Quantum Oscillations without Quantum Coherence

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We study numerically the damping of quantum oscillations and the dynamics of the density matrix in model many-spin systems decohered by a spin bath. We show that oscillations of some density matrix elements can persist with considerable amplitude long after other elements, along with the entropy, have come close to saturation, i.e., when the system has been decohered almost completely. The oscillations exhibit very slow decay, and may be observable in experiments.

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For a quantum system prepared in a linear superposition of its eigenstates, some observables can oscillate with time. Interaction of the system with its environment leads to a decay of the system's initial pure state into a mixture of several states; i.e., nondiagonal elements of the density matrix vanish, and diagonal elements achieve their equilibrium values. This causes an increase of the system's entropy and damping of quantum oscillations with time [1,2]. Rabi oscillations have been observed for many microscopic systems, and even for some mesoscopic (e.g., Josephson-junction based [3]) systems. Detailed theoretical study of decoherence has become experimentally relevant and important. The standard picture of the evolution of an open quantum system [1,2], based on earlier derivations of the master equation [4,5], suggests that the increase of entropy and the saturation of the diagonal elements, along with the decrease of nondiagonal elements and the damping of quantum oscillations, are very fast, and usually obey an exponential $[\exp(-t/\tau)]$ or Gaussian $[\exp(-t^2/\tau^2)]$ law. After the initial fast decay, the system becomes quasiclassical. Rapid quantum motions are absent, the system's entropy changes slowly, and the dynamics of the density matrix is determined mainly by slow transitions between different decohered states (thermalization of the system).

In this work, we consider the first stage of evolution, studying decoherence of an open system made of several strongly coupled spins, $s_i = 1/2$, by a spin bath. We show that, for an even number of the spins s_i in the system, the decoherence process can demonstrate unusual properties which do not fit in the standard picture. Namely, decoherence starts with conventional fast Gaussian decay, which sharply increases the entropy of the system and brings most of the density matrix elements close to saturation. In standard situations, this would lead to complete damping of all quantum oscillations. But in many-spin systems containing an even number of spins, some nondiagonal elements of the density matrix survive the initial rapid decay. These oscillating density matrix elements demonstrate very slow damping, which is not related to thermalization of the system. The existence of rapid quantum oscillations in a decohered system is in striking contrast with the standard scenario of decoherence, and, to our knowledge, has not been discussed before.

We consider a system weakly coupled to the environment, when the characteristic energies of the system are much larger than environmental ones. In this case, the final states are the eigenstates $|\phi_n\rangle$ of the system's Hamiltonian [6]. The damping of the nondiagonal elements $\langle\phi_n|\rho|\phi_m\rangle$ of the density matrix ρ is fast Gaussian, and its rate is proportional to the magnitude of the interaction Hamiltonian [6]. But detailed analytical studies of this dynamical process are difficult, and often include quite stringent approximations (e.g., Markovian behavior of the bath). In this work, we numerically solve the compound "system-plus-bath" time-dependent Schrödinger equation, using Suzuki-Trotter decomposition and Chebyshev polynomial expansion. These techniques are described in detail in Ref. [7]. The analytical approximations we use are compared with the exact numerical solution. We do not consider the case of a single central spin; although there are analogies [8], a two-step decoherence is not clearly seen.

Consider the system of two central spins $\mathbf{s}_1$ and $\mathbf{s}_2$ ($s_1 = s_2 = 1/2$) coupled by Heisenberg exchange, so that the system's Hamiltonian is $\mathcal{H}_S = 2J\mathbf{s}_1\mathbf{s}_2$. This system is coupled to a spin bath made of spins $\mathbf{I}_k$ ($I_k = 1/2,\ k = 1, \ldots, N$) via Heisenberg interactions, so the Hamiltonian $\mathcal{V} = \sum_k A_k^{(1)}\mathbf{s}_1\mathbf{I}_k + A_k^{(2)}\mathbf{s}_2\mathbf{I}_k$ describes the interaction between the central system and the bath. Below, we consider only strongly coupled central spins, when $J \gg A_k^{(1)}, A_k^{(2)}$. Then, the difference between $A_k^{(1)}$ and $A_k^{(2)}$ is not important, even if all $A_k^{(2)} = 0$. This is justified by the cumulant expansion [9] of the evolution operator, and is confirmed by our numerical results. Therefore, below we discuss only the case where $A_k^{(1)} = A_k^{(2)} = A_k$. The total Hamiltonian determining the overall "system-plus-bath" dynamics is

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{V} = \mathcal{H}_S + \mathcal{H}_B + \mathcal{V}, \tag{1}$$

where $\mathcal{H}_S$ and $\mathcal{H}_B$ are the Hamiltonians of the central system and the bath, respectively, and $\mathcal{V}$ is the system-bath interaction. Here, we consider both the case of the "static" bath, with $\mathcal{H}_B = 0$, and the case of a slow bath possessing chaotic dynamics (see below).

The models considered here are rather general, and can be used to describe a number of systems [e.g., superconducting quantum interference devices (SQUIDs), quantum dots, magnetic molecules, etc.] where a spin bath, such as nuclear spins, constitutes an important decoherence mechanism [10]. Spin-bath decoherence has been discussed in Ref. [10], but consideration there is restricted to a single central spin. Phonons or conduction electrons (if weakly coupled with the central spins) do not overdamp quantum oscillations [2], and corresponding decoherence rates can be much slower than the rate of the spin-bath decoherence at low temperatures. Oscillations in two coupled SQUIDs have been detected experimentally [11], and observation of the effect predicted here may become feasible. Detailed theoretical assessment of specific experiments requires separate consideration, beyond the scope of this Letter, but essential physical details are captured in the models considered.

Considering decoherence caused by nuclear spins, we assume that the couplings A_k are random, uniformly distributed from zero to $A_k^{\max}$. Initially, the system and the bath are in a product state $|\phi\rangle \otimes |b\rangle$; the state of the bath $|b\rangle$ is a random superposition of all possible basis states. This corresponds to the temperature $J \gg T \gg A_k$, which is true for low-temperature experiments (down to fractions of milliKelvin) and for strong coupling inside the central system. In Fig. 1, we present the results for $N = 13$ bath spins, $\mathcal{H}_B = 0$, with the system-bath couplings distributed from 0 to $A_k^{\max} = 0.5$. The exchange between the central spins $J = 8.0$. The initial state of the system $|\phi\rangle = |\uparrow\rangle|\downarrow\rangle$, i.e., a symmetric superposition of the triplet $|s = 1, s_z = 0\rangle$ and the singlet $|s = 0\rangle$ states (where $\mathbf{s} = \mathbf{s}_1 + \mathbf{s}_2$ is the total spin and s_z is its z component). We present only the oscillations of the z component of the first spin $s_1^z(t)$: oscillations of $s_2^z(t)$ are just shifted in phase by π, and all other components of the central spins remain practically constant. We also present the time dependence of quadratic entropy $S_e(t) = 1 - \mathrm{Tr}\rho^2(t)$; see Fig. 1(b). This quantity, as well as the von Neumann's entropy ($S_{vN} = -\mathrm{Tr}\rho \ln\rho$), characterizes how strongly mixed is the state of the system [1,6], but $S_e(t)$ is technically more convenient.

The graphs in Fig. 1 clearly show a two-step process. Initially, decoherence is very fast: in agreement with the standard picture, the correlations $C_{12}^{\alpha\beta} = \langle s_1^\alpha s_2^\beta \rangle$ between the central spins diminish sharply, and the entropy of the system rapidly increases. In a standard situation, e.g., for decoherence by a boson bath [1,2,6], this would lead to fast disappearance of all quantum features. However, the results demonstrate that this does not always happen: for the two-spin system, after the first step, the oscillations of z components of the central spins $s_1^z(t)$ and $s_2^z(t)$ persist and decay very slowly.

In Fig. 2 we present the dynamics of different elements of the density matrix ρ of the central system. The density matrix is more suitable for detailed analysis than $S_e(t)$, $s_1^z(t)$, or $s_2^z(t)$. For example, even in a completely decohered system which has not yet achieved a thermal equilibrium, entropy still slowly increases with time due to changes in the diagonal density matrix elements, but this long-time tail is not related to decoherence. Both $S_e(t)$ and $s_1^z(t)$ [or $s_2^z(t)$] depend on all elements of the matrix ρ, and clearly different behavior of different matrix elements becomes "smoothed out" in $S_e(t)$ and $s_1^z(t)$.

Figure 2 shows that initially part of the $|s = 1, s_z = 0\rangle$ spectral weight is transferred equally to the $|s = 1, s_z = \pm 1\rangle$ states. The direction of the system's total spin randomizes (although incompletely) due to rotation around the randomly oriented effective field generated by the

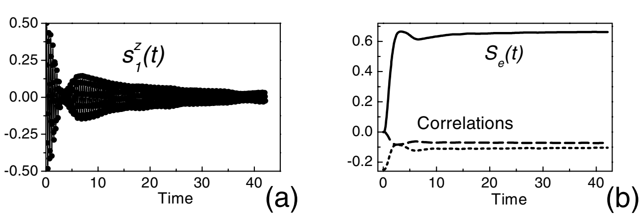

FIG. 1. Decoherence of two coupled spins by a spin bath. (a) Oscillations of $s_1^z(t)$; (b) entropy $S_e(t)$ (solid line), and correlations between the central spins, C_{12}^{zz} (dotted line) and $C_{12}^{xx} = C_{12}^{yy}$ (dashed line).

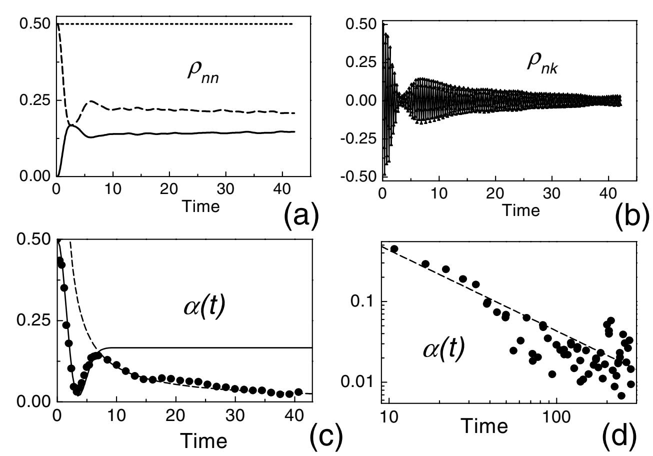

FIG. 2. Dependence of the density matrix elements vs time. (a) Diagonal elements for the $|s = 1, s_z = 0\rangle$ state (solid line), $|s = 1, s_z = \pm 1\rangle$ states (dashed line), and $|s = 0\rangle$ state (dotted line); (b) nondiagonal element $\langle s = 0|\rho|s = 1, s_z = 0\rangle$. All other matrix elements are very small. (c) Comparison of the numerical results for $\alpha(t)$ (dots) with the analytical short-time solution (solid line) and long-time approximation (dashed line). (d) The same comparison for longer times, on log-log scale (the analytical short-time solution is omitted).

bath. Also, the nondiagonal element of the density matrix element $\langle s=0|\rho|s=1, s_z=0\rangle$ decays rapidly. These changes of the density matrix are in agreement with the standard scenario of decoherence. After the initial fast decoherence, the diagonal elements do not show any fast dynamics [Fig. 2(a)], but the nondiagonal element $\langle s=0|\rho|s=1, s_z=0\rangle$ exhibits slowly damped oscillations, Fig. 2(b).

Conclusive analytical treatment of the system under consideration is difficult, and we are not aware of any means of obtaining an exact solution. The compound "system-plus-bath" evolution operator is $U(t) = \exp[-iJ\mathbf{s}^2 t - i\mathbf{s}\mathbf{B}t]$, where $\mathbf{B} = \sum_k A_k \mathbf{I}_k$ is the operator of the effective field acting on the central spins. To obtain an approximate analytical description of the system's dynamics, we consider the bath in the mean-field manner similar to the Mermin model [12]. Since the effective field $\mathbf{B}$ is created by a large number of independent bath spins, we replace $B_{x,y,z}$ by Gaussian random fields with the mean square $b^2 \approx \sum_k A_k^2/4$. The mean-field evaluation gives

$$\alpha(t) = (1/6)[1 - 2(b^2t^2 - 1)\exp(-b^2t^2/2)], \qquad (2)$$

where $\alpha(t)$ denotes the envelope of the oscillating quantity $\langle s=0|\rho|s=1, s_z=0\rangle$. That is, the initial decoherence proceeds as fast Gaussian decay, with the final value $1/6$ rather than zero. This prediction, valid for short times, is in good agreement with the numerical results; see Fig. 2(c). The subsequent slow damping of oscillations cannot be described within the mean-field treatment. The second step of the decoherence process is associated with the temporal changes of the effective field $\mathbf{B}$. We are not aware of analytical solution; in analogy with the single-spin considerations [8], we can assume a power-law decay $1/t$. As seen from Figs. 2(c) and 2(d), this approximation agrees with the numerical results, but at $t > 100$, the mean value of $\alpha(t)$ becomes smaller than the fluctuations, so that conclusions on the form of the long-time decay are difficult to make, and further detailed study is needed. However, the central result of the present work, the drastic difference in the rate between the two steps of decoherence, is clearly seen independently of the exact form of decay.

The long-time oscillations do not take place inside decoherence-free subspaces [13]: they take place between the singlet $|s=0\rangle$ and triplet $|s=1, s_z=0\rangle$ states. To consider a more general situation, we include the dynamics inside the triplet manifold using the initial condition $|\phi\rangle = \alpha^2|\uparrow\downarrow\rangle + \beta^2|\downarrow\uparrow\rangle + \alpha\beta|\uparrow\uparrow\rangle + \alpha\beta|\downarrow\downarrow\rangle$, which involves the states $|s=1, s_z=\pm1\rangle$. The dynamics of different elements of the density matrix for $\alpha^2 = 0.5(1+\sqrt{0.8})$ and $\beta^2 = 0.5(1-\sqrt{0.8})$ is shown in Fig. 3. One can see that the behavior of the nondiagonal elements connecting the states within the triplet subspace [Fig. 3(b)] is similar to the behavior of the diagonal elements: after the fast initial decoherence, they remain almost constant, and their changes are much smaller than the changes of the amplitude of oscillations of the element $\langle s=0|\rho|s=1, s_z=0\rangle$ [Fig. 3(d)].

Also, we have checked the role of the slow dynamics of the bath. In reality, the dynamics of the nuclear spins is indeed very slow, due to very small interactions between them, and chaotic. To model a chaotic bath, we use the Hamiltonian suggested in [14]:

$$\mathcal{H}_B = h\sum_k I_k^z + \sum_{k'k''}\Gamma_{k'k''} I_{k'}^x I_{k''}^x, \qquad (3)$$

with random nearest-neighbor exchanges $\Gamma_{k',k''}$. We have checked the level statistics, and confirmed that it follows the Wigner-Dyson distribution. In our simulations, we used $h = 0.1$ and $\Gamma_{k',k''}$ randomly distributed in the interval $[-0.013, 0.013]$. Again, the two-step scenario is seen, and the behavior of the elements of the density matrix is qualitatively the same as in the case $\mathcal{H}_B = 0$. The long-lasting oscillations, along with the motion of the bath spins, are shown in Fig. 4. Other models for a slow chaotic bath give essentially identical results.

The conclusions presented here have been confirmed by calculations for different sets of system parameters, for environments of different sizes (up to 20 bath spins), etc. Our qualitative conclusions also hold for larger central

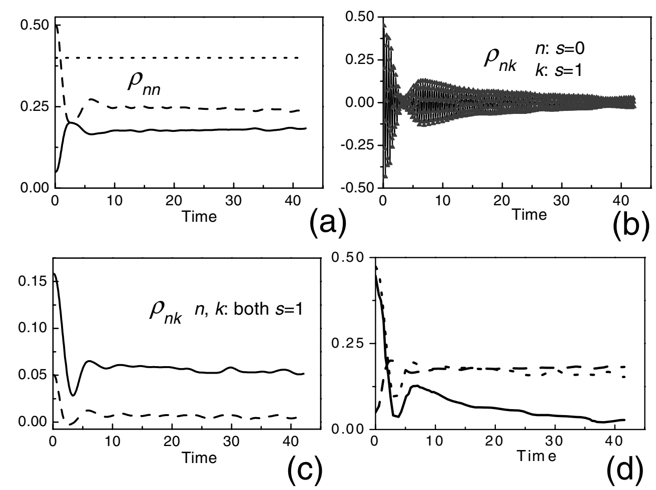

FIG. 3. Dependence of the density matrix elements vs time. (a) Diagonal elements for $|s=1, s_z=0\rangle$ state (solid line), $|s=1, s_z=\pm1\rangle$ states (dashed line), and $|s=0\rangle$ state (dotted line); (b) nondiagonal element $\langle s=0|\rho|s=1, s_z=0\rangle$; (c) nondiagonal elements $\langle s=1, s_z=0|\rho|s=1, s_z=1\rangle$ (solid line) and $\langle s=1, s_z=-1|\rho|s=1, s_z=1\rangle$ (dashed line); (d) comparison of the envelope of oscillations of $\langle s=0|\rho|s=1, s_z=0\rangle$ and the changes in the nondiagonal $\langle s=1, s_z=0|\rho|s=1, s_z=1\rangle$ and diagonal $\langle s=1, s_z=1|\rho|s=1, s_z=1\rangle$ elements vs time. The value of the element $\langle s=1, s_z=0|\rho|s=1, s_z=1\rangle$ has been increased by three to match the scale of other curves on the graph (d). All other matrix elements are either very small or similar to those presented here.

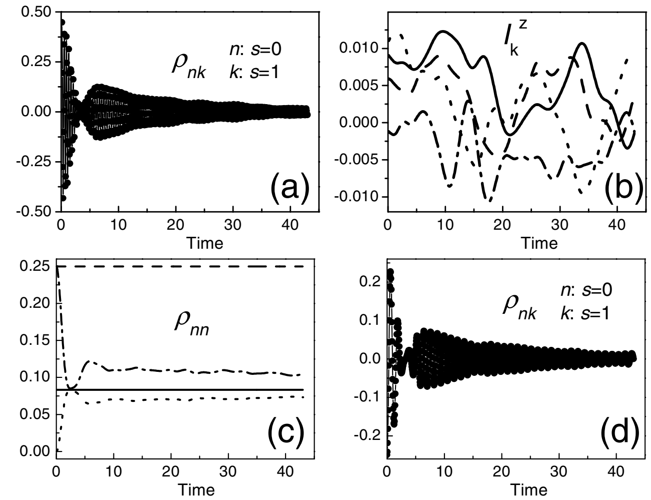

FIG. 4. Oscillation dynamics for a slow chaotic bath. (a) The oscillations of the nondiagonal element $\langle s=0|\rho|s=1, s_z=0\rangle$. (b) Time dependence of the I_k^z for some of the bath spins. No qualitative changes in the oscillations are seen, in spite of the chaotic motion of the bath spins occurring during oscillations. Also shown, (c) and (d), is the evolution of the density matrix for the system of four coupled spins. (c) Evolution of the diagonal density matrix elements; (d) dynamics of the nondiagonal element $\langle x|\rho|y\rangle$, where $|x\rangle$ has $s=s_a=s_b=0$, and $|y\rangle$ has $s=1$, $s_z=0$, $s_a=0$, $s_b=1$.

systems. For example, in Figs. 4(c) and 4(d), we show the density matrix dynamics of four central spins coupled to each other by Heisenberg exchange with $J=2.5$. The states of such a system are characterized by the values of s and s_z(total spin and its z projection), and by the quantities s_a and s_b defined as $(\mathbf{s}_2+\mathbf{s}_3)^2 = s_a(s_a+1)$, $(\mathbf{s}_1+\mathbf{s}_4)^2 = s_b(s_b+1)$. In all the cases we have considered, oscillations of the nondiagonal elements of the density matrix show up in the long-living oscillations of $s_1^z(t)$. Thus, in experiments, the oscillations can be registered by monitoring the dynamics of individual spins in the central system.

In summary, we have studied the decoherence process which takes place in some generic systems containing an even number of interacting spins $1/2$ coupled to a spin bath. We analyzed the dynamics of different elements of the density matrix, and found that the decoherence proceeds in two steps. Initially, a conventional fast Gaussian decoherence takes place when the diagonal elements of the density matrix and some of the nondiagonal elements decrease very rapidly. Simultaneously, the system's entropy rises quickly. But this stage is not final, and some of the nondiagonal elements still exhibit oscillations which decay very slowly, showing presumably power-law damping. These long-living oscillations are robust with respect to the chaotic dynamics of the bath, and are present for different initial conditions, different sizes of the central system and couplings to the bath, etc. Therefore, in some cases, significant quantum oscillations can be seen even in a decohered system. This is in striking contrast with the standard scenario of decoherence, which implies rapid single-step decoherence and quick suppression of fast quantum dynamics. Corresponding experiments are possible, although they require significant effort and further development.

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