Relaxation and decoherence in quantum spin system
Yuan, Shengjun

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Chapter 5

Importance of Bath Dynamics for Decoherence in Spin Systems

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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 computers. Therefore, understanding the decoherence in quantum spin systems is a subject of numerous works (for review, 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. Most of the problems cannot be solved analytically, in particular if there is more than one spin in the central system, but we can use the computer to simulate the dynamics and find useful information.
An unusual two-step decoherence was reported in Ref. [5]. This is an important phenomenon since it implies that, generally speaking, the observation of the Rabi oscillations does not guarantee access to sectors of the Hilbert space that may be essential for efficient quantum computation. Its origin is still poorly understood; it was described analytically in a framework of an exactly solvable model of noninteracting spins in the bath [6] but it is not clear how sensitive it is to the details of spin-spin interactions. In the real world, the environment has its own dynamics, which could be much slower or comparable to the central dynamics. First attempts to investigate numerically the effects of the environment dynamics [7] did not lead to definite conclusions.

The behavior of an open quantum system crucially depends on the ratio of typical energy differences of the central system $\delta E_c$ and the energy $E_{ce}$ which characterizes the interaction of the central system with 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 [8, 9]: As a result of time evolution, the central system passes to one of the “pointer states” [9] which, in this case, are the eigenstates of the interaction Hamiltonian. 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 of the central system, but this is proven only for a very simple model [10]. 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 (e.g., if one considers the possibility of quantum computation using molecular magnets [11, 12]).

In fact, as we will show, the selection of an eigenstate as the pointer state is also determined by the state and the dynamics of the environment. Elsewhere [13, 14], we have already shown that if the environment is a spin glass and initially in the ground state, then independent of the initial state of the central system, the central system relaxes to a state that is very close to its ground state: The ground state is selected as the point state of the central system. In this chapter, we consider a realistic model of decoherence of a system of two spins by an environment of nuclear spins at elevated temperatures. We will demonstrate that the decoherence of the central system depends in a significant, nonintuitive manner on the details of the dynamics of the environment.
5.1 Model

We consider a generic quantum spin model described by the Hamiltonian $H = H_c + H_{ce} + H_e$ where

\begin{align*}
H_c &= -J S_1 \cdot S_2, \\
H_e &= -\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \sum_{\alpha} \Omega^{(\alpha)}_{i,j} I_{i}^{\alpha} I_{j}^{\alpha}, \\
\text{and} \\
H_{ce} &= -2 \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{\alpha} \Delta^{(\alpha)}_{i,j} S_{i}^{\alpha} I_{j}^{\alpha}, \quad (5.1)
\end{align*}

are the Hamiltonians of the central system, the environment, and the interaction of the central system and the environment, respectively. In Eq.(5.1), the exchange integrals $J$ and $\Omega^{(\alpha)}_{i,j}$ determine the strength of the interaction between spins $S_n = (S_n^x, S_n^y, S_n^z)$ of the central system $H_c$, and the spins $I_n = (I_n^x, I_n^y, I_n^z)$ in the environment $H_e$, respectively. The exchange integrals $\Delta^{(\alpha)}_{i,j}$ control the interaction $H_{ce}$ of the central system with its environment. In Eq.(5.1), 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” $H_e$ to indicate that each $\Omega^{(\alpha)}_{i,j}$ is a uniform random number in the range $[-\Omega|J|, \Omega|J|]$, $\Omega$ being a free parameter. We will consider two different kinds of $H_{ce}$, namely rotational invariant Heisenberg interactions $\Delta^{(\alpha)}_{i,j} \equiv \Delta$ and “Ising-like” interactions for which $\Delta^{(x)}_{i,j} = \Delta^{(y)}_{i,j} = 0$ and $\Delta^{(z)}_{i,j}$ are dichotomic random variables, taking the values $\pm \Delta$. Obviously, if $H_{ce}$ is “Ising like”, the total magnetization of the central system ($M = S_1^z + S_2^z$) is a conserved quantity.

As we demonstrate in this chapter, the connectivity of the spins in the environment affects the decoherence in a nontrivial manner. We characterize this connectivity by the number $K$, the number of environment spins with which a spin in the environment interacts. If $K = 0$, each spin in the environment interacts with the central system only. If $K = 2$, the structure of the environment is assumed to be that of a ring, that is each spin in the environment interacts with two other spins only. Likewise, $K = 4$ and $K = 6$ correspond environments in which the spins are placed on a 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 $H_{ce}$ [9]. In the opposite case, that is the regime $|\Delta| \ll |J|$ that we explore in this chapter, the pointer states are supposed to be eigenstates of $H_c$ [10]. The latter are given by $|1\rangle \equiv |T_1\rangle = |\uparrow\uparrow\rangle$, $|2\rangle \equiv |S\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$, $|3\rangle \equiv |T_0\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$, and $|4\rangle \equiv |T_{-1}\rangle = |\downarrow\downarrow\rangle$, satisfying $H_c|S\rangle = (3J/4)|S\rangle$ and $H_c|T_i\rangle = (-J/4)|T_i\rangle$ for $i = -1, 0, 1$. To check this conjecture is one of the main aims of our simulations.

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 [13, 14], we know 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. The numerical method that we use is described in Ref. [15]. It conserves the energy of the whole system to machine precision. We monitor the effects of the decoherence by plotting the time dependence of the matrix elements of the reduced density matrix of the central system. As explained earlier, in the regime of interest $|\Delta| \ll |J|$, the pointer states are the eigenstates of the central systems, hence we compute the matrix elements of the density matrix in the basis of eigenvectors of the central system.

### 5.2 Isotropic Heisenberg Coupling

In Fig. 5.1, we show the time evolution of the elements of the reduced density matrix of the central system for different connectivity numbers $K$ and Heisenberg or Heisenberg-like interactions between central system and the spins in the environment. We conclude that:
5.2. Isotropic Heisenberg Coupling

Figure 5.1: (Color online) The time evolution of the real part of the off-diagonal element \( \rho_{23} \) (right panel) and the diagonal elements \( \rho_{11}, \ldots, \rho_{44} \) (left panel) of the reduced density matrix of a central system (with \( J = -5 \)), interacting with a Heisenberg-like environment \( H_e \) (with \( \Omega = 0.15 \)) via an isotropic Heisenberg Hamiltonian \( H_{ce} \) (with \( \Delta = -0.075 \)) for different connectivity numbers \( K \) of the spins in the environment: (a) \( K = 0 \); (b) \( K = 2 \); (c) \( K = 4 \); (d) \( K = 6 \); (e) \( K = N - 1 \).

1. In agreement with earlier work [5, 6], we find that in the absence of interactions between the environment spins (\( K = 0 \)) and after the initial fast decay, the central system exhibits long-time oscillations (see Fig. 5.1(a)(left)). In this case and in the limit of a large environment,
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we have [6]

\[ \text{Re} \rho_{23}(t) = \left[ \frac{1}{6} + \frac{(1 - b t^2) e^{-c t^2}}{3} \right] \cos \omega t, \quad (5.2) \]

where \( b = N \Delta^2 / 4, \ c = b/2 \) and \( \omega = J - \Delta \). Equation (5.2) 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 [6]. Notice that because of conservation laws, this behavior does not change if the environment is described by an isotropic Heisenberg Hamiltonian (\( \Omega^{(\alpha)}_{i,j} \equiv \Omega \) for all \( \alpha, i \) and \( j \)), whatever the value of \( K \). If, as in Ref. [5], we take \( \Delta^{(x)}_{i,j} = \Delta^{(y)}_{i,j} = \Delta^{(z)}_{i,j} \in [0, \Delta] \) random instead of the same, the amplitude of the long-living oscillations is no longer constant but decays very slowly [5].

2. The presence of Heisenberg-like (non-isotropic, random) interactions between the spins of the environment leads to a reduction and a decay of the amplitude of the long-living oscillations (see Fig. 5.1(b-e)(left)). The larger the connectivity number \( K \), the faster is the decay of the amplitude. When \( K \) reaches its maximum \( K = N - 1 \) (spin glass), the second step in the decoherence process is no longer separated from the initial decay. In fact, it seems as if it has merged with the final stage of the first step (see Fig. 5.1(e)(left)). For \( K = N - 1 \), the time evolution of \( \rho_{23}(t) \) can be fitted well by the function

\[ \text{Re} \rho_{23}(t) = \left[ e^{-a' t} / 6 + \frac{(1 - b' t^2) e^{-c' t^2}}{3} \right] \cos \omega' t, \quad (5.3) \]

with \( a' = 0.13403, \ b' = 0.00659, \ c' = 0.01085 \) and \( \omega' = 5.01037 \). For comparison, the values that enter Eq.(5.2) are \( b = 0.0225, \ c = 0.01125 \) and \( \omega = 4.925 \). It is of interest to note that if the dynamics of the environment is sufficiently slow (\( \Omega \approx 0.01 \) in Ref. [5]), this dynamics apparently does not affect the decoherence of the central spins [5]. Thus, the effectiveness of the decoherence process not only depends on \( K \) but also on the details of the interactions within the environment.

3. According to the general picture of decoherence [9], 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
5.2. Isotropic Heisenberg Coupling

![Figure 5.2](image.png)

**Figure 5.2:** (Color online) The time evolution of the real part of the off-diagonal element $\rho_{23}$ of the reduced density matrix of a central system (with $J = -1$), interacting with a Heisenberg-like environment $H_e$ (with $\Omega = 0.15$) via an Ising-like Hamiltonian $H_{ee}$ (with $\Delta = 0.075$) for different connectivity numbers $K$ of the spins in the environment: (a) $K = 0$; (b) $K = 2$; (c) $K = 4$; (d) $K = 6$; (e) $K = N - 1$.

will cause all the off-diagonal elements of the reduced density matrix to vanish with time. Moreover, the weight of the degenerate eigenstates $|T_0\rangle$, $|T_{-1}\rangle$, and $|T_1\rangle$ in this mixed state are expected to be the same. As shown in Fig. 5.1(b-e)(right), our simulations confirm that this picture is correct in all respects. Furthermore, the results depicted in Fig. 5.1(b-e)(right) demonstrate that the connectivity number $K$ has no effect on the value of $\rho_{11}$, $\rho_{22}$, $\rho_{33}$ and $\rho_{44}$ for long times.
Table 5.1: Frequency of oscillation $\omega''$ and decoherence time $\tau''$ for different connectivity $K$. In case 1 and case 2, for each $K$, the values of $\Omega_{i,j}^{(a)}$ are the same but the values of $\Delta_{i,j}^{(a)}$ are different. In case 2 and case 3, for each $K$, the values of $\Delta_{i,j}^{(a)}$ are the same but the values of $\Omega_{i,j}^{(a)}$ are different.

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<th>$K = 6$</th>
<th>$K = N - 1$</th>
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<tr>
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<td>110.0</td>
<td>111.7</td>
</tr>
</tbody>
</table>

5.3 Anisotropic Ising-like Coupling

Next, we change the interactions between central system and the spins in the environment from Heisenberg-like to Ising-like but keep the interactions between different spins in the environment Heisenberg-like. In fact, in our simulations, the Hamiltonian $H_e$ is the same for both cases. As explained earlier, in the Ising-like case, the total magnetization of the central system is conserved during the time evolution. Thus, as the initial state of the central system is $(|S\rangle + |T_0\rangle)/\sqrt{2}$, at any time $t$ the state of the whole system can be written as

$$|\Psi(t)\rangle = |2\rangle|\phi_2(t)\rangle + |3\rangle|\phi_3(t)\rangle,$$

(5.4)

where $|\phi_2(t)\rangle$ and $|\phi_3(t)\rangle$ denote the states of the environment. In other words, only $\rho_{22}(t)$, $\rho_{23}(t)$, $\rho_{32}(t)$, and $\rho_{33}(t)$ can be nonzero.

On general grounds, we may expect that the presence of an additional conservation law slows down the decoherence and indeed, as shown in Fig. 5.2, this is the case. Note that the results of Fig. 5.2 have been obtained for $J = -1$ instead of for $J = -5$, the value used to compute the results shown in Fig. 5.1 (the latter value was chosen to facilitate the comparison with the results of Ref. [5]), but this factor of five in the value of $J$ cannot account for the large difference in the observed decoherence times.

From Fig. 5.2, we conclude that
1. We never observe the two-step process that we find in the case of Heisenberg-like $H_{ce}$. For $K = 0$ (Fig. 5.2(a), there is no decoherence.

2. For $K > 0$, $\text{Re } \rho_{23}(t)$ vanishes with time, in agreement with the general picture of decoherence [9]. However, quite unexpectedly, the rate of decoherence increases with $K$, in contrast to the case of Heisenberg-like $H_{ce}$ in which the rate of decoherence decreases with $K$. The data presented in Figs. 5.2(b-d) can all be fitted very well by

$$\text{Re } \rho_{23}(t) = \frac{1}{2} e^{-t/\tau''} \cos \omega'' t,$$

where $\omega'' \approx |J|$ and the values of $\tau''$ depend on $K$. In Table 5.1, we give some typical results for these parameters. Cases 1 and 2 illustrate that (random) changes in $H_{ce}$ may affect the value of the decoherence time $\tau''$ significantly but the general trend, the increase of $\tau''$ with $K$ seems generic.

### 5.4 Summary

In conclusion, we have shown that (1) the pure quantum state of the central spin system evolves into the classical, mixed state, and (2) 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 [9].

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 (1) changing the internal dynamics of the environment may change the qualitative features of the decoherence of the central spin system, and that (2) the dependence of the decoherence time of the central spin system on the connectivity of the interactions between spins of the environment is counterintuitive.

### References


