Decoherence by a spin thermal bath: Role of the spin-spin interactions

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(Dated: March 3, 2010)

We study the decoherence of two coupled spins that interact with a spin-bath environment. It is shown that the connectivity and the coupling strength between the spins in the environment are of crucial importance for the decoherence of the central system. Changing the connectivity or coupling strengths changes the decoherence of the central system from Gaussian to exponential decay law.

PACS numbers: 03.67.Mn 05.45.Pq 75.10.Nr

It is commonly accepted that decoherence by nuclear spins is the main obstacle for realization of quantum computations in magnetic systems; see, e.g., discussions of specific silicon [1] and carbon [2] based quantum processors. Therefore, understanding the decoherence in quantum spin systems is a subject of numerous works (for reviews, see Refs [3, 4]). The issue seems to be very complicated and despite many efforts, even some basic questions about character of the decoherence process are unsolved yet. Due to the interactions with and between the spin of the bath, an analytical treatment can be carried out in very exceptional cases, even if the central systems contains one spin only. Recent work suggests that the internal dynamics of the environment can be crucial to the decoherence of the central system [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. In this Letter, we present results of extensive simulation work of a two-spin system interacting with a spin-bath environment and show that the decoherence of the two-spin system can exhibit different behavior, depending on the characteristics of the coupling with the environment and of the internal dynamics of the latter. We also provide a simple physical picture to understand this behavior.

In general, the behavior of an open quantum system crucially depends on the ratio of typical energy differences of the central system and the energy of the environment. The case \( \delta E_c \ll E_{ce} \) has been studied extensively in relation to the "Schrödinger cat" problem and the physics is quite clear [18, 19]: As a result of time evolution, the central system passes to one of the "pointer states" [19] which, in this case, are the eigenstates of the interaction Hamiltonian \( H_{ce} \). The opposite case, \( \delta E_c \gg E_{ce} \) is less well understood. There is a conjecture that in this case the pointer states should be eigenstates of the Hamiltonian \( H_c \) of the central system but this has been proven for a very simple model only [20]. On the other hand, this case is of primary interest if, say, the central system consists of electron spins whereas the environment are nuclear spins, for instance if one considers the possibility of quantum computation using molecular magnets [21, 22].

We consider a generic quantum spin model described by the Hamiltonian \( H = H_c + H_{ce} + H_e \) where \( H_c = -JS_1 \cdot S_2 \) is the Hamiltonian of the central system and the Hamiltonians of the environment and the interaction of the central system with the environment are given by

\[
H_c = -\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \sum_{\alpha} \Omega_{ij}^{(\alpha)} I_{i\alpha}^x I_{j\alpha}^x,
\]

\[
H_{ce} = -2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \sum_{\alpha} \Delta_{ij}^{(\alpha)} S_i^y \Delta_{ij}^{(\alpha)} S_j^y,
\]

respectively. The exchange integrals \( J \) and \( \Omega_{ij}^{(\alpha)} \) determine the strength of the interaction between spins \( S_i = (S_{ix}, S_{iy}, S_{iz}) \) of the central system, and the spins \( I_n = (I_{nx}, I_{ny}, I_{nz}) \) in the environment, respectively. The exchange integrals \( \Delta_{ij}^{(\alpha)} \) control the interaction of the central system with its environment. In Eq. (1), the sum over \( \alpha \) runs over the \( x, y \) and \( z \) components of spin-1/2 operators \( S \) and \( I \). In the sequel, we will use the term "Heisenberg-like" \( H_c \) (\( H_{ce} \)) to indicate that each \( \Omega_{ij}^{(\alpha)} \) (\( \Delta_{ij}^{(\alpha)} \)) is a uniform random number in the range \([-\Omega], \Omega \) (\([-\Delta], \Delta \)), \( \Omega \) and \( \Delta \) being free parameters. In earlier work [16, 17], we found that a Heisenberg-like \( H_c \) can induce close to perfect decoherence of the central system and therefore, we will focus on this case only.

The bath is further characterized by the number of environment spins \( K \) with which a spin in the environment interacts. If \( K = 0 \), each spin in the environment interacts with the central system only. \( K = 2, K = 4 \) or \( K = 6 \) correspond to environments in which the spins are placed on a ring, square or triangular lattice, respectively and interact with nearest-neighbors only. If \( K = N - 1 \), each spin in the environment interacts with all the other spins in the environment and, to give this case a name, we will refer to this case as "spin glass".

If the Hamiltonian of the central system \( H_c \) is a perturbation relative to the interaction Hamiltonian \( H_{ce} \), the pointer states are eigenstates of \( H_{ce} \) [19]. In the opposite case, that is the regime \( |\Delta| \ll |J| \) that we explore in this Letter, the pointer states are conjectured to be eigenstates of \( H_c \) [20]. The latter are given...
by $|1\rangle \equiv |T_1\rangle = |1\rangle$, $|2\rangle \equiv |S\rangle = (|1\rangle - |1\rangle)/\sqrt{2}$, $|3\rangle \equiv |T_0\rangle = (|1\rangle + |1\rangle)/\sqrt{2}$, and $|4\rangle \equiv |T_{-1}\rangle = |1\rangle$, satisfying $H_e|S\rangle = (3J/4)|S\rangle$ and $H_e|T_i\rangle = (-J/4)|T_i\rangle$ for $i = -1, 0, 1$.

The simulation procedure is as follows. We generate a random superposition $|\phi\rangle$ of all the basis states of the environment. This state corresponds to the equilibrium density matrix of the environment at infinite temperature. The spin-up – spin-down state $|\{\uparrow\downarrow\}\rangle$ is taken as the initial state of the central system. Thus, the initial state of the whole system reads $|\Psi(t = 0)\rangle = |\{\uparrow\downarrow\}\rangle |\phi\rangle$ and is a product state of the state of the central system and the random state of the environment which, in general is a (very complicated) linear combination of the $2^N$ basis states of the environment. In our simulations we take $N = 16$ which, from earlier work [16, 17], is sufficiently large for the environment to behave as a “large” system.

For a given, fixed set of model parameters, the time evolution of the whole system is obtained by solving the time-dependent Schrödinger equation for the many-body wave function $|\Psi(t)\rangle$, describing the central system plus the environment [23]. It conserves the energy of the whole system to machine precision. We monitor the effects of the decoherence by computing the the matrix elements of the reduced density matrix of the central system. Hence we compute the matrix elements of the density matrix in the basis of eigenvectors of the central system. We also compute the time dependence of quadratic entropy $S_c(t) = 1 - Tr \rho^2(t)$ and the Loschmidt echo $L(t) = Tr(\rho(t) \rho_0(t))$ [24], where $\rho_0(t)$ is the density matrix for $H_{ee} = 0$.

In Fig. 1 and Fig. 2, we show the time evolution of the elements of the reduced density matrix $\rho(t)$ for different connectivity $K$ and $\Omega$, for the case that $H_{ee}$ is an isotropic Heisenberg model.

If $|\Delta| \gg K\Omega$, in agreement with earlier work [25, 26], we find that in the absence of interactions between the environment spins ($K\Omega = 0$) and after the initial decay, the central system exhibits long-time oscillations (see Fig. 1(a)(left)). In this case and in the limit of a large environment, we have [26]

$$\text{Re } \rho_{23}(t) = \left[\frac{1}{6} + \frac{1}{3} \frac{b t^2}{(c + b t^2)} \right] \cos \omega t,$$

where $b = N\Delta^2/4$, $c = b/2$ and $\omega = J - \Delta$. Equation (2) clearly shows the two-step process, that is, after the initial Gaussian decay of the amplitude of the oscillations, the oscillations revive and their amplitude levels of [26].

Due to conservation laws, this behavior does not change if the environment consists of an isotropic Heisenberg system ($\Omega_{i,j}^{(a)} \equiv \Omega$ for all $a$, $i$ and $j$), independent of $K$. If, as in Ref. [25], we take $\Delta_{i,j}^{(x)} = \Delta_{i,j}^{(y)} = \Delta_{i,j}^{(z)} \in [0, \Delta]$ random instead of the identical, the amplitude of the long-living oscillations is no longer constant but decays very slowly [25].

If $|\Delta| \approx K\Omega$, the presence of Heisenberg-like interactions between the spins of the environment has little effect on the initial Gaussian decay of the central system, but it leads to a reduction and to a decay of the amplitude of the long-living oscillations. The larger $K$ (see Fig. 1(b-e)(left)) or $\Omega$ (see Fig. 2(a,c)), the faster the decay is. Note that for the sake of clarity, we have suppressed the fast oscillations by plotting instead of the real part, the absolute value of the matrix elements.

If $|\Delta| \ll K\Omega$, keeping $K$ fixed and increasing $\Omega$ smoothly changes the initial decay from Gaussian (fast) to exponential (slow), and the long-living oscillations are completely suppressed (see Fig. 2(b,d)). For large $\Omega$, the
FIG. 2: (Color online) The time evolution of the off-diagonal element \(\rho_{23}\) of the reduced density matrix of a central system (with \(J = -5\)), interacting with a Heisenberg-like environment \(H_c\) via an isotropic Heisenberg Hamiltonian \(H_{ce}\) (with \(A = -0.075\)) for the same geometric structures in the environment: (a,b) \(K = 2\) and (c,d) \(K = N - 1\). The number next to each curve is the corresponding value of \(\Omega\).

FIG. 3: (Color online) Same as Fig. 2 except that \(H_{ce}\) is Heisenberg-like and \(A = 0.15\).

Simulation data fits very well to

\[ |\rho_{23}(t)| = \frac{1}{2} e^{-A_K(\Omega)t}, \]

with \(A_K(\Omega) \approx \Omega \tilde{A}_K\), \(\tilde{A}_2 = 9.13\) and \(\tilde{A}_{N-1} = 26.73\).

Physically, the observed behavior can be understood as follows. If \(|\Delta| \approx K\Omega\), a bath spin is affected by roughly the same amount by the motion of both the other bath spins and by the two central spins. Therefore, each bath spin has enough freedom to follow the original dynamics, much as if there were no coupling between bath spins. This explains why the initial Gaussian decay is insensitive to the values of \(K\) or \(\Omega\). After the initial decay, the whole system is expected to reach a stationary state, but because of the presence of Heisenberg-like interactions between the bath spins, a new stationary state of the bath is established, suppressing the long-living oscillations.

For increasing \(K\), the distance between two bath spins, defined as the minimum number of bonds connecting the two spins, becomes smaller. For instance, for \(K = 2\), this distance is \((N - 2)/2\), and for \(K = N - 1\), it is zero. Therefore, for fixed \(\Omega\) and increasing \(K\) the fluctuations in the spin bath can propagate faster and the evolution to the stationary state will be faster. Similarly, for fixed \(K\), increasing the coupling strength between the bath spins will speed up the dynamics of the bath, that is, the larger \(\Omega\) the faster will be the evolution to the stationary state.

In the opposite case \(|\Delta| \ll K\Omega\), \(H_{ce}\) is a small perturbation relative to \(H_e\) and the coupling between bath spins is the dominant factor in determining the dynamics of the bath spins. Therefore, by increasing \(K\) or \(\Omega\), the bath spin will have less freedom to follow the dynamics induced by the coupling to the two central spins, the influence of the bath on the central system will decrease, and the (exponential) decay will become slower.

According to the general picture of decoherence [19], for an environment with nontrivial internal dynamics that initially is in a random superposition of all its eigenstates, we expect that the central system will evolve to a stable mixture of its eigenstates. In other words, the decoherence will cause all the off-diagonal elements of the reduced density matrix to vanish with time. In the case of an isotropic Heisenberg coupling between the central system and the environment, \(H_e\) commutes with the Hamiltonian \(H\), hence the energy of the central system is a conserved quantity. Therefore, the weight of the singlet \(|S\rangle\) in the mixed state should be a constant \((1/2)\), and the weights of the degenerate eigenstates \(|T_0\rangle\), \(|T_{-1}\rangle\) and \(|T_1\rangle\) are expected to become the same \((1/6)\). As shown in Fig. 1(b-e)(right), our simulations confirm that this picture is correct in all respects.

It is important to note that although in the foregoing discussion we have compared \(K\Omega\) to \(|\Delta|\), this does not imply that \(K\Omega\) can be used to fully characterize the decoherence process. In order to clarify the role of \(K\) and \(\Omega\), we change the coupling between the central system and the bath from Heisenberg to Heisenberg-like. From a comparison of the data in Fig. 2 and Fig. 3, it is clear that the roles of \(K\) and \(\Omega\) are the same in both cases, no matter whether the central-bath coupling is isotropic or anisotropic. However, there are some differences in the decoherence process.

If \(|\Delta| \gg K\Omega\), in the presence of anisotropic interactions between the central system and the environment spins, even in the absence of interactions between the bath spins, the second step of the oscillations decays and finally disappear as \(K\) increases. This is because the anisotropic interactions break the rotational symmetry of the coupling between central system and environment.
which is required for the long-living oscillations to persist.

If $|\Delta| \ll K\Omega$, $|\rho_{23}(t)|$ can still be described by Eq. (3), but now $A_K(\Omega)$ is no longer a linear function of $\Omega$. For an anisotropic $H_{ce}$, the energy of the central system is no longer a conserved quantity. Therefore there will be energy transfer between the central system and the environment and the weight of each pointer state (eigenstate) in the final stable mixture need not be the same for all $K$ or $\Omega$.

For a change, we illustrate this point by considering the quadratic entropy $S_c(t)$ and Loschmidt echo $L(t)$ of a central system (with $J = -5$), interacting with a Heisenberg-like environment $H_e$ (with different $\Omega$) via a Heisenberg $\langle a,b, \Delta = -0.075 \rangle$ or Heisenberg-like $\langle c,d, \Delta = 0.15 \rangle$ Hamiltonian $H_{ce}$ for the case $K = 2$. The number next to each curve is the corresponding value of $\Omega$.

In conclusion, we have shown how a pure quantum state of the central spin system evolves into a mixed state, and that if the interaction between the central system and environment is much smaller than the coupling between the spins in the central system, the pointer states are the eigenstates of the central system. Both these observations are in concert with the general picture of decoherence [19]. Furthermore, we have demonstrated that, in the case that the environment is a spin system, the details of this spin system are important for the decoherence of the central system. In particular, we have shown that changing the internal dynamics of the environment (geometric structure or exchange couplings) may change the decoherence of the central spin system from Gaussian to exponential decay.

Acknowledgement

M.I.K. acknowledges a support by the Stichting Fundamenteel Onderzoek der Materie (FOM).