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Giant enhancement of quantum decoherence by frustrated environments

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This Letter studies the decoherence in a system of two antiferromagnetically coupled spins that interact with a spin bath environment. Systems are considered that range from the rotationally invariant to highly anisotropic spin models, have different topologies and values of parameters that are fixed or are allowed to fluctuate randomly. We explore the conditions under which the two-spin system clearly shows an evolution from the initial spin-up – spin-down state towards the maximally entangled singlet state. We demonstrate that frustration and, especially, glassiness of the spin environment strongly enhances the decoherence of the two-spin system.

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The interaction between a quantum system, called central system in what follows, and its environment affects the state of the former. Intuitively, we expect that by turning on the interaction with the environment, the fluctuations in the environment will lead to a reduction of the coherence in the central system. This process is called decoherence [1, 2]. In general, there are two different mechanisms that contribute to decoherence. If the environment is dissipative (or coupled to a dissipative system), the total energy is not conserved and the central system + environment relax to a stationary equilibrium state, for instance the thermal equilibrium state. In this paper, we exclude this class of dissipative processes and restrict ourselves to closed quantum systems in which a small, central system is brought in contact with a larger quantum system that is prepared in its ground state. Then, decoherence is solely due to fact that the initial product state (wave function of the central system times wave function of the environment) evolves into an entangled state of the whole system. The interaction with the environment causes the initial pure state of the central system to evolve into a mixed state, described by a reduced density matrix [3], obtained by tracing out all the degrees of freedom of the environment [1, 2, 4, 5].

Not all initial states are equally sensitive to decoherence. The class of states that is "robust" with respect to the interaction with the environment are called pointer states [2]. If the Hamiltonian of the central system is a perturbation, relative to the interaction Hamiltonian $H_{\rm int}$, the pointer states are eigenstates of $H_{\rm int}$ [2, 6]. In this case, the pointer states are essentially "classical states", such as states with definite particle positions or with definite spin directions of individual particles for magnetic systems. In general, these states, being a product of states of individual particles forming the system, are not entangled. On the other hand, decoherence does not necessarily imply that the central system evolves to a classical-like state. If $H_{\rm int}$ is much smaller than the typical energy differences in the central system, the pointer states are eigenstates of the latter, that is, they may be "quantum" states such as standing waves, stationary electron states in atoms, tunnelling-split states for a particle distributed between several potential wells, singlet or triplet states for magnetic systems, etc. [6]. This may explain, for example, that one can observe linear atomic spectra – the initial states of an atom under the equilibrium conditions are eigenstates of its Hamiltonian and not arbitrary superpositions thereof.

Let us now consider a central system for which the ground state is a maximally entangled state, such as a singlet. In the absence of dissipation and for an environment that is in the ground state before we bring it in contact with this central system, the loss of phase coherence induces one of following qualitatively different types of behavior.

1. The interaction/bath dynamics is such that there is very little relaxation.

2. The system as a whole relaxes to some state (which may or may not be close to the ground state) and

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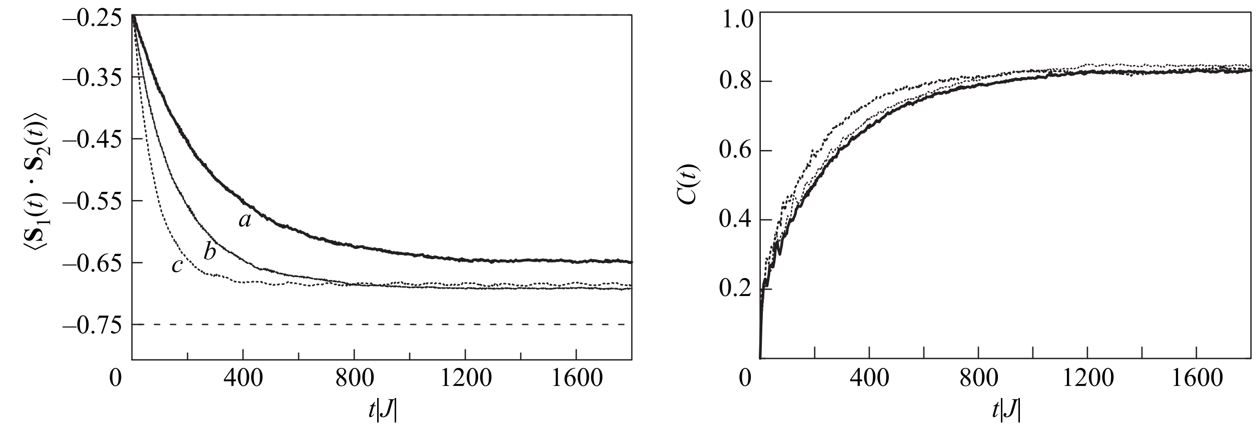

Fig.1 (color online). Left: Time evolution of the correlation $\langle\Psi(t)|\mathbf{S}_1\cdot\mathbf{S}_2|\Psi(t)\rangle$ of the two spins in the central system. Dashed horizontal line at $-1/4$: Correlation in the initial state ($\langle\Psi(t=0)|\mathbf{S}_1\cdot\mathbf{S}_2|\Psi(t=0)\rangle=-1/4$); Horizontal line at $-3/4$: Expectation value in the singlet state; (*a*) Environment containing $N=14$ quantum spins; (*b*) $N=16$; (*c*) $N=18$. The parameters $\Omega_{i,j}^{(\alpha)}$ and $\Delta_{i,j}^{(\alpha)}$ are uniform random numbers in the range $[-0.15|J|,0.15|J|]$. Right: Time evolution of the concurrence $C(t)$ for three different random realizations of a spin glass environment. The parameters are uniform random numbers in the range $-0.15|J|\le\Omega_{i,j}^{(\alpha)},\Delta_{i,j}^{(\alpha)}\le 0.15|J|$ and the environment contains $N=14$ quantum spins. The transition from an unentangled state ($C(t)=0$) to a nearly fully entangled state ($C(t)=1$) is clearly seen

this state is a complicated superposition of the states of the central system and the environment.

3. The system as a whole relaxes to a state that is (to good approximation) a direct product of the states of the central system and a superposition of states of the environment. In this case there are two possibilities:

   (a) The central system does not relax to its ground state;

   (b) The central system relaxes to its maximally entangled ground state.

Only case 3b is special: The environment and central system are not entangled (to a good approximation) but nevertheless the decoherence induces a very strong entanglement in the central system. In this paper, we demonstrate that, under suitable conditions, dissipation free decoherence forces the central system to relax to a maximally entangled state which itself, shows very little entanglement with the state of the environment.

Most theoretical investigations of decoherence have been carried out for oscillator models of the environment for which powerful path-integral techniques can be used to treat the environment analytically [4, 5]. On the other hand, it has been pointed out that a magnetic environment, described by quantum spins, is essentially different from the oscillator model in many aspects [7]. For the simplest model of a single spin in an external magnetic field, some analytical results are known [7]. For the generic case of two and more spins, numerical simulation [8, 9] is the main source of theoretical information. Not much is known now about which physical properties of the environment are important for the efficient selection of pointer states. Recent numerical simulations [9] confirm the hypothesis [10] on the relevance of the chaoticity of the environment but its effect is actually not drastic.

In this paper, we report on the results of numerical simulations of quantum spin systems, demonstrating the crucial role of frustrations in the environment on decoherence. In particular, we show that, under appropriate conditions, decoherence can cause an initially classical state of the central system to evolve into the most extreme, maximally entangled state. We emphasize that we only consider systems in which the total energy is conserved such that the decoherence is not due to dissipation.

We study a model in which two antiferromagnetically coupled spins, called the central system, interact with an environment of spins. The model is defined by

$$
\begin{gathered}
H = H_c + H_e + H_{int} \quad , \quad H_c = -J\mathbf{S}_1\cdot\mathbf{S}_2, \\
H_e = -\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\sum_{\alpha}\Omega_{i,j}^{(\alpha)} I_i^{\alpha} I_j^{\alpha}, \\
H_{int} = -\sum_{i=1}^{2}\sum_{j=1}^{N}\sum_{\alpha}\Delta_{i,j}^{(\alpha)} S_i^{\alpha} I_j^{\alpha},
\end{gathered}
\tag{1}
$$

where the exchange integrals $J<0$ and $\Omega_{i,j}^{(\alpha)}$ determine the strength of the interaction between spins $\mathbf{S}_n=(S_n^x,S_n^y,S_n^z)$ in the central system (H_c), and the

Table: **Minimum value of the correlation of the central spins and the energy of the whole system (which is conserved), as observed during the time evolution corresponding to the curves listed in the first column. The correlations $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle_0$ and the ground state energy E_0 of the whole system are obtained by numerical diagonalization of the Hamiltonian Eq.(2)**

	$\langle \Psi(t)\|H\|\Psi(t)\rangle$	E_0	$\min_t \langle \mathbf{S}_1(t) \cdot \mathbf{S}_2(t)\rangle$	$\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle_0$
Fig. 1 (a)	-1.299	-1.829	-0.659	-0.723
Fig. 1 (b)	-1.532	-2.065	-0.695	-0.721
Fig. 1 (c)	-1.856	-2.407	-0.689	-0.696
Fig. 2	-4.125	-4.627	-0.744	-0.749
Fig. 3 (a)	-1.490	-1.992	-0.746	-0.749
Fig. 3 (b)	-0.870	-1.379	-0.260	-0.741
Fig. 3 (c)	-1.490	-1.997	-0.737	-0.744
Fig. 3 (d)	-2.654	-3.160	-0.742	-0.745
Fig. 3 (e)	-7.791	-8.293	-0.716	-0.749
Fig. 3 (f)	-3.257	-3.803	-0.713	-0.718
Fig. 4 (b)	-0.884	-1.388	-0.424	-0.733
Fig. 4 (c)	-1.299	-1.829	-0.659	-0.723
Fig. 4 (d)	-1.299	-1.807	-0.741	-0.743
Fig. 4 (e)	-1.843	-2.365	-0.738	-0.735

spins $\mathbf{I}_n = (I_n^x, I_n^y, I_n^z)$ in the environment (H_e), respectively. The exchange integrals $\Delta_{i,j}^{(\alpha)}$ control the interaction (H_{int}) of the central system with its environment. In Eq. (2), the sum over α runs over the x, y and z components of spin 1/2 operators. The number of spins in the environment is N.

Initially, the central system is in the spin-up – spin-down state and the environment is in its ground state. Thus, we write the initial state as $|\Psi(t=0)\rangle = |\uparrow\downarrow\rangle|\Phi_0\rangle$. The time evolution of the 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. [11]. It conserves the energy of the whole system to machine precision.

By changing the parameters of model (1), we explore the conditions under which the central system clearly shows an evolution from the initial spin-up – spin-down state towards the maximally entangled singlet state. We consider systems that range from the rotationally invariant Heisenberg case to the extreme case in which H_e and $H_{\rm int}$ reduce to the Ising model, topologies for which the central system couples to two and to all spins of the environment, and values of parameters that are fixed or are allowed to fluctuate randomly. Illustrative results of these calculations are shown in Figs.1–4. In Table, we present the corresponding numerical data of the energy $\langle \Psi(0)|H|\Psi(0)\rangle = \langle \Psi(t)|H|\Psi(t)\rangle$ and of the two-spin correlation $\langle \mathbf{S}_1(t) \cdot \mathbf{S}_2(t)\rangle = \langle \Psi(t)|\mathbf{S}_1 \cdot \mathbf{S}_2|\Psi(t)\rangle$. For comparison, Table also contains the results of the energy E_0 and of the two-spin correlation $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle_0$ in

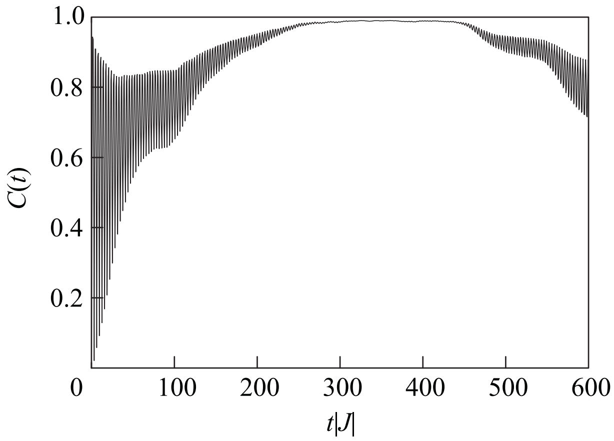

Fig.2 (color online). Time evolution of the concurrence $C(t)$ for the case of a frustrated antiferromagnetic environment. The interactions of the central system and the environment are uniform random numbers in the range $-0.15|J| \le \Delta_{i,j}^{(\alpha)} \le -0.05|J|$. The environment contains 14 quantum spins, arranged on a triangular lattice and interacting with nearest neighbors only. The nonzero exchange integrals are uniform random numbers in the range $-0.55|J| \le \Omega_{i,j}^{(\alpha)} \le -0.45|J|$. The transition from an unentangled state ($C(t) = 0$) to a nearly fully entangled state ($C(t) = 1$) is evident, as is the onset of recurrent behavior due to the finite size of the environment

the ground state of the whole system, as obtained by numerical diagonalization of the Hamiltonian Eq.(2).

We monitor the effects of decoherence by computing the expectation value $\langle \Psi(t)|\mathbf{S}_1 \cdot \mathbf{S}_2|\Psi(t)\rangle$. The central system is in the singlet state if $\langle \mathbf{S}_1(t) \cdot \mathbf{S}_2(t)\rangle = -3/4$,

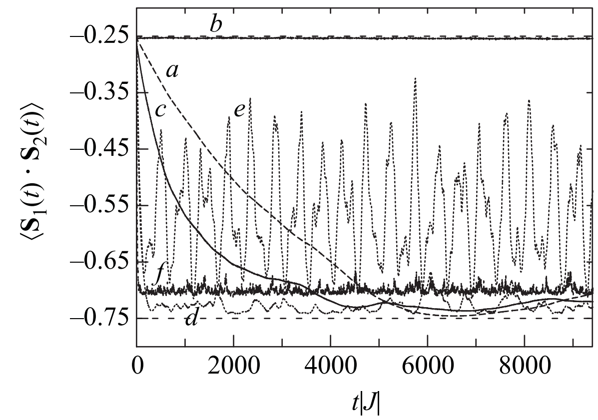

Fig.3 (color online). Time evolution of the correlation $\langle\Psi(t)|\mathbf{S}_1\cdot\mathbf{S}_2|\Psi(t)\rangle$ of the two spins in the central system. Environment containing $N=16$ quantum spins. Dashed horizontal line at $-1/4$: Correlation in the initial state ($\langle\Psi(t=0)|\mathbf{S}_1\cdot\mathbf{S}_2|\Psi(t=0)\rangle=-1/4$); Horizontal line at $-3/4$: Correlation in the singlet state. For all curves $(a-f)$ $\Delta_{i,j}^{(x)}=\Delta_{i,j}^{(y)}=0$, that is $H_{\rm int}$ is Ising like. The values of $\Delta_{i,j}^{(z)}$ are: (a) random $-0.0375\,|J|$ or $0.0375\,|J|$, $(b-e)$ random $-0.075\,|J|$ or $0.075\,|J|$, (f) random $-0.15\,|J|$ or $0.15\,|J|$. The values of $\Omega_{i,j}^{(\alpha)}$ are uniform random numbers in the range: (b) $[-0.0375|J|,0.0375|J|]$, (a,c) $[-0.15|J|,0.15|J|]$, (d,f) $[-0.3|J|,0.3|J|]$ and (e) $[-|J|,|J|]$

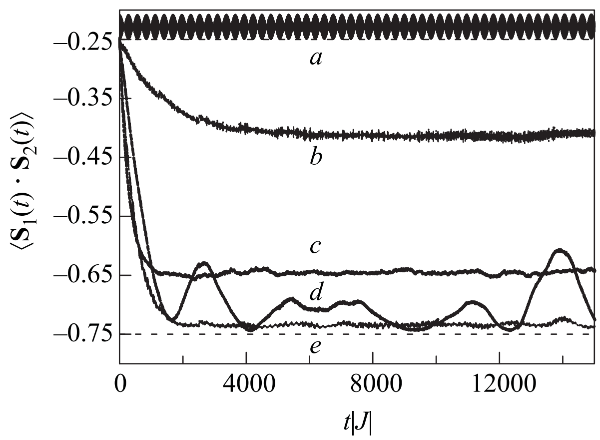

Fig. 4 (color online). Effect of the symmetry of the exchange interactions $\Omega_{i,j}^{(\alpha)}$ and $\Delta_{i,j}^{(\alpha)}$ on the time evolution of the correlation $\langle\Psi(t)|\mathbf{S}_1\cdot\mathbf{S}_2|\Psi(t)\rangle$ of the two spins in the central system. Dashed horizontal line at $-1/4$: Correlation in the initial state ($\langle\Psi(t=0)|\mathbf{S}_1\cdot\mathbf{S}_2|\Psi(t=0)\rangle=-1/4$); Horizontal line at $-3/4$: Correlation in the singlet state; Other lines from top to bottom (at $t|J|=6000$): (a) Ising $H_{\rm int}$ with Ising H_e, $N=14$; (b) Heisenberg-like $H_{\rm int}$ with Ising H_e, $N=14$; (c) Heisenberg-like $H_{\rm int}$ with Heisenberg-like H_e, $N=14$; (d) Ising $H_{\rm int}$ with Heisenberg-like H_e, $N=14$; (e) Same as (d) except that $N=18$. We use the term Heisenberg-like $H_{\rm int}$ (H_e) to indicate that $\Delta_{i,j}^{(\alpha)}$ ($\Omega_{i,j}^{(\alpha)}$) are uniform random numbers in the range $[-0.15\,|J|\,,0.15\,|J|]$. Likewise, Ising $H_{\rm int}$ (H_e) means that $\Delta_{i,j}^{(x,y)}=0$ ($\Omega_{i,j}^{(x,y)}=0$), and $\Delta_{i,j}^{(z)}$ ($\Omega_{i,j}^{(z)}$) are random $-0.075\,|J|$ or $0.075\,|J|$

that is if $\langle\mathbf{S}_1(t)\cdot\mathbf{S}_2(t)\rangle$ reaches its minimum value. We also study the time evolution of the concurrence $C(t)$, which is a convenient measure for the entanglement of the spins in the central system [12]. The concurrence is equal to one if the central system is in the singlet state and is zero for an unentangled pure state such as the spin-up – spin-down state [12].

A very extensive search through parameter space leads to the following conclusions:

- The maximum amount of entanglement strongly depends on the values of the model parameters $\Omega_{i,j}^{(\alpha)}$ and $\Delta_{i,j}^{(\alpha)}$. For the case in which there is strong decoherence, increasing the size of the environment will enhance the decoherence in the central system (compare the curves of Fig.1(a,b,c) and Fig.4(d,e)). Keeping the size of the environment fixed, different realizations of the random parameters do not significantly change the results for the correlation and concurrence (right panel of Fig.1). However, the range of random values $\Omega_{i,j}^{(\alpha)}$ and $\Delta_{i,j}^{(\alpha)}$ for which maximal entanglement can be achieved is narrow, as illustrated in Figs.3 and 4. In Fig.3 we compare results for the same type of $H_{\rm int}$ (Ising like) and the same type of H_e (anisotropic Heisenberg like), but with different values of the model parameters. In Fig.4, we present results for different types of $H_{\rm int}$ and H_e but for parameters within the same range.

- Environments that exhibit some form of frustration, such as spin glasses or frustrated antiferromagnets, may be very effective in producing a high degree of entanglement between the two central spins, see Figs.1–4.

- Decoherence is most effective if the exchange couplings between the system and the environment are random (in a limited range) and anisotropic, see Figs. 3 and 4.

- The details of the internal dynamics of the environment affects the maximum amount of entanglement that can be achieved [9], and also affects the speed of the initial relaxation (compare the curves of Fig.3(b,c,d,e), Fig.4(a,d) and Fig.4(b,c)).

- For the case in which there is strong decoherence, for the same H_e and the same type of $H_{\rm int}$, decreasing the strengh of $H_{\rm int}$ will reduce the relaxation to the finial state, and the final state comes closer to the singlet state (compare the curves of Fig.3(a,c) and Fig.3(d,f)).

Earlier simulations for the Ising model in a transverse field have shown that time-averaged distributions of the energies of the central system and environment agree with those of the canonical ensemble at some effective temperature [13, 14]. Our results do not contradict these findings but show that there are cases in which the central system relaxes from a high energy state to its ground state while the environment starts in the ground state and ends up in state with slightly higher energy. As shown in Fig.4(e), this state is extremely robust and shows very little fluctuations.

For the models under consideration, the efficiency of decoherence decreases drastically in the following order: Spin glass (random long-range interactions of both signs); Frustrated antiferromagnet (triangular lattice with the nearest-neighbour interactions); Bipartite antiferromagnet (square lattice with the nearest-neighbour interactions); One-dimensional ring with the nearest-neighbour antiferromagnetic interactions. This can be understood as follows. A change of the state of the central system affects a group of spins in the environment. The suppression of off-diagonal elements of the reduced density matrix can be much more effective if the group of disturbed spins is larger. The state of the central system is the most flexible in the case of a coupling to a spin glass for which, in the thermodynamic limit, an infinite number of infinitely closed quasi-equilibrium configurations exist [15, 16]. As a result, a very small perturbation leads to the change of the system *as a whole*. This may be considered as a quantum analog of the phenomenon of "structural relaxation" in glasses. This suggests that frustrated spin systems that are close to the glassy state should provide extremely efficient decoherence.

To conclude, we have demonstrated that frustrations and, especially, glassiness of the spin environment result in a very strong enhancement of its decohering action on the central spin system. Our results convincingly show that this enhancement can be so strong that solely due to decoherence, a fully disentangled state may evolve into a fully entangled state, even if the environment contains a relatively small numbers of spins.

1. D. Giulini, E. Joos, C. Kiefer et al., *Decoherence and the Appearance of a Classical World in Quantum Theory*, Springer, Berlin, 1996.
2. W. H. Zurek, Rev. Mod. Phys. **75**, 715 (2003).
3. J. von Neumann, *Mathematical Foundations of Quantum Mechanics*, Princeton University Press, Princeton, 1955.
4. R. P. Feynman and F. L. Vernon, Ann. Phys. (N.Y.) **24**, 118 (1963).
5. A. J. Leggett, S. Chakravarty, A. T. Dorsey et al., Rev. Mod. Phys. **59**, 1 (1987).
6. J.-P. Paz and W. H. Zurek, Phys. Rev. Lett. **82**, 5181 (1999).
7. N. V. Prokof'ev and P. C. E. Stamp, Rep. Prog. Phys. **63**, 669 (2000).
8. V. V. Dobrovitski, H. A. De Raedt, M. I. Katsnelson et al., Phys. Rev. Lett. **90**, 210401 (2003).
9. J. Lages, V. V. Dobrovitski, M. I. Katsnelson et al., Phys. Rev. E **72**, 026225 (2005).
10. W. H. Zurek, Nature **412**, 712 (2001).
11. V. V. Dobrovitski and H. A. De Raedt, Phys. Rev. E **67**, 056702 (2003).
12. W. K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).
13. R. V. Jensen and R. Shankar, Phys. Rev. Lett. **54**, 1879 (1985).
14. K. Saito, S. Takasue, and S. Miyashita, Phys. Rev. Lett. **65**, 1243 (1996).
15. K. Binder and A. P. Young, Rev. Mod. Phys. **58**, 801(1986).
16. M. Mezard, G. Parisi, and M. A. Virasoro, *Spin Glass Theory and Beyond*, World Scientific, Singapore, 1987.