^x \tilde{\rho}_b(t)]$, we readily obtain $\hat{M}_1^c(z) = -g(z)(\mathbf{1} - \sigma^x) \otimes \sigma^x$. Next we invoke the second-order perturbation approximation with respect to the coupling constants C_k/ω_k. This has been verified for a reasonable scaling rule $C_k/\omega_k \sim 1/\sqrt{N}$, where N is the number of bath spins (cf. [23]). We find for the Ohmic dissipation $A(t) = q(\beta)(1 + \omega_c^2 t^2)^{-\alpha}$, where $q(\beta) = \prod_k \tanh(\beta \hbar \omega_k/2)$ is a time-independent coefficient. With the Laplace transform of $A(t)$, the function $g(z)$ reads

$$g(z) = \frac{i}{2} \frac{\Delta_0}{\omega_c} \frac{\sqrt{\pi}}{2^{1/2+\alpha}} q(\beta)z\left(\frac{\omega_c}{z}\right)^{1/2-\alpha} \Gamma(1 - \alpha)$$

$$\times \left[\mathbf{H}_{1/2-\alpha}\left(\frac{z}{\omega_c}\right) - \mathbf{N}_{1/2-\alpha}\left(\frac{z}{\omega_c}\right) \right], \qquad (5)$$

where $\mathbf{H}$ is the Struve function and $\mathbf{N}$ is the Bessel function of the second kind [24]. Similarly, we find the correlation part of the second-order self-energy matrix contribution $\hat{M}_{2,c}^c(z) = -f(z)(\mathbf{1} - \sigma^z) \otimes \mathbf{1}$, where $f(z) = z\Delta_0^2 \mathcal{L}\{\int_0^t \Phi(u,t)du\} + \text{c.c.}$ with $\Phi(u,t) = \text{Tr}[\prod_k \otimes \sigma_k^x \prod_k \otimes \tilde{\sigma}_k^x(-u)\tilde{\rho}_b(t-u)]$. For the Ohmic dissipation we obtain $\Phi(u,t) \equiv A_1(u) \exp\{i[B(u) - B(t) + B(t - u)]\}$, where the amplitude $A_1(u) = (1 + \omega_c^2 u^2)^{-\alpha}$ and the "phase" term $B(s)$ reads

$$B(s) = 2\alpha \sum_{n=0}^{\infty} (-1)^n \left\{ \tan^{-1}\left(\frac{\omega_c s}{1 + n\omega_c \beta \hbar}\right) \right.$$

$$\left. - \tan^{-1}\left(\frac{\omega_c s}{1 + (n+1)\omega_c \beta \hbar}\right) \right\}. \qquad (6)$$

Note that the amplitude $A_1(u)$ is independent of temperature. The influence of temperature is manifested through the three phase terms. At zero temperature, i.e., $\beta \to \infty$, we find $B(t) = 2\alpha \tan^{-1}(\omega_c t)$. In addressing the dynamics in a meaningful domain, i.e., $t \gg \omega_c^{-1}$ or $\tan^{-1}(\omega_c t) = \pi/2$, one gets $\Phi(u,t) = e^{i\pi/2}A_1(u) \exp\{i[B(u) + B(t - u)]\} + \text{c.c.}$ By virtue of the convolution theorem, we obtain $f(z) = z\Delta_0^2 e^{i\pi/2} \mathcal{L}\{A_1(t) \exp[iB(t)]\}\mathcal{L}\{\exp[iB(t)]\} + \text{c.c.}$ At a very high temperature, i.e., $\beta \to 0$, $B(s)$ vanishes. Thus one gets $f(z) = \mathcal{L}\{A_1(t)\}$. In the following we will focus on the dynamics at zero and infinite temperatures.

Recognizing that $M_{2,u}^c(z) = -[M_1^c(z)]^2/z$, we know all three contributions to the self-energy matrix $\langle M_2^c(z) \rangle_b$. The behavior of $P(t)$ for times much larger than ω_c^{-1} is determined by the leading order term of $\hat{P}(z)$ for $|z\omega_c^{-1}| \ll 1$ and it suffices to examine the asymptotic

properties of $\langle M_2^c(z)\rangle_b$ or functions $g(z)$ and $f(z)$ as $z \to 0$. By virtue of the known features of the Struve and Bessel functions, one can show that, for $z \to 0$, $g(z) \sim z^{2\alpha}$ if $\alpha < 1/2$, and $g(z) \sim z$ for $\alpha > 1/2$ [cf. Eq. (5)]. At zero temperature, one finds that, for $\alpha < 1$, $f(z) = \Delta_{\mathrm{eff}}^{2(1-\alpha)} z^{2\alpha-1} + O[z(\Delta_0/\omega_c)^2]$, where

$$\Delta_{\mathrm{eff}} = [\cos(\alpha\pi)\Gamma(1-2\alpha)]^{1/2(1-\alpha)}(\Delta_0/\omega_c)^{\alpha/1-\alpha}\Delta_0$$

coincides precisely with the effective tunneling frequency defined in the spin-boson model [1]. If $\alpha > 1$, $f(z)$ is linear in z. In the opposite limit of *high* temperatures we find that $f(z) = -2i\Delta_0 g(z)/zq(\beta)$. Thus, for $\alpha < 1/2$ we obtain $f(z) = \bar{\Delta}_{\mathrm{eff}}^{2(1-\alpha)} z^{2\alpha-1} + O(\Delta_0^2/\omega_c)$, where

$$\bar{\Delta}_{\mathrm{eff}} = \left[\frac{\Gamma(1-\alpha)\Gamma(1/2-\alpha)}{\sqrt{\pi}}\right]^{1/2(1-\alpha)}$$
$$\times (\Delta_0/2\omega_c)^{\alpha/1-\alpha}\Delta_0$$

is the effective (high temperature) tunneling frequency. In contrast, for $\alpha > 1/2$, one finds $f(z) = \gamma + O(z^{2\alpha-1}\Delta_0^2/\omega_c^{2\alpha})$, where $\gamma = \sqrt{\pi}\,\Delta_0^2\Gamma(\frac{1}{2}+\alpha)/[\omega_c(2\alpha-1)\Gamma(\alpha)]$ is the corresponding decay rate. We should stress that these formulas are valid for the dissipation coefficient α being not close to $1/2$. Of course, a more accurate asymptotic analysis is possible for all values of α.

Results for the quantum coherence dynamics.—Let us focus on the *zero-temperature* behavior of the quantum coherence function $P(t)$. Comparing the three contributions to the self-energy [recall that $\hat{M}_{2,u}^c(z) \sim g^2(z)/z$] we find that $\hat{M}_{2,c}^c(z)$ dominantly rules the expression for the self-energy if $\alpha < 1$. Upon replacing $\langle M^c(z)\rangle_b$ simply by $\hat{M}_{2,c}^c(z)$ in the averaged Liouvillian propagator yields $\langle \hat{Q}(z)\rangle_b = [z - \hat{M}_{2,c}^c(z)\rangle_b]^{-1}$, we obtain $\hat{P}(z) = [z + f(z)]^{-1}$. This is exactly the result of the spin-boson model within the noninteracting blip approximation (NIBA), being a valid approximation in the case considered herein [1–3]. The prominent feature of $P(t)$ is a crossover from coherent (i.e., oscillatory) exponentially damped decay to pure incoherent decay at $\alpha = 1/2$; see Refs. [1,2] for details. When $\alpha > 1$, all of the leading terms of the three self-energy contributions are linear in z, as $z \to 0$. In this case, we obtain $\hat{P}(z) = z^{-1}[1 + O((\Delta_0/\omega_c)^2)]$. Put differently, for $\alpha > 1$, $P(t) = 1$, i.e., localization takes place [5]. Thus, these findings confirm that the spin-boson model and the spin-spin-bath model exhibit the same physics at *zero* temperature.

At high temperatures $\beta \to 0$, the correlation term $\hat{M}_{2,c}^c(z)$ always dominates the self-energy for small z, which leads to $\hat{P}(z) = [z + f(z)]^{-1}$. From the foregoing discussion about the property of $f(z)$, one thus expects similar behavior from $P(t)$. Note that $\hat{P}(z)$ has a branch point at $z = 0$. The complex z plane is cut along the negative real axis. By calculating the inverse Laplace transform it is clear that $P(t)$ contains two parts, $P_{\mathrm{coh}}(t)$

and $P_{\mathrm{inc}}(t)$, for $\alpha < 1/2$. The *coherent* contribution $P_{\mathrm{coh}}(t)$ emerges from the conjugate pair of simple poles z_0 and z_0^* in the principal sheet, and the *incoherent* contribution $P_{\mathrm{inc}}(t)$ results from the cut. Performing the required manipulations gives us $z_0 = \Gamma_0 + i\Omega_0$, where $\Gamma_0 = \bar{\Delta}_{\mathrm{eff}}\cos[(1-2\alpha)\pi/(2-2\alpha)]$ and $\Omega_0 = \bar{\Delta}_{\mathrm{eff}}\sin[(1-2\alpha)\pi/(2-2\alpha)]$. After some algebra we arrive at $P_{\mathrm{coh}}(t) = \cos(\Omega_0 t)\exp(-\Gamma_0 t)/(1-\alpha)$ and

$$P_{\mathrm{inc}}(t) = -\frac{\sin(2\alpha\pi)}{\pi}\int_0^\infty dx$$
$$\times \frac{x^{1-2\alpha}\exp(-xy)}{x^{2-2\alpha}[1 + 2\cos(2\alpha\pi) + 1]},$$

where $y = \bar{\Delta}_{\mathrm{eff}}t$. $P_{\mathrm{coh}}(t)$ exhibits damped oscillations while $P_{\mathrm{inc}}(t)$ obeys a power law. Therefore, if $\alpha < 1/2$, $P(t)$ manifests similar characteristics, both at zero and infinite temperatures. The only difference is a change of the effective tunneling frequency. By direct comparison we know that the ratio of the two effective tunneling frequencies $R(\alpha) = \bar{\Delta}_{\mathrm{eff}}/\Delta_{\mathrm{eff}}$ [$R(0) = 1$] is an increasing function of α: For instance, $R(0.1) = 1.05$. If α becomes larger than $1/2$, however, a qualitatively *different* behavior, is expected. In fact, we find that $P(t) = \exp(-\gamma t)$, where $\gamma = \sqrt{\pi}\,\Delta_0^2\Gamma(\frac{1}{2}+\alpha)/[\omega_c(2\alpha-1)\Gamma(\alpha)]$, i.e., an exponential decay. The decay rate γ decreases as α increases. It is interesting to note that, at $\alpha = 1$, the decay rate $\gamma = \pi\Delta_0^2/2\omega_c$ is identical to that of the spin-boson model for $\alpha = 1/2$ at zero temperature. The dynamics of $P(t)$ is subtle in a *critical* regime at about $\alpha = 1/2$ and defies (in clear contrast to the spin-boson case) an exact solution. The main feature is, of course, that a crossover from coherent relaxation to exponential decay occurs [25].

At finite temperatures, we find $\hat{P}(z) = [z + f(z)]^{-1}$, where

$$f(z) = z\Delta_0^2\mathcal{L}\left\{\int_0^t du\frac{e^{i[B(u)-B(t)+B(t-u)]}}{(1+\omega_c^2 u^2)^\alpha}\right\} + \mathrm{c.c.}$$

Here the phase $B(t)$ is proportional to the dissipation coefficient and to some degree its value reflects quantum dissipation. Since $B(t)$ is a monotonic increasing function of β, decoherence is partially *suppressed* by increasing temperature. Therefore, temperature plays, though weakly, a positive role in maintaining coherent dynamics. This means that *the spin-spin-bath model prefers coherent dynamics in the whole range of temperatures if the dissipation coefficient α is sufficiently small*, i.e., $\alpha < 1/2$. To get an idea of the temperature dependence, we turn to the expression of the phase $B(t)$ [Eq. (6)]. Taking the first term ($n = 0$) in the series on the rhs leads to $B(s) = 2\alpha\{\tan^{-1}(\omega_c s) - \tan^{-1}[\omega_c s/(1 + \omega_c\beta\hbar)]\}$. When the temperature is sufficiently low, say, $\beta \gg t/\hbar$, to first order in $1/\beta$, $f(z)$ does not depend on β for $\omega_c t \gg 1$. A similar behavior is also observed for very high temperatures. Therefore, temperature only weakly affects the dynamics at low and high temperatures. We suspect that this is also true at any finite temperatures.

In *summary*, we have investigated the properties of the quantum coherence dynamics in a two-level system that are coupled to a sea of thermally prepared spin-1/2 particles. Using the resolvent operator method we have shown that the spin-spin-bath model exhibits at *nonzero* temperatures a distinctly *different* physics as compared to spin-boson model. At zero temperature, however, the dissipative dynamics of the two models is identical. In particular, we could assess that for the spin-spin-bath the decoherence measure $P(t)$ is effectively temperature independent at low and high temperatures. For weak couplings ($\alpha < 1/2$), quantum coherence, i.e., the oscillatory decay of coherence, sustains up to infinite temperature. For strong couplings ($\alpha > 1/2$), however, the system obeys an exponential decay law at high temperatures, and its decay rate becomes smaller as the coupling parameter α becomes larger. The most interesting effect is that temperature helps the system suppress decoherence. The difference between the finite temperature behavior of this spin-spin-bath model and the spin-boson model (or, equivalently, also the spin-Fermion-bath model with its infinitely many excitation energies [3,26]) can be traced back to the severe restriction of the thermal induced excitation possibilities of the bath degrees of freedom (only a single level in each individual two-level system composing the spin bath); i.e., the mechanism of thermal excitation of many levels of a single bath degree of freedom that characterizes the crossover behavior from quantum coherent to quantum incoherent tunneling at weak coupling $\alpha < 1/2$ in the spin-boson model is simply not at work in this spin-spin-bath case. Clearly, our findings may have an impact on studies involving the decoherence properties in nanomagnets and, as well, the (spin) decoherence-limited efficiency of interacting qubits in realistic quantum computing schemes. In particular, the result that temperature favors the coherent dynamics is *good news* for the quantum computing efforts.

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