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# Numerical simulations of decoherence suppression in open quantum spin systems *

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**Abstract**

Understanding decoherence in open quantum many-spin systems is important for many fields of physics, from quantum computations (QC) to the nuclear and electronic spin resonance. We use numerical simulations to study some particularly interesting situations where the destructive impact of environment can be suppressed, so that the quantum oscillations in the system fall off very slowly, demonstrating a power-law decay. Such a slow decay may be experimentally relevant for the QC architectures based on electron spins in quantum dots or nuclear spins in semiconductors.

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## 1 Introduction

Recently, much attention has been devoted to the study of quantum computation (QC) [1]. Numerous physical systems have been proposed as promising candidates for implementation of QC, and for many architectures the

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basic quantum gates have been experimentally demonstrated. Among others, the solid-state spin-based QC architectures utilizing e.g. electron spins in quantum dots [2] or nuclear spins in semiconductors [3–5], to mention a few, look particularly promising due to their intrinsic scalability. Also, impressive experimental progress has been achieved recently in controlling and measuring a single spin [6–8]. However, many challenges are yet to be met. To be practical, a quantum computer should contain a large number of qubits (some estimates give up to $10^6$ qubits [9]), and be able to reliably perform many hundreds of quantum gate operations. These requirements are not easy to satisfy in experiments. A real system of quantum spins 1/2 is different from an ideal set of qubits. The system interacts with its environment, and this causes a loss of phase relations between different states of the quantum computer (decoherence) [10–12]. As a result, the system goes from its original pure state into an incoherent mixture of different quantum states, thus leading to rapid generation of errors. A detailed theoretical understanding of the decoherence process is needed for finding the ways to prevent or to suppress the destructive influence of environment.

Moreover, decoherence is an interesting many-body quantum phenomenon which is important for many areas of fundamental and applied physics, from foundations of quantum mechanics [10, 11] to the advanced electron spin resonance (ESR) and nuclear magnetic resonance (NMR) techniques [13, 14]. E.g., interaction of the electon spin with the bath of nuclear spins (one of the most important decoherence sources) leads to broadening of the ESR lines. Interaction of a single atom with the engineered electromagnetic environment leads to the wave function collapse thus quickly destroying the "Schrödinger cat"-type superpositions [15] and quickly bringing the system into a mixture of different quantum states. Even in more conventional solid state systems, decoherence may have considerable consequences, e.g. may suppress the spin tunneling in magnetic molecules and nanoparticles [16, 17], or destroy the Kondo effect in a dissipationless manner [18].

Therefore, it is highly desirable to find ways of suppressing decoherence. One well known approach to this problem is the use of the spin-echo-like techniques [19], where the Hamiltonian of the system is changed in such a manner that the interaction with the environment changes sign, and the unwanted evolution caused by the system-environment interaction is reversed. Extension of the spin-echo-like approach to quantum computations is known as the "bang-bang control" [20]. Here, we consider a similar situation, where the inversion of the system-bath interaction is achieved by static interactions inside the system, instead of periodic field pulses. We show that this, indeed, leads to suppression of the environment-induced evolution, and the decay

of quantum oscillations in the system becomes very slow (power-law). This approach may be experimentally relevant for the QC architectures based on electron spins in quantum dots or impurity spins in semiconductors.

The rest of the paper is organized as follows. Section 2 briefly describes the numerical approach we use for simulation of open many-spin systems. In Section 3, we present the models and the results of our simulations. Section 4 presents our conclusions.

## 2 Numerical approach

The theoretical description of decoherence, i.e. the description of the evolution of the central system from its initial pure state $\psi_0$ to the final mixed state, along with the corresponding transformation of the environment, is a very difficult problem of quantum many-body theory. Some simple models can be solved analytically, for some more complex models different approximations can be employed, such as the Markov approximation (which assumes that the memory effects in the bath dynamics are negligible), or the short-time approximation [21]. A special case of environment consisting of uncoupled oscillators, so-called "boson bath", is also rather well understood theoretically [12]. Although the boson bath description is applicable for many types of environment (phonons, photons, conduction electrons, etc.) [12], it is not universal. A particularly important situation where the boson bath model is inapplicable is the decoherence caused by an enviroment made of spins, e.g. nuclear spins, or impurity spins (so called "spin bath" environment). Analytical studies of the spin-bath decoherence are difficult, and the spin-bath decoherence of many-body systems still remains poorly explored.

The most direct approach to study the spin-bath decoherence is to simulate numerically the evolution of the whole compound system (the central system plus the bath) by directly solving the time-dependent Schrödinger equation of the compound system. This approach allows to avoid any kind of approximation, except for the obvious limitation on the total number of spins modeled. Our previous experience shows that this limitation is not too restrictive, and for many interesting problems reliable simulations can be run with the baths containing only 15–20 spins 1/2 (depending on specific problem). However, even such a modest number of spins requires considerable computational resources, because the dimensionality of the Hilbert space of $N$ quantum spins 1/2 grows very fast (as $2^N$), and because the dynamical evolution of the system should be followed over substantial periods

of time. To make such simulations feasible, high-performance computational schemes are needed.

Here, we use the simulation method based on the Chebyshev's polynomial expansion [22–25]. This approach is applicable when the Hamiltonian is not explicitly dependent on time, and as we have shown before [24, 25], is very efficient for simulating many-spin systems. For time-dependent Hamiltonians, a high-performance method based on the Suzuki-Trotter decomposition [28] can be used [26, 27]. Application of the Chebyshev's polynomial expansion to the modeling of the many-spin systems has been discussed in detail elsewhere [24, 25], and here we give only a brief description of the method.

Let us consider a system of $N$ quantum spins 1/2, which is initially in the state $\Psi_0$, and whose evolution is governed by the time-independent Hamiltonian $\mathcal{H}$. Our goal is to solve efficiently the time-dependent Schrödinger equation

$$i\, d\Psi(t)/dt = \mathcal{H}\Psi(t), \tag{1}$$

i.e. the system of $2^N$ first-order ordinary differential equations with the initial condition $\Psi(t=0) = \Psi_0$. The length of the vector $\Psi$ is $2^N$; for a system of $N = 20$ spins, an exact solution of about $10^6$ differential equations becomes a serious task. Moreover, the interaction between the central spins is often much bigger than the coupling with environment or coupling between the bath spins, so that the system (1) is often stiff. Simple methods, e.g. predictor-corrector schemes, perform rather poorly in this case, and very small integration steps are needed to obtain a reliable solution.

For a time-independent Hamiltonian, the solution of Eq. (1) can be formally written as

$$\Psi(t) = \exp\left(-it\mathcal{H}\right)\Psi_0 = U(t)\Psi_0 \tag{2}$$

where $U(t) = \exp\left(-it\mathcal{H}\right)$ is the evolution operator. An effective way of calculating the exponent of a large matrix $\mathcal{H}$ is to expand it in a series of the Chebyshev polynomials of the operator $\mathcal{H}$. The Chebyshev's polynomials $T_k(x) = \cos\left(k \arccos x\right)$ are defined for $x \in [-1, 1]$. Thus, the Hamiltonian $\mathcal{H}$ first should be rescaled by the factor $E_0$ (the range of the values of the system's energy) and shifted by $E_c$ (median value of the systems' energy). For spin systems, both $E_0$ and $E_c$ can be easily estimated, see [24], to produce the rescaled operator $\mathcal{G} = 2(\mathcal{H} - E_c)/E_0$ bounded by $-1$ and 1. The Chebyshev's expansion of the evolution operator $U(t)$ (see Eq. 2) now looks like

$$U(t) = \exp\left(-i\tau\mathcal{G}\right) = \sum_{k=0}^{\infty} c_k T_k(\mathcal{G}) \tag{3}$$

where $\tau = E_0 t/2$. The expansion coefficients $c_k$ can be calculated using the orthogonal property of the polynomials $T_k(x)$ to give:

$$c_k = \frac{a_k}{\pi} \int_{-1}^{1} \frac{T_k(x) \exp(-ix\tau)}{\sqrt{1-x^2}}\, dx = a_k (-i)^k J_k(\tau), \tag{4}$$

where $J_k(\tau)$ is the Bessel function of $k$-th order, and $a_k = 2$ for $k = 0$ and $a_k = 1$ for $k \geq 1$. The successive terms in the Chebyshev's series can be efficiently determined using the recursion

$$T_{k+1}(\mathcal{G}) = 2\mathcal{G} T_k(\mathcal{G}) + T_{k-1}(\mathcal{G}) \tag{5}$$

with the conditions $T_0(\mathcal{G}) = 1$, $T_1(\mathcal{G}) = \mathcal{G}$. Thus, to find the vector $\Psi(t)$, we just need to sum successively the terms of the series (3), using Eq. (5) for calculation of the subsequent terms, until we reach some pre-defined value $K$ of $k$, which is determined by the required precision. The high efficiency and precision of this scheme is due to the fact that, for $k \gg \tau$, the value of a Bessel function decreases super-exponentially $J_k(\tau) \sim (\tau/k)^k$, so that termination of the series (3) at $k = K$ leads to an error which decreases super-exponentially with $K$; in practice, $K = 1.5\tau$ already gives precision of $10^{-7}$ or better in most cases.

## 3 The model and the results of simulations

It is instructive to start from an exactly solvable, but experimentally relevant model of a single central spin $\mathbf{S}$ ($S = 1/2$) interacting with a bath of nuclear spins $\mathbf{I}_k$ ($I_k = 1/2$), $k = 1, \ldots M$. We assume that a strong quantizing magnetic field is applied to the system (an ESR/NMR-like situation) along the $z$-direction, and an rf field $h$ is applied along the $x$-axis at a frequency $\omega_{rf}$ close to the resonance frequency $\omega_0$ of the central spin (we assume that the $S$ and $I_k$ are "unlike" spins, i.e. they have very different resonance frequencies). In the rotating coordinate frame, after omitting the extremely small non-secular terms [19] in a standard way, the Hamiltonian describing such a situation is

$$\mathcal{H} = \omega S^z + h S^x + \sum_{k=1}^{M} A_k S^z I_k^z \tag{6}$$

where $\omega = \omega_0 - \omega_{rf}$, and the interaction between the nuclear spins $I_k$, which is much smaller than $A_k$, is neglected. E.g., one can think of an electron spin of a phosphorus donor center in the matrix of silicon. The P

electron is delocalized in Si over a range of few tens of the lattice constants, so that the electron spin interacts with many nuclear spins 1/2 of $^{29}$Si (all other Si isotopes have zero nuclear spins). Similar situation is encountered in quantum dots, where the electron is also delocalized in the dot, and the electron spin interacts with the nuclear spins of Ga and As (the fact that the nuclear spins of Ga and As are not 1/2 is not important here). In all these cases, neglecting the interaction between $I_k$ is valid, since the magnitude of these dipolar interactions (few kHz) is 3 orders smaller than $A_k$ (few MHz).

A few remarks are in order here. Decoherence of the P electron spin with the nuclear spins $^{29}$Si has been studied both theoretically and experimentally from early 1960s [29, 30] till very recently [31, 32]. However, the studies we are aware of are focused on "normal" ESR/NMR situation, with either small $h$ (continuous-wave resonance experiments) or strong fields $h$ applied during small time intervals, as in pulsed resonance experiments, free-induction decay (FID) or the spin echo decay (SED). In these cases, the most important physics is connected with the slow dynamics of the bath. Here, we consider a situation of a rather strong ($h^2 \gg \sum_k A_k^2$) constant rf field, and the dynamics of the bath is irrelevant. Also, for an electron spin in a quantum dot, a FID and a SED have been studied [31], and the energy (longitudinal) relaxation of the electron spin by the nuclear spin bath [33]. Again, totally different physical processes have been considered, and we are not aware of the studies of this system with strong constant field $h$.

The model described by the Hamiltonian (6) is exactly solvable due to the fact that the operator $B = \omega + \sum_{k=1}^{M} A_k I_k^z$ commutes with all the terms in the Hamiltonian, and therefore can be treated essentially as a $c$-number (with little precautions). The evolution operator is $U(t) = \cos \Omega t - i(BS^z + hS^x)\Omega^{-1} \sin \Omega t$, where $\Omega = (1/2)[h^2 + B^2]^{1/2}$. The observables of the central spin can be estimated, because the state of the nuclear spins is completely random at the temperature higher than few nK. It is easy to show that in this case, for $2^M \gg 1$, the trace over the bath spins is equivalent to averaging over the Gaussian random field $B$ with zero average and dispersion $b^2 \approx \sum_k (1/4) A_k^2$. Note that $b$ is just a width of the resonance line: it is easy to see that for $h \ll b$, the FID of the central spin demonstrates Gaussian decoherence with the $T_2^*$ time of $1/b$. For P donors in Si the linewidth is 2.5 G, and even for small GaAs quantum dots its value is about 20 G (the linewidth decreases with the dot size), so it is possible to satisfy the condition $h \gg b$ in experiments.

Let us consider the case where $h \gg b$ and $\omega = 0$ (i.e., we are at the center of the resonance line), and the spin $S$ is initially uncorrelated with

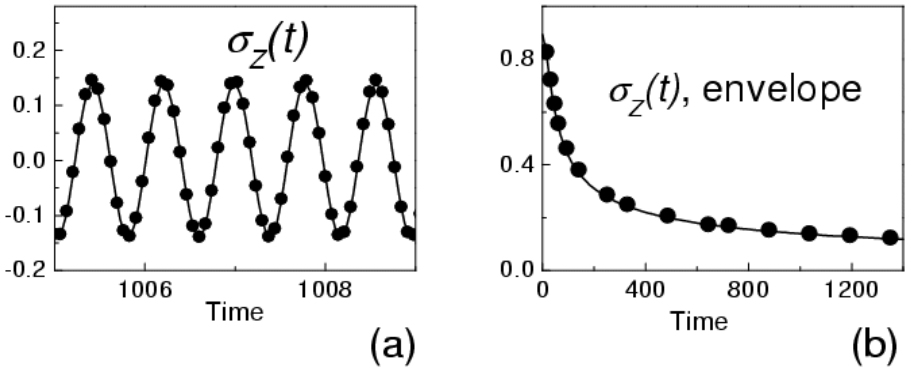


Figure 1: Decoherence of a single spin coupled to a spin bath, comparison of the analytical solution (solid line) with the numerical results (dots) for the envelope of $\sigma^z$ oscillations (b) and for oscillations themselves (a). In (b), most of numerical data points have been removed to make the solid line visible.

the bath. Then for $\sigma^z(t) = 2\langle S^z(t)\rangle$ we have:

$$\sigma^z(t) = \frac{\sigma^z(0)}{\sqrt{2\pi}b}\,\mathrm{Re}\int dB \exp\left[-iht - iB^2t/(2h) - B^2/(2b^2)\right], \qquad (7)$$

and the envelope of the $\sigma^z(t)$ oscillations is

$$\sigma^{(\mathrm{env})z}(t) = \sigma^z(0)\left[1 + (2t/\tau_1)^2\right]^{1/4},$$

where $\tau_1 = 2h/b^2$. Similar results hold also for the $\sigma^y(t) = 2\langle S^y(t)\rangle$ oscillations. Thus, initially there is the usual Gaussian damping (quadratic with time), but afterwards it changes to a slow power-law decay $1/\sqrt{2t/\tau_1}$. We have performed the simulations for the system described above in order to provide cross-check between analytics and numerics. The results of the simulations are shown in Fig. 1 for $M = 14$ bath spins and $h = 2$ (we use dimensionless units for the field, energy and time). Initial state of the central spin is characterized by $\sigma^x(0) = 0.447$, $\sigma^y(0) = 0$ and $\sigma^z(0) = 0.894$, and the initial state of the bath is a superposition of all possible basis states with random coefficients. This state is known [34] to approximate the high-temperature bath's density matrix $\rho = \mathbf{1}_M$ with the error of order of $2^{-M/2}$ (which is less than 1% for $M = 14$), avoiding the use of many realizations of the bath's initial state. The period of the oscillations is much smaller than

the decay time, thus we perform comparison at two different time scales. Fig. 1a shows the results at fine timescale, corresponding to a few oscillations periods. Fig. 1b demonstrates the overall picture of the decay of the oscillations envelope, and the individual oscillations can not be resolved at this coarse timescale. The analytical results for the envelope, and for the oscillations of $\sigma^z(t)$ themselves, coincide perfectly with the numerical simulations.

We have considered the high-temperature case (random unpolarized state of the bath), which is adequate for the bath of nuclear spins at the temperature higher than few nK. For the polarized bath described by the inverse spin temperature $\beta$ (i.e., for the bath's initial state described by the density matrix $\rho_0 = (1/Z)\exp(-\beta\sum_k I_k^z)$), the solution (7) remains valid, although with slightly renormalized temperature-dependent values of $h$ and $b$, and the long-time decay retains $1/\sqrt{t}$ character.

The analytical solution makes clear that the rapidness of the system's dynamics ($h \gg b$ in our case) is needed for long-time oscillations in a decohered system. Fast motion of the system eliminates from the evolution operator the decohering terms which are of first order in the system-bath coupling, and only second-order terms survive, as seen from Eq. 7, and the destructive impact of the spin bath is strongly suppressed, although not eliminated completely, as it would be in the spin echo experiments. On the other hand, the spin echo trains refocus the central spin only for a very short time, of order of the FID time $T_2^*$, after which time the ESR signal disappears again, while for the situation above the Rabi oscillations of the central spin are present constantly.

It is clear from the discussion above that the oscillations in many-spin central systems can also be sustained in a similar manner, by introducing in the spin Hamiltonian the terms which invert the system-bath interaction. In this case, the application of the external rf field $h$ (which may present some technical difficulties) is not necessary. For example, let us consider a central system of two isotropically coupled spins 1/2, $S_1$ and $S_2$:

$$\mathcal{H} = J\mathbf{S_1}\mathbf{S_2} + \sum_{k=1}^{M} A_k S_1^z I_k^z + \sum_{k=1}^{M} C_k S_2^z I_k^z \tag{8}$$

with different couplings between $S_1$ and the bath ($A_k$), and $S_2$ and the bath ($C_k$). This model can describe the two electron spins of P donors in Si coupled by applying the voltage to an external gate, as in Ref. [3], or the electon spins in two coupled quantum dots. This model is hard to solve explicitly, and we use numerical simulations to study this case for

different system parameters. Fig. 2 presents typical simulations results for the envelope of the $\sigma_1^z(t)$ oscillations (the envelope $\sigma_2^z(t)$ is identical to $\sigma_1^z(t)$), for $M = 14$ and $J = 1.0$. The central system initially was disentangled from the bath, with the spin $S_1$ directed up and $S_2$ directed down. Note that the difference between $A_k$ and $C_k$ is not important for $J \gg A_k, C_k$. One can see that again, the oscillations of the central spins decay very slowly, in a power-law $t^{-1/2}$ manner.

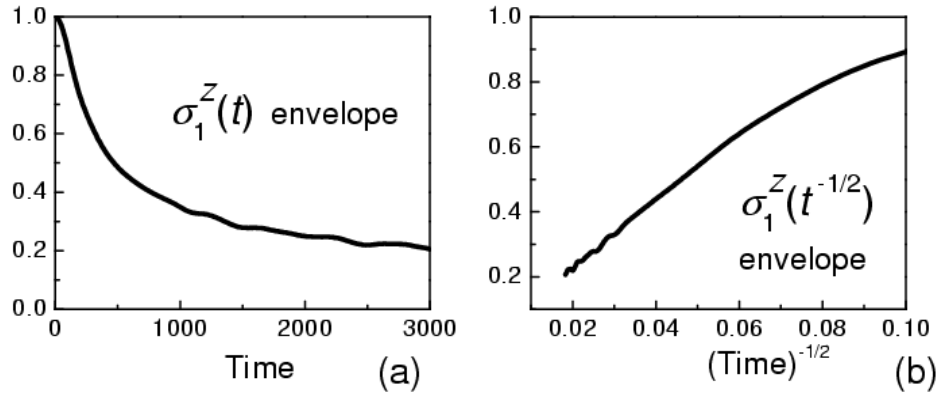


Figure 2: Decoherence of a two-spin system coupled to the spin bath. (a) The envelope of the $\sigma_1^z$ oscillations vs. time. (b) The envelope of the the $\sigma_1^z$ oscillations plotted vs. $1/\sqrt{t}$; the long-time power-law decay $t^{-1/2}$ is seen: the calculated points lay on the straight line for small values of the abscissas, which corresponds to large $t$.

Using the values of $b$ (given above) for P donor electron in Si, and for an electron in small GaAs quantum dots, it seems possible to satisfy the condition $J \gg b$ in experiments.

## 4 Conclusions

We use numerical simulations to study how the destructive impact of environment on an open many-spin system can be suppressed. The dynamics has been simulated by directly solving the time-dependent Schrödinger equation for the compound system (the central system plus the environment). We consider a situation similar to the "bang-bang control", where the static interactions inside the central system invert the system-bath coupling,

and show that this leads to suppression of the environment-induced evolution. The decay of quantum oscillations in the system becomes very slow (power-law $t^{-1/2}$). This approach may be experimentally relevant for the QC architectures based on electron spins in quantum dots or impurity spins in semiconductors.

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