Efficient scheme for numerical simulations of the spin-bath decoherence

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We demonstrate that the Chebyshev expansion method is a very efficient numerical tool for studying spin-bath decoherence of quantum systems. We consider two typical problems arising in studying decoherence of quantum systems consisting of a few coupled spins: (i) determining the pointer states of the system and (ii) determining the temporal decay of quantum oscillations. As our results demonstrate, for determining the pointer states, the Chebyshev-based scheme is at least a factor of 8 faster than existing algorithms based on the Suzuki-Trotter decomposition. For problems of the second type, the Chebyshev-based approach is 3–4 times faster than the Suzuki-Trotter-based schemes. This conclusion holds qualitatively for a wide spectrum of systems, with different spin baths and different Hamiltonians.

I. INTRODUCTION

Recently, a great deal of attention has been devoted to the study of quantum computation [1,2]. For many physical systems, basic quantum operations needed for implementation of quantum gates have been demonstrated. To be practical, a quantum computer should contain a large number of qubits (some estimates give up to 10^6 qubits [3]) and be able to perform many hundreds of quantum gate operations. However, these requirements are not easy to satisfy in experiments. A real two-state quantum system is different from the ideal qubit. The system interacts with its environment, and this leads to a loss of phase relations between different states of the quantum computer (decoherence) [4–7], causing rapid accumulation of errors. Detailed theoretical understanding of the decoherence process is needed to prevent this.

More generally, decoherence is an interesting many-body quantum phenomenon which is fundamental for many areas of quantum mechanics, quantum measurement theory, etc. [4,5]. It also plays an important role in solid state systems and might suppress quantum tunneling of defects in crystals [7] and spin tunneling in magnetic molecules and nanoparticles [8,9], or destroy the Kondo effect in a dissipationless manner [10]. That is, decoherence in many physical systems can have experimentally detectable (and sometimes considerable) consequences, and extensive theoretical studies of decoherence are needed to understand the behavior of these systems.

Formally speaking, decoherence is a dynamical development of quantum correlations (entanglement) between central system and its environment. Let us assume that initially the central system is in the state $|\psi_0\rangle$ and the environment is in the state $|\chi_0\rangle$, so that the state of the compound system (central system plus bath) is $|\Psi(t=0)\rangle = |\psi_0\rangle \otimes |\chi_0\rangle$. In the course of dynamical evolution, the direct product structure of the state $|\Psi(t)\rangle$ is no longer conserved. If we need to study only the properties of the central system, we can consider the reduced density matrix of the central system, i.e., the matrix $\rho_S(t) = \mathrm{Tr}_B |\Psi(t)\rangle \langle \Psi(t)|$, where Tr_B means tracing over the environmental degrees of freedom. Initially, $\rho_S(0) = |\psi_0\rangle \langle \psi_0|$, the system is in a pure state, and

its density matrix is a projector, i.e., $\rho_S^2(0) = \rho_S(0)$. At $t>0$, this property is lost, and the system appears in a mixed state. It has been shown that, even for relatively small integrable and nonintegrable systems, the mixing is sufficient for the time-averaged, quantum dynamical properties of the subsystem to agree with their statistical mechanics values [11]. Diagonalizing the density matrix ρ_S, we can find the (instantaneous) states of the system $|q_i(t)\rangle$ and (instantaneous) occupation numbers of these states $w_i(t)$. It is generally assumed (and is true for all cases we know) that in "regular" situations, the states $|q_i(t)\rangle$ quickly relax to some limiting states $|p_i\rangle$, called "pointer states." This process (decoherence) is, in most cases, much faster than the relaxation of the occupation numbers $w_i(t)$ to their limiting values (which correspond to thermal equilibrium of the system with the bath).

The theoretical description of decoherence, i.e., a description of the evolution of the central system from its initial pure state ψ_0 to the final mixed state, and finding the final pointer states $|p_i\rangle$, 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 for the bath, which assumes that the memory effects in the bath dynamics are negligible. The special case of the environment consisting of uncoupled oscillators, the so-called boson bath, is also rather well understood theoretically. But, although the model of the boson bath is applicable for description of a large number of possible types of environments (phonons, photons, conduction electrons, etc.) [7], it is not universal.

A particularly important case where the boson bath description is inapplicable is the decoherence caused by an environment made of spins, e.g., nuclear spins or impurity spins (the so-called spin-bath environment). Similarly, decoherence caused by some other types of quantum two-level systems can be described in terms of the spin bath. Analytical studies of the spin-bath decoherence are difficult, and the spin-bath decoherence of many-body systems is practically unexplored yet. In this situation, numerical modeling of spin-bath decoherence becomes an invaluable research tool.

The most direct approach to studying spin-bath decoherence is to compute the dynamical evolution of the whole compound system by directly solving the time-dependent Schrödinger equation of the model system. Even for a modest number of spins, say 20, such calculations require considerable computational resources, in particular because to study decoherence we have to follow the dynamical evolution of the system over substantial periods of time. Therefore it is worthwhile to explore ways to significantly improve the efficiency of these simulations.

In this paper, we apply the Chebyshev expansion method to simulate models for the spin-bath decoherence. This method has been widely applied before [12–18] to study the dynamics of large quantum systems, but, to our knowledge, has never been used for simulations of systems made of large numbers of coupled quantum spins. We show that for realistic problems and typical values of parameters this method is a very efficient tool. We compare this approach with algorithms based on the Suzuki-Trotter decomposition [21] and the short-time iterative Lanczos (SIL) method [14,22,23]. We find that for a large class of problems relevant for decoherence studies, the Chebyshev polynomial expansion method gives a significant increase in the simulation speed, sometimes up to a factor of 8, in comparison with algorithms [19,20] based on Suzuki-Trotter decompositions [21]. We illustrate this point by test examples that we have encountered in our previous studies of the dynamics of spin-bath decoherence. We also find that the short-time iterative Lanczos method is significantly slower than both Suzuki-Trotter and Chebyshev's methods.

The remainder of the paper is organized as follows. In Sec. II, we describe the model and the approaches used for the decoherence simulations. In Sec. III, we describe the specific details of application of Chebyshev's expansion method to the spin-bath decoherence simulations. In Sec. IV, we present the results of our test simulations. A brief summary is given in the Sec. V.

II. SIMULATIONS OF THE SPIN-BATH DECOHERENCE: THE MODEL AND NUMERICAL APPROACHES

We focus on decoherence in quantum systems of several coupled spins. This type of quantum system is of particular interest for quantum computations, since a qubit can be represented as a quantum spin 1/2, and qubit-based quantum computation is, in fact, the controlled dynamics of a system made of many spins 1/2. Such systems are also of primary interest for studying many solid state problems, since an electron is a particle with spin 1/2, and its orbital degrees of freedom are often irrelevant. Thus, a system made of several coupled spins 1/2 is a good model for investigating a large class of important problems both in quantum computing and in solid state theory. The approach described below can be easily extended to arbitrary spin values, but discussion of simulations with arbitrary spins is beyond the scope of this paper.

We consider the following class of models. There is a central system made of M coupled spins $\mathbf{S}_m$ ($S_m = 1/2$, $m = 1, \ldots, M$). The spins $\mathbf{S}_m$ interact with a bath consisting of

N environmental spins $\mathbf{I}_n$ ($I_n = 1/2$, $n = 1, \ldots, N$). The Hamiltonian governing behavior of the whole "compound" system (the central spins $\mathbf{S}_m$ plus the bath spins $\mathbf{I}_n$) 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 "bare" Hamiltonians of the central system and the bath, respectively, and $\mathcal{V}$ is the system-bath interaction. Below, we present simulation results for the following general forms of the Hamiltonians:

$$\mathcal{H}_S = \sum_{\langle m,m' \rangle} \sum_{\alpha=x,y,z} J^\alpha_{mm'} S^\alpha_m S^\alpha_{m'} + \sum_m \sum_{\alpha=x,y,z} H^\alpha_m S^\alpha_m,$$

$$\mathcal{H}_B = \sum_{\langle n,n' \rangle} \sum_{\alpha=x,y,z} \Gamma^\alpha_{nn'} I^\alpha_n I^\alpha_{n'} + \sum_n \sum_{\alpha=x,y,z} H^\alpha_n I^\alpha_n,$$

$$\mathcal{V} = \sum_{\langle m,n \rangle} \sum_{\alpha=x,y,z} A^\alpha_{mn} S^\alpha_m I^\alpha_n. \tag{2}$$

We assume that the Hamiltonian $\mathcal{H}$ does not explicitly depend on time, i.e., all exchange interaction constants J, Γ, and A, and all external magnetic fields $\mathbf{H}$ are constant in time. Although this makes it impossible to model a time-dependent quantum gate operation, the investigation of the fundamental properties of spin-bath decoherence is not seriously affected by this requirement. The dynamics of the model (1) is already too complex to be studied analytically, and for general $\mathcal{H}$, when no *a priori* knowledge is available, the only option is to solve the time-dependent Schrödinger equation of the whole compound system numerically. That is, we choose some basis states for the Hilbert space of the compound system (the simplest choice is the direct product of the states $|\uparrow\rangle$ and $|\downarrow\rangle$ for each spin $\mathbf{S}_m$, $\mathbf{I}_n$). We represent an initial state of the compound system Ψ_0 as a vector in this basis set, and the Hamiltonian $\mathcal{H}$ is represented as a matrix, so that the Schrödinger equation

$$i d\Psi(t)/dt = \mathcal{H}\Psi(t) \tag{3}$$

is a system of first-order ordinary differential equations with the initial condition $\Psi(t=0) = \Psi_0$.

The length of the vector Ψ is 2^{M+N}; for typical values $M = 2$ and $N = 20$, an exact solution of about 4×10^6 differential equations becomes a serious task. Moreover, the interaction between the central spins is often much bigger than the coupling with the environment or coupling between the bath spins, so that the system (3) 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.

Algorithms based on the Suzuki-Trotter decomposition [19,20] can solve Eq. (3) for sufficiently long times (essential to determine the pointer states of the central system). They can handle Hamiltonians with explicit dependence on time, are unconditionally stable, exactly preserve the unitarity of quantum evolution, and the time step can be made more than an order of magnitude bigger than in the typical predictor-corrector method. Moreover, as our experience shows, for a

scheme based on the Suzuki-Trotter decomposition, a large part of the total numerical error is accumulated in the total phase of the wave function $|\Psi(t)\rangle$, and does not affect any measurable physical quantities (observables). However, for reasonably large systems, this scheme is still slow, and simulations of decoherence last for up to 200 CPU hours on a SGI 3800 supercomputer. The problem of long simulation times becomes especially prominent if we need to find the pointer states, or if the dynamics of the central system is much faster than the decoherence rate. We found that in these circumstances the method based on Chebyshev's expansion becomes a very efficient tool to study problems of decoherence.

Along with the Chebyshev expansion method, the short iterative Lanczos approach [14,22,23], which is also based on the power-series expansion of the evolution operator, was found to be efficient for many similar problems of quantum chemistry. We have tested this method, but our results are negative. The low-order SIL method (with a small number of Lanczos iterations per step, usually less than 25) gives an unacceptable error, even for very short time steps. On the other hand, the high-order SIL method (with more than 25 Lanczos iterations per step) is noticeably slower than the approach based on Chebyshev's expansion. We believe that the poor performance of the SIL method originates from the fact that for a small number of Lanczos iterations (i.e., for the low-order SIL method), only a very limited part of the spectrum is described correctly. For a typical problem where the SIL method is known to be very effective (e.g., wave packet propagation), most of the relevant basis states have energy close to the energy of a wave packet. Only these relevant states should be accurately described, while an accurate description of the whole energy spectrum is excessive. In contrast, in a typical spin-bath decoherence problem, a large number of bath states with very different energies are involved in the decoherence process. Correspondingly, a large part of the spectrum should be taken into account, and the high-order SIL integrator should be employed, reducing the performance of the SIL method.

Significant speed-up can be achieved by employing a radically different approach, by using an approximate form of the wave function of the total system (central system plus bath). In particular, the multiconfigurational time-dependent Hartree (MCTDH) method [24–26] is known to be very efficient, e.g., for modeling boson-bath decoherence. The MCTDH approach uses an approximate representation of the wave function, based on the assumption that the wave function of the total system can be written as a superposition of a relatively small number of "configurations," i.e., products of time-varying spin wave functions. The MCTDH method is the method of choice when the dimensionality of a single-particle Hilbert space is large, and the multiparticle quantum correlations are associated with a superposition of a small number of products of single-particle wave functions. The problems considered in our paper present an opposite situation. The bath consists of many spins 1/2, i.e., we have only two orbitals per particle (spin), and the single-particle evolution is very simple, while the complex many-particle quantum correlations are responsible for most of the physical effects (i.e., the number of important single-spin wave functions products is very large). It is probable that many problems of spin-bath decoherence can be efficiently treated by the MCTDH method, but the corresponding study requires a separate extensive research effort, which is beyond the framework of our paper.

III. CHEBYSHEV'S METHOD FOR SPIN-BATH DECOHERENCE

For a time-independent Hamiltonian, the solution of Eq. (3) can be formally written as

$$\Psi(t) = \exp(-it\mathcal{H})\Psi_0 = U(t)\Psi_0, \qquad (4)$$

where $U(t) = \exp(-it\mathcal{H})$ is the evolution operator. An effective way [12–18] of calculation of the exponent of a large matrix $\mathcal{H}$ is to expand it in a series of the Chebyshev polynomials of the operator $\mathcal{H}$. Below, we describe the specific details of application of the Chebyshev method to spin-bath decoherence simulations.

The Chebyshev polynomials $T_k(x) = \cos(k \arccos x)$ are defined for $x \in [-1,1]$. Thus, the Hamiltonian $\mathcal{H}$ first should be rescaled by the factor E_0 (the range of values of the system's energy) and shifted by E_c (median value of the system's energy):

$$E_c = \frac{1}{2}(E_{max} + E_{min}), \quad E_0 = E_{max} - E_{min},$$

$$E_{min} = \min\langle\mathcal{H}\rangle = \min_{\langle\Phi|\Phi\rangle=1} \langle\Phi|\mathcal{H}|\Phi\rangle,$$

$$E_{max} = \max\langle\mathcal{H}\rangle = \max_{\langle\Phi|\Phi\rangle=1} \langle\Phi|\mathcal{H}|\Phi\rangle. \qquad (5)$$

In this way, the rescaled operator $\mathcal{G} = 2(\mathcal{H} - E_c)/E_0$ is also bounded by -1 and 1: $-1 \leq \langle\mathcal{G}\rangle \leq 1$, i.e., $-1 \leq \langle\Phi|\mathcal{G}|\Phi\rangle \leq 1$ for any state vector $|\Phi\rangle$ such that $\langle\Phi|\Phi\rangle = 1$. For spin systems, the Hamiltonian is bounded both from above and from below, and the operator $\mathcal{G}$ can be found.

In the specific case considered in this paper, when the Hamiltonian $\mathcal{H}$ is defined by Eq. (2), we take $E_0 = 2\max(|E_{min}|, |E_{max}|)$. For this choice, $-E_0/2 \leq \langle\mathcal{H}\rangle \leq E_0/2$. Correspondingly, we can take $E_c = 0$; this choice is legitimate, and, although it might be not optimal for some problems, it still results in very good performance of Chebyshev's method (see below). Since $\max\langle\mathcal{H}\rangle = \|\mathcal{H}\|$ is the norm of the Hamiltonian, the value of E_0 can be estimated using Cauchy's inequality: $E_0/2 \leq \|\mathcal{H}_S\| + \|\mathcal{H}_B\| + \|\mathcal{V}\|$. Similarly,

$$\|\mathcal{H}_S\| \leq \sum_{\langle m,m'\rangle} \sum_{\alpha=x,y,z} |J_{mm'}^\alpha| \|S_m^\alpha\| \|S_{m'}^\alpha\|$$

$$+ \sum_m \sum_{\alpha=x,y,z} |H_m^\alpha| \|S_m^\alpha\|$$

$$= \sum_{\langle m,m'\rangle} \sum_{\alpha=x,y,z} \frac{1}{4}|J_{mm'}^\alpha| + \sum_m \sum_{\alpha=x,y,z} \frac{1}{2}|H_m^\alpha|, \quad (6)$$

and $\|\mathcal{H}_B\|$ and $\|\mathcal{V}\|$ can be estimated in the same manner. As a result, we have an estimate $E_0 \lesssim E_1$, where

$$E_1 = \sum_{\langle m,m' \rangle} \sum_{\alpha=x,y,z} \frac{1}{2} |J^\alpha_{mm'}| + \sum_{\langle n,n' \rangle} \frac{1}{2} |\Gamma^\alpha_{nn'}| + \sum_{\langle m,n \rangle} \frac{1}{2} |A^\alpha_{mn}|$$

$$+ \sum_m |H^\alpha_m| + \sum_n |H^\alpha_n|, \qquad (7)$$

and the operator $\mathcal{G}$ can be defined as $\mathcal{G} = 2\mathcal{H}/E_1$, which satisfies the inequality $-1 \leq \langle \mathcal{G} \rangle \leq 1$.

The Chebyshev expansion of the evolution operator $U(t)$ [see Eq. (4)] now looks like

$$U(t) = \exp(-i\tau\mathcal{G}) = \sum_{k=0}^{\infty} c_k T_k(\mathcal{G}), \qquad (8)$$

where $\tau = E_1 t/2$. The expansion coefficients c_k can be calculated using the orthogonal property of the polynomials $T_k(x)$:

$$c_k = \frac{a_k}{\pi} \int_{-1}^{1} \frac{T_k(x)\exp(-ix\tau)}{\sqrt{1-x^2}} dx = a_k(-i)^k J_k(\tau), \quad (9)$$

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

$$T_{k+1}(\mathcal{G}) = 2\mathcal{G}T_k(\mathcal{G}) - T_{k-1}(\mathcal{G}) \qquad (10)$$

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 (8), using Eq. (10) for calculation of the subsequent terms, until we reach some predefined value K of k, which is determined by the required precision.

The high precision of this scheme originates from the fact that, for $k \gg \tau$, the value of a Bessel function decreases superexponentially $J_k(\tau) \sim (\tau/k)^k$, so that termination of the series (8) at $k = K$ leads to an error that decreases superexponentially with increasing K. In practice, $K = 1.5\tau$ already gives a precision of 10^{-7} or better in most cases. For the same reason, this scheme is asymptotically more efficient than any time-marching scheme. For given sufficiently small error ϵ, the number of operations N_{op} needed for finding the wave function at time T, i.e., $\Psi(T)$, grows linearly with T for the Chebyshev-based scheme. For a marching scheme of order r with the time step Δt, the numerical error is $\epsilon \sim (\Delta t)^r T$, so that for given ϵ and T, the number of operations needed is $N_{op} = T/\Delta t \sim T^{1+1/r}$, growing superlinearly with increasing T. For very long-time simulations, and when very high precision is necessary, the Chebyshev method is more efficient than any time-marching scheme known to us. However, in practice, a precision better than 0.5–1 % is very rarely needed. Similarly, very long-time simulations are rarely of interest: in most cases, the simulations are interesting only until the dynamics of the system exhibits some nontrivial behavior. Therefore, in spite of its asymptotic effi-
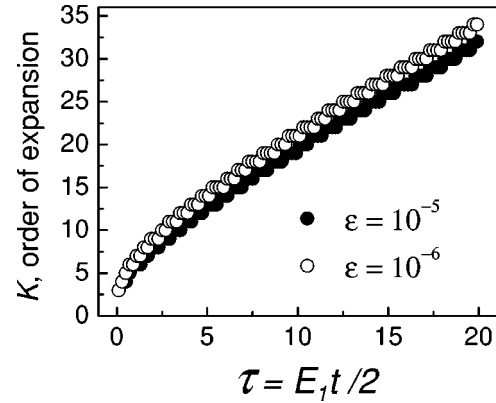

FIG. 1. Dependence of the order of the Chebyshev expansion K on the value of $\tau = E_1 t/2$. The solid circles correspond to the minimum value $\epsilon = 10^{-5}$ of the expansion coefficient c_k; the open circles correspond to $\epsilon = 10^{-6}$.

ciency, the Chebyshev method is not always the best choice for real research, and its efficiency should be studied in every separate case.

IV. SIMULATION RESULTS

We assess the usefulness of the Chebyshev method for a wide spectrum of decoherence problems, by considering two central problems of decoherence, the description of damping of quantum oscillations in a system, and determination of the pointer states. In fact, there is no strict boundary: in studying both problems, we track the evolution of the system, checking its state at regular intervals of length T, but in studying the oscillation decay the interval T is much smaller than the characteristic decoherence time T_{dec}, while in studying the pointer states, T is larger than T_{dec}.

In spite of the asymptotic advantages of the Chebyshev-based scheme, it is not *a priori* clear if it is efficient for realistic problems, when the required numerical error δ is modest (say, $\delta = 10^{-2} - 10^{-3}$). Also, if we track the dynamics of the decoherence process, we make many steps of modest length T, and the overhead associated with the use of the Chebyshev expansion might be significant (see Fig. 1).

To study this issue, we have performed several types of numerical tests. The timing information reported in this paper has been obtained from calculations on a SGI Origin 3800 (500 MHz) system, using sequential, single-processor code. The order of Chebyshev's expansion K has been defined by the prespecified precision ϵ. We determined the minimum value of K such that $|c_k| < \epsilon$ for $k \geq K$, starting from the value $K_0 = [1.1\tau]$ ([x] is the integer part of x), and adjusting it as needed. Each simulation has been performed three times: (i) using the Chebyshev method with $\epsilon = 10^{-12}$, the reference run, (ii) using Chebyshev's method with $\epsilon = 10^{-5} - 10^{-6}$, and (iii) using the scheme based on Suzuki-Trotter decomposition [19,20]. Previously we have used the latter to study spin-bath decoherence [10,27]. In this paper, we have chosen to consider the same problems as in our previous work on this subject, in order to avoid the impression that the tests have been constructed to favor one particular method.
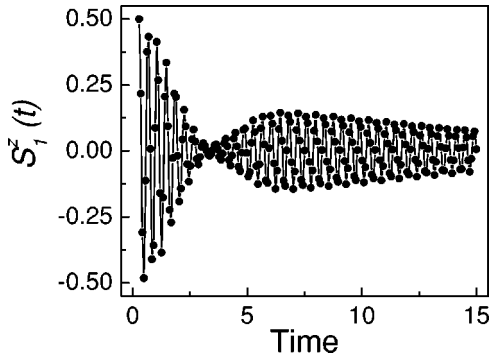
FIG. 2. Time dependence of the oscillations of the expectation value of $S_1^z(t)$ in the two-spin system decohered by a spin bath.

First, we consider the problem of oscillations damping in the central system of two spins coupled by Heisenberg exchange, interacting with the bath. We studied this problem using the Suzuki-Trotter scheme in Ref. [27]. The Hamiltonians describing the bath and the system are

$$\mathcal{H}_S = J\mathbf{S}_1 \cdot \mathbf{S}_2, \quad \mathcal{H}_B = 0, \quad \mathcal{V} = \sum A_n(\mathbf{S}_1 + \mathbf{S}_2)\cdot \mathbf{I}_n, \quad (11)$$

with $N = 16$ bath spins. The exchange parameter $J = 16.0$ (antiferromagnetic coupling between the central spins), while A_n are uniformly distributed between 0 and -0.5. The initial state of the compound system $|\Psi_0\rangle = |\psi_0\rangle \otimes |\chi_0\rangle$ is the product of the initial state $|\psi_0\rangle$ of the central system, and $|\chi_0\rangle$ of the bath. In this case, $|\psi_0\rangle = |\uparrow\downarrow\rangle$, i.e., the first central spin is in the state $S_1^z(t=0) = +1/2$, and the second spin is in the state $S_2^z(t=0) = -1/2$. The initial state of the bath $|\chi_0\rangle$ is the linear superposition of all basis states with random coefficients. Physically, this situation corresponds to the case of the temperature θ which is high in comparison with the bath energies A_n, but is much lower than the system's energy J (note that $J \gg A_n$ in this case).

The initial state of the central system is a superposition of two eigenstates of $\mathcal{H}$: the state with the total spin $S=1$ and $S_z=0$, and the state with the total spin $S=0$. These states have different energies, and, for example, the dynamics of $S_1^z(t)$ is represented by oscillations with the frequency J. Due to interaction with the spin bath, these oscillations are damped (see Fig. 2). To study this damping in detail, we take the Suzuki-Trotter time step $\Delta t = 0.035$, $T = 2\Delta t$, and watch the system from $t=0$ until $t_{max} = 800T$. If we do not need

such a high resolution, we increase T. In Table I, we present the CPU time needed to perform the simulations using the Suzuki-Trotter and Chebyshev methods, along with the resulting error δ (which should not be confused with the "nominal" precision of the Chebyshev scheme, ϵ). The error δ has been obtained from comparison with the "reference" Chebyshev run ($\epsilon = 10^{-12}$), and is equal to the maximum of the absolute errors of the quantities (all normalized to unity) $2S_1^\alpha$, $2S_2^\alpha$, $4S_1^\alpha S_1^\beta$ ($\alpha, \beta = x, y, z$), and the so-called "quadratic entropy" [28] $S^{(2)} = 1 - \text{Tr}\,\rho_S^2$. These quantities have been calculated and compared at regular intervals of length T. Their calculation increases the number of computations, so that the tests 1, 2, and 3, which are otherwise equivalent for the Suzuki-Trotter method, require more and more CPU time.

As one can see from Table I, for realistic values of the maximum error $\delta \sim 0.5 \times 10^{-2}$, and even for not very long runs, the Chebyshev scheme can be faster than the Suzuki-Trotter method by a factor of up to 4, and the efficiency of the Chebyshev scheme grows fast with increasing T. However, this straightforward comparison is too crude, and Table I is only an illustration of basic features of the Chebyshev method. To model fast oscillations which decay slowly (often with a decay time of the order of the decoherence time T_{dec}), we should make T significantly smaller than the oscillation period $t_{osc} = 2\pi/J$, in order to correctly determine the amplitude of oscillations at a given time.

Therefore, to track the damping of oscillations, we use the two-leap approach: first, we make a large time leap of length T_1 ($T_1 \gg t_{osc}$, but $T_1 \ll T_{dec}$), and then we make a number n_2 (usually 15–20) of smaller steps T_2 such that $T_2 \ll t_{osc}$ but $n_2 T_2 \gtrsim t_{osc}$, resolving in detail one period of oscillations and extracting the amplitude. By repeating this two-stage sequence n_{tot} times, we can reliably track the change of the oscillation amplitude with time. The test examples of this approach have been taken from our recent work [29]. We have performed the same kind of simulations as described above, with $N = 16$ bath spins, repeating the two-leap sequence $n_{tot} = 8$ times, each time making one long leap T_1 followed by $n_2 = 21$ short leaps T_2. The results of these tests are presented in Table II. Again, the Chebyshev-based method can be up to three times faster than the Suzuki-Trotter algorithm [19,20].

Finally, we have tested the Chebyshev scheme in the problem of determining the pointer states, employing an example from our work [10]. This example is interesting also

TABLE I. Comparison of the Suzuki-Trotter scheme (abbreviated as ST) with the Chebyshev scheme (abbreviated as Ch) for the problem of oscillation decay.

Test	Δt	T	t_{max}	δ	ϵ	CPU time
1, Ch		$200\Delta t$	$8T$	1×10^{-5}	10^{-6}	22 min
1, ST	0.035	$200\Delta t$	$8T$	0.44×10^{-2}		80 min
2, Ch		$8\Delta t$	$200T$	0.3×10^{-4}	10^{-6}	59 min
2, ST	0.035	$8\Delta t$	$200T$	0.48×10^{-2}		89 min
3, Ch		$2\Delta t$	$800T$	0.55×10^{-3}	10^{-6}	226 min
3, ST	0.035	$2\Delta t$	$800T$	0.48×10^{-2}		156 min

TABLE II. Comparison of the Suzuki-Trotter scheme (abbreviated as ST) with the Chebyshev scheme (abbreviated as Ch) for the problem of oscillation decay, employing the two-leap approach with different T_1 and T_2.

Test	Δt	T_1	T_2	δ	ϵ	CPU time
4, Ch		$150\Delta t$	Δt	0.4×10^{-4}	10^{-6}	61 min
4, ST	0.02	$150\Delta t$	Δt	0.2×10^{-2}		144 min
5, Ch		$300\Delta t$	Δt	0.4×10^{-4}	10^{-6}	75 min
5, ST	0.02	$300\Delta t$	Δt	0.3×10^{-2}		221 min

because it deals with the physically important case of a spin bath possessing chaotic internal dynamics, which is relevant for the majority of realistic spin baths (such as nuclear spins or impurity spin baths). The Hamiltonian describing the system is

$$\mathcal{H}_S = J\mathbf{S}_1 \cdot \mathbf{S}_2, \quad \mathcal{V} = \sum A_n \mathbf{S}_1 \cdot \mathbf{I}_n, \tag{12}$$

i.e., the bath spins are coupled only with the first central spin, and the bath Hamiltonian is now

$$\mathcal{H}_B = \sum_n h_z I_k^z + \sum_{\langle n,n' \rangle} U_{nn'} I_n^x I_{n'}^x. \tag{13}$$

In our simulations we used $h = 0.1$ and $U_{nn'}$ randomly distributed in the interval $[-0.013, 0.013]$. This Hamiltonian is known to result in stochastic behavior [30]; we have checked the level statistics independently, and found that it closely follows the Wigner-Dyson distribution.

To determine the pointer states, we need to find the elements of the reduced density matrix $\rho_S(t)$ in the long-time limit $t \to \infty$. We start at $t = 0$ from the state of the compound system which is the product of the states of the bath and the central system (as above), but the initial state of the central spins now is the singlet $|\psi_0\rangle = (1/\sqrt{2})[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]$. Because of decoherence, the final state of the central system is mixed, and $\rho_S = w_1 |p_1\rangle\langle p_1| + w_2 |p_2\rangle\langle p_2|$, where $|p_1\rangle$ and $|p_2\rangle$ are the pointer states, which are superpositions of the states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ $|\uparrow\downarrow\rangle$, and $|\downarrow\uparrow\rangle$. As we found in [10], the form of this superposition is determined by the ratio J/b, where $b = \sum_n A_n^2$. For $J/b \sim 1$, the pointer states are very close to the singlet $S = 0$ and triplet $S = 1$, $S_z = 0$ states, and for $J \ll b$, the pointer states are close to $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$. Thus, the quantities characterizing the type of the pointer state are the values of the nondiagonal elements of the density matrix ρ_S in the basis $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ $|\uparrow\downarrow\rangle$, and $|\downarrow\uparrow\rangle$. In particular, the element $\rho_S^{12} = \langle\uparrow\downarrow|\rho_S|\downarrow\uparrow\rangle$ is a very suitable quantity to characterize the pointer state. This nondiagonal element is close to zero for $J \ll b$, and gradually increases in absolute value with increasing J.

Typical results for temporal evolution of the elements of the density matrix ρ_S are shown in Fig. 3. One can see that in this situation we *do not* need to use the two-leap approach with different T_1 and T_2. The relaxation (after some initial period) is slow, and no fast oscillations of considerable amplitude exist at long times, so that the one-leap approach is sufficient. Thus, the efficiency of the Chebyshev-based

scheme is expected to be very good. This is indeed the case, as Table III demonstrates. The results presented there correspond to $J = 0.1$. The Chebyshev-based scheme is faster than the Suzuki-Trotter method by up to a factor of 8.

We checked our conclusions on many other cases, with the central systems made of up to $M = 4$ spins, and with the baths made of up to $N = 22$ spins, with different Hamiltonians and different values of the Hamiltonian parameters. We found that the Chebyshev-based method gives a significant increase in the simulation speed for all problems where the value of T can be made sufficiently large.

V. SUMMARY

Theoretical studies of spin-bath decoherence are important for many areas of physics, including quantum mechanics and quantum measurement theory, quantum computing, solid state physics, etc. Decoherence is a complex many-body phenomenon, and numerical simulation is an important tool for its investigation. In this paper, we studied the efficiency of a numerical scheme based on the Chebyshev expansion. We presented specific details of the application of this method to spin-bath decoherence modeling. To assess the efficiency of the simulation method, we used model problems which we have encountered in our previous studies of
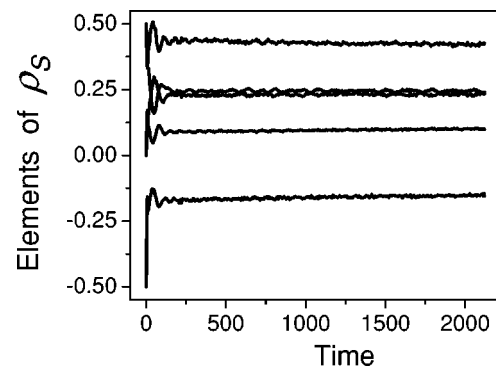

FIG. 3. Temporal evolution of different elements of the density matrix ρ: diagonal elements corresponding to the states $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$ (the four upper curves), and the nondiagonal element ρ_S^{12} (the lowest curve). Very slow relaxation is better seen for the uppermost curve (the diagonal element corresponding to the state $|\uparrow\uparrow\rangle$) which has a small negative slope. Note that the two lines in the middle (the second and the third lines from the top, the diagonal elements corresponding to the states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$, respectively) are very close to each other at $t \gtrsim 200$, as expected for a near-equilibrium (although not completely relaxed) situation.

TABLE III. Comparison of the Suzuki-Trotter scheme (abbreviated as ST) with the Chebyshev scheme (abbreviated as Ch) for the problem of determining the pointer states.

Test	Δt	T	t_{max}	δ	ϵ	CPU time
6, Ch		$100\Delta t$	$500T$	0.2×10^{-3}	10^{-6}	19 min
6, ST	0.14	$100\Delta t$	$500T$	0.7×10^{-2}		105 min
7, Ch		$10\Delta t$	$5000T$	0.1×10^{-2}	10^{-6}	52 min
7, ST	0.14	$10\Delta t$	$5000T$	0.8×10^{-2}		117 min
8, Ch		$1000\Delta t$	$50T$	0.3×10^{-6}	10^{-6}	13 min
8, ST	0.14	$1000\Delta t$	$50T$	0.8×10^{-2}		107 min

spin-bath decoherence. We compared the Chebyshev-based scheme with a fast method based on the Suzuki-Trotter decomposition. We found that in many cases the former gives a considerable increase in the speed of simulations, sometimes by up to a factor of 8 (for the problem of finding the system's pointer states), while in studying the decoherence dynamics, the increase in speed is less drastic (a factor of 2–3), but still considerable. This conclusion holds for many types of central systems and spin baths, with different Hamiltonians.

[1] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2000).

[2] D. P. DiVincenzo, e-print quant-ph/0002077.

[3] J. Preskill, Proc. R. Soc. London, Ser. A **454**, 385 (1998).

[4] *Decoherence: Theoretical, Experimental and Conceptual Problems*, edited by Ph. Blanchard, D. Giulini, E. Joos, C. Kiefer, and I.-O. Stamatescu (Springer-Verlag, Berlin, 2000).

[5] D. Giulini, E. Joos, C. Kiefer, J. Kupsch, I.-O. Stamatescu, and H. D. Zeh, *Decoherence and the Appearance of a Classical World in Quantum Theory* (Springer-Verlag, Berlin, 1996).

[6] W. H. Zurek, Phys. Rev. D **24**, 1516 (1981); **26**, 1862 (1982); E. Joos and H. D. Zeh, Z. Phys. B: Condens. Matter **59**, 223 (1985).

[7] A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).

[8] *Quantum Tunneling of Magnetization—QTM'94*, edited by L. Gunther and B. Barbara, Vol. 31 of *NATO Advanced Study Institute, Series E: Applied Physics* (Kluwer, Dordrecht, 1995).

[9] K. Saito, S. Miyashita, and H. De Raedt, Phys. Rev. B **60**, 14 553 (1999).

[10] M. I. Katsnelson, V. V. Dobrovitski, H. A. De Raedt, and B. N. Harmon, e-print cond-mat/0205540.

[11] K. Saito, S. Takesue, and S. Miyashita, J. Phys. Soc. Jpn. **65**, 1243 (1996).

[12] H. Tal-Ezer, SIAM (Soc. Ind. Appl. Math.) J. Numer. Anal. **23**, 11 (1986); **26**, 1 (1989).

[13] H. Tal-Ezer and R. Kosloff, J. Chem. Phys. **81**, 3967 (1984).

[14] C. Leforestier, R.H. Bisseling, C. Cerjan, M.D. Feit, R. Friesner, A. Guldberg, A. Hammerich, G. Jolicard, W. Karrlein, H.-D. Meyer, N. Lipkin, O. Roncero, and R. Kosloff, J. Comput. Phys. **94**, 59 (1991).

[15] R. Kosloff, Annu. Rev. Phys. Chem. **45**, 145 (1994).

[16] T. Iitaka, S. Nomura, H. Hirayama, X. Zhao, Y. Aoyagi, and T. Sugano, Phys. Rev. E **56**, 1222 (1997).

[17] R. N. Silver and H. Röder, Phys. Rev. E **56**, 4822 (1997).

[18] Y. L. Loh, S. N. Taraskin, and S. R. Elliott, Phys. Rev. Lett. **84**, 2290 (2000); **84**, 5028 (2000).

[19] P. de Vries and H. De Raedt, Phys. Rev. B **47**, 7929 (1993).

[20] H. De Raedt, A.H. Hams, K. Michielsen, and K. De Raedt, Comput. Phys. Commun. **132**, 1 (2000).

[21] M. Suzuki, S. Miyashita, and A. Kuroda, Prog. Theor. Phys. **58**, 1377 (1977).

[22] U. Manthe, H. Köppel, and L. S. Cederbaum, J. Chem. Phys. **95**, 1708 (1991).

[23] J. Jaklič and P. Prelovšek, Adv. Phys. **49**, 1 (2000).

[24] M. H. Beck, A. Jäckle, G. A. Worth, and H.-D. Meyer, Phys. Rep. **324**, 1 (2000).

[25] H. Wang, J. Chem. Phys. **113**, 9948 (2000).

[26] M. Thoss, H. Wang, and W. H. Miller, J. Chem. Phys. **115**, 2991 (2001).

[27] V. V. Dobrovitski, H. A. De Raedt, M. I. Katsnelson, and B. N. Harmon, e-print quant-ph/0112053.

[28] Quadratic entropy $S^{(2)}=1-\text{Tr}\,\rho_S^2$ characterizes how mixed is the state of the central system; for pure states $S^{(2)}=0$.

[29] A. Melikidze, V. V. Dobrovitski, H. A. De Raedt, M. I. Katsnelson, and B. N. Harmon (unpublished).

[30] B. Georgeot and D. L. Shepelyansky, Phys. Rev. E **62**, 6366 (2000).