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Decoherence by a chaotic many-spin bath

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We numerically investigate decoherence of a two-spin system (central system) by a bath of many spins 1/2. By carefully adjusting parameters, the dynamical regime of the bath has been varied from quantum chaos to regular, while all other dynamical characteristics have been kept practically intact. We explicitly demonstrate that for a many-body quantum bath, the onset of quantum chaos leads to significantly faster and stronger decoherence compared to an equivalent non-chaotic bath. Moreover, the non-diagonal elements of the system’s density matrix decay differently for chaotic and non-chaotic baths. Therefore, knowledge of the basic parameters of the bath (strength of the system-bath interaction, bath’s spectral density of states) is not always sufficient, and much finer details of the bath’s dynamics can strongly affect the decoherence process.

Real physical systems are never isolated. Interaction of a quantum system with its environment leads to decoherence: the initial pure state of the system quickly decays into an incoherent mixture of several states [1, 2]. Modern experiments provide much information about the decoherence dynamics of single (or few) ions [3], Cooper pairs [4], or spins [5], and require a comprehensive theory for adequate understanding. Decoherence is also a major obstacle to building a practical quantum computer, which, for a wide class of problems, is exponentially more efficient than classical computers [6]. Interaction of a quantum computer with the bath leads to a fast generation of errors, and an accurate theory is needed to find a way of controlling this process.

Decoherence is a complex quantum many-body phenomenon, and its detailed description is a challenging problem. Many theoretical approaches eliminate the environment from consideration, approximating its influence by suitably chosen operators (deterministic or stochastic), and retaining only basic information: the strength of the system-bath interaction, characteristic energies/times of the bath, etc. [2] Such methods often work well, but many situations require detailed account of the bath’s internal dynamics. Recently, the role of quantum chaos [7] in the decoherence process has become a subject of debate [8, 9, 10]. Qualitative semiclassical arguments indicate that the chaotic bath (i.e., the bath having only a few trivial integrals of motion) is “a stronger decoherer” [8] than an integrable bath (i.e., the bath possessing a complete set of the integrals of motion). Perturbative arguments lead to the opposite answer [9]. However, these and related works [10], eliminate the central system from discussion, considering instead a static perturbation acting on a bath, and/or treat the bath semiclassically, as a particle (or a single large spin) with an integrable or a chaotic Hamiltonian.

Although many valuable insights have been obtained in previous work, an important question remains unanswered: is the onset of quantum chaos important for the real-world situation when both the system and the bath are fundamentally quantum many-body objects with non-trivial dynamics? In this paper, we give an affirmative answer to this question. In contrast with previous work, we do not replace the system or the bath by perturbation. We go beyond the semiclassical one-body description, realistically considering the spin environment as many interacting spins 1/2, which have no well-defined semiclassical limit. We show that the chaotic bath decoheres the central system stronger and faster than an equivalent non-chaotic one, and changes the dynamics of the decay of non-diagonal elements of the system’s density matrix.

The bath of spins 1/2 (nuclear or electron spins, magnetic impurities) constitutes a major source of decoherence for nuclear magnetic resonance (NMR) experiments, decoherence of phosphorus spins in Si [11], spins in magnetic molecules [12] and quantum dots [13]. Two-level defects, governing decoherence in Josephson junctions [14], can also be modeled as spins 1/2. Even small coupling between the bath spins can make the bath chaotic, and we need to understand, at least qualitatively, how this affects the decoherence process. The dynamics of a system decohered by the spin bath is affected by many factors. In order to conclusively separate the impact of chaos in the bath, and to provide the knowledge needed for more complex studies, we need a simple, well-characterized, but realistic model. Here, we consider a central system of two exchange-coupled spins 1/2, $S_1$ and $S_2$, where $S_1$ interacts with a bath of spins $I_k$ ($I_k = 1/2, k = 1, \ldots, N$). The corresponding Hamiltonian is

$$H = J S_1 S_2 + S_1 \sum_k A_k I_k + H_B$$

(1)

where $A_k$ are the system-bath coupling constants, and $H_B$ is the Hamiltonian of the bath. Similar models describe cross-relaxation and double resonance in NMR [15], and destruction of the Kondo effect by decoherence [16]. Detailed theoretical assessment of specific experiments requires separate consideration, beyond the scope of this paper, but this simplified model captures essential...
physical details of decoherence by the chaotic spin bath. Due to similar reasons, we describe the bath by the "spin glass shard" model [17] with the Hamiltonian

$$H_B = \sum_{k,l} \Gamma_{kl} I_k^x I_l^x + \sum_k h_k^x I_k^x + \sum_k h_k^z I_k^z$$  \hspace{1cm} (2)$$

with random $\Gamma_{kl}$ and $h_k^{x,z}$, uniformly distributed in the intervals $[-\Gamma_0, \Gamma_0]$ and $[0, \hbar_0]$ respectively. This model describes the regular-to-chaotic transition in a simple and clear way, and permits straightforward control of the bath’s dynamics [17]. For small $\Gamma_0$, the bath is integrable, and becomes chaotic for $\Gamma_0 > \Gamma_{cr} \sim \hbar_0 / (zN)$ where $N$ is the number of bath spins and $z$ is the number of neighbors coupled via the term $\Gamma_{kl} I_k^z I_l^z$. Therefore, in real baths with large $N$, the chaotic regime can be relevant even for very small couplings $\Gamma_{kl}$.

We study decoherence by numerically solving the time-dependent Schrödinger equation for the wave function $|\Psi(t)\rangle$ of the compound system (the central system plus bath), using the Hamiltonians (1)-(2), and considering

up to $N = 16$ bath spins (the results do not change much already for $N > 10$). We use Chebyshev’s polynomial expansion, in order to work with large Hilbert spaces and to study the system’s dynamics at extremely long times [18, 19]. The initial state of the compound system is $|\Psi(0)\rangle = |\psi\rangle |\chi\rangle$, where the state of the central system is maximally entangled, $|\psi\rangle = \frac{1}{\sqrt{2}}(|1\uparrow\downarrow\rangle - |1\downarrow\uparrow\rangle)$ (singlet), and the state of the environment $|\chi\rangle$ is a superposition of all basis states with random coefficients (which corresponds e.g. to the bath of nuclear spins at temperatures above few tenths of Kelvin). A wide range of the parameters $J$, $\hbar_0$, $\Gamma_0$, $N$, and different sets of $A_k$ have been explored, and typical results are presented below.

It is convenient to describe the system’s evolution by the reduced density matrix $\rho(t) = \text{Tr}_B|\Psi(t)\rangle\langle\Psi(t)|$ where $\text{Tr}_B$ means trace over the bath states. Dynamics of some elements of $\rho(t)$ is shown in Fig. 1a. Two stages are clearly seen: first, the bath rapidly decoheres the system, excites the triplet states, and the system oscillates between the singlet and triplet states. Much later, thermalization takes place at much slower rate (note the log scale of the time axis). Fig. 1b shows the evolution of the real part of the non-diagonal element $\rho_{12} = \text{Re}(|1\uparrow|\langle\rho|1\downarrow\rangle)$ for different system-bath couplings, with the coupling parametrized by the quantity $b = \left(\sum_{k=1}^{N} A_k^2\right)^{1/2}$. For every $b$ two curves are shown, corresponding to $\Gamma_0 > \Gamma_{cr}$ (i.e., chaotic bath) and $\Gamma_0 < \Gamma_{cr}$ (regular bath); for the bath here, $\Gamma_{cr} \sim 0.013$. The chaotic bath changes the system’s evolution both at long time (clearly seen on Fig. 1b), and at short times (see below). We verified the onset of chaos by calculating the level spacing statistics $P(s)$ [7], which agrees with the Wigner-Dyson distribution for chaotic bath and with Poisson for a regular
FIG. 3: The value $p^I_{12}$ vs. $J/b$ for the chaotic environment $\Gamma_0 = 0.04$, $h_0 = 0.014$ (•), and for the regular environment $\Gamma_0 = 0.008$, $h_0 = 0.014$ (□). The inset shows $p^I_{12}$ as a function of $J/b$ for $h_0 = 1/\sqrt{2}$, $\Gamma = 0.008$ (regular bath); for different sizes $N$ of the environment and different values $b$ of the coupling between the central system and the environment: $N = 8$, $b = 0.518$ (□), $N = 10$, $b = 0.562$ (o), $N = 12$, $b = 0.683$ (△). $N = 12$, $b = 0.608$ (■), $N = 12$, $b = 0.965$ (●), $N = 12$, $b = 1.365$ (▲).

The bath (insets (a),(b) in Fig. 2). It is important that other parameters of the bath remain practically intact: the large-scale structure of the bath’s spectrum (see Eq. 2) is governed by the local fields $h^Z_k$, since $\Gamma_{cr} \ll h_0$. E.g., Fig. 2 shows that the spectral density of states is practically the same for the regular and the chaotic bath.

Decoherence can be quantified by the system’s entropy, concurrence, etc., but particular, does not affect the conclusions. The element $\rho_{12} = \text{Re} \langle \mid \mid | \rho | \mid \mid \rangle$ is particularly suitable for our model: it has an obvious physical meaning, and its evolution can be understood from the Hamiltonian (1). The coupling $JS_1S_2$ inside the central system preserves the initial singlet correlation between $S_1$ and $S_2$, thus steering the value of $\rho_{12}$ towards $-1/2$. The system-bath coupling $\sum A_k I_k$ entangles the spin $S_1$ with the bath and destroys the correlations between $S_1$ and $S_2$, thus leading $\rho_{12}$ towards zero. Competition between the two tendencies determines the value of $\rho_{12}$ at $t \to \infty$. Inset in Fig. 3 shows that $p^I_{12} = \rho_{12}(t \to \infty)$ is determined by the single ratio $J/b$ (where $b^2 = \sum A_k^2$), independently of the size of the bath $N$ and particular values of $A_k$. But the bath’s internal dynamics noticeably affects the dependence $p^I_{12}(J/b)$, as Fig. 1b shows. Fig. 3 presents the results of many simulations, comparing the curves $\rho^I_{12}(J/b)$ for chaotic and regular environments. The chaotic bath, for the same value of $J/b$, is more efficient in steering $\rho^I_{12}$ towards zero, i.e. in breaking the correlations between $S_1$ and $S_2$.

But the most obvious difference between the chaotic and the regular baths emerges at short times, $t < 100$–300 (Fig. 4). For $J \gg b$ (small system-bath coupling), $\rho_{12}(t)$ oscillates with the frequency $\omega \sim J$, mirroring the quantum oscillations of the central system between the singlet and triplet states. For $b$ larger than the spectral width $W$ of the bath (here, $W \sim 0.1$, see Fig. 2), the oscillations of $\rho_{12}(t)$ are identical for the chaotic and the regular baths (Fig. 4a). The envelope of the oscillations is Gaussian, i.e. $\rho^G_{12}(t) = \alpha + \beta \exp \left( -t^2/T_s^2 \right)$ where $\alpha$ and $\beta$ are constants, and $T_s$ is the decay time. However, when $b$ becomes smaller than $W$, prominent differences appear (Fig. 4b). For the regular bath, the decay remains Gaussian, but the chaotic bath leads to the exponential decay, with the envelope $\rho^E_{12}(t) = \alpha' + \beta' \exp \left( -t/T_s \right)$. The decay time $T_s$ also becomes different, see Fig. 5, where $T_s$ is plotted as a function of $1/b$. The values of $T_s$ were determined from the least-square fits of $\rho^G_{12}(t)$ to both Gaussian and exponential forms; both forms give similar $T_s$. For $b < W$ (large $1/b$), the chaotic-bath decoherence is faster by a factor of $2–2.5$ [20].

It is important to note that the curves $\rho_{12}(t)$ for the regular bath are insensitive to $\Gamma_0$, but the drastic difference emerges as soon as $\Gamma_0$ exceeds $\Gamma_{cr}$, when the bath becomes chaotic.

In our model, the central system can not be considered as a Hamiltonian perturbation acting on the bath: $S_1$ can not be replaced by a fictitious magnetic field since the intra-system and the system-bath couplings are isotropic [21]. Also, our bath has no semiclassical limit. Nonetheless, there is a striking analogy between our results and the Loschmidt echo decay in semiclassical systems [19]. Following Ref. [8], if the central system could be replaced by a perturbation $\Delta$ of the bath’s internal Hamiltonian (2), then the states $| \uparrow \rangle$ and $| \downarrow \rangle$ of the central system would correspond to different perturbations $\Delta'$ and $\Delta''$, which would produce different bath states $| \chi^{\prime}_n \rangle = \exp(-i[H_B + \Delta'|t]|\chi_0 \rangle$ and $| \chi''_{n} \rangle = \exp(-i[H_B + \Delta''|t]|\chi_0 \rangle$. The strength of the system-bath interaction $b$ then would correspond to the magnitude of $| \Delta |$, and the matrix element $\langle \downarrow | \mid \rho | \uparrow \rangle$ would correspond to the overlap $\langle \chi^{\prime}_n | \chi''_{n} \rangle$. It is known [19]
that the quantity $F(t) = |\langle \phi^s | \phi^r \rangle|^2$ (called Loschmidt echo) exhibits Gaussian decay when $||\Delta||$ is larger than the bath’s spectral width $W$, and our results for $p_{12}(t)$ at $b > W$ also show Gaussian decay. At $||\Delta|| < W$ (in Lyapunov’s regime), the Loschmidt echo of the chaotic bath decays exponentially with the rate independent of $||\Delta||$, while for the regular bath the decay is Gaussian. Our simulations give the same picture, with the decay time $T_s$ almost independent of $b$ for chaotic bath ($T_s$ changes by only $\sim 20\%$ for $0.005 < b < 0.1$). So, it is likely that the $b < W$ regime of decoherence corresponds to the Lyapunov’s regime of the bath, in spite of the fact that our bath has no semiclassical analogy [22]. The study of the Lyapunov’s exponents is an interesting problem for further research.

Summarizing, we compare decoherence of a two-spin system by regular and chaotic spin baths. We go beyond the standard one-body semiclassical description, considering environments of many spins $1/2$. We do not replace the system by a perturbation acting on the bath, thus going beyond the Loschmidt echo studies. At $t \rightarrow \infty$, the chaotic bath leads to smaller values of the system’s density matrix element $|\langle \uparrow | \rho | \downarrow \rangle|^2$ than the regular bath, i.e. at long times the chaotic bath decoheres the system more efficiently. At short times, the chaotic bath leads to faster decay of quantum oscillations in the system, and changes the form of the decay from Gaussian to exponential. Therefore, the onset of chaos in the bath drastically changes the decoherence dynamics. Also, based on the analogy with the Loschmidt echo studies, we give arguments that the chaotic bath is in the Lyapunov’s regime.

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[20] It is interesting that at $0.01 < b < 0.1$, for the regular bath, $T_s$ decreases by a factor of $\sim 2$ with decreasing $b$, i.e. the system is decohered faster for smaller system-bath interaction, while for the chaotic bath $T_s$ is almost constant (the change is $\sim 13\%$). We will discuss this effect elsewhere.
[21] The Loschmidt echo decay depends on the direction of