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10 Decoherence in Quantum Spin Systems

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Abstract. Computer simulations of decoherence in quantum spin systems require the solution of the time-dependent Schrödinger equation for interacting quantum spin systems over extended periods of time. We use exact diagonalization, the Chebyshev polynomial technique, four Suzuki-formula algorithms, and the short-iterative-Lanczos method to solve a simple model for decoherence of a quantum spin system by an environment consisting of quantum spins, and compare advantages and limitations of different algorithms.

10.1 Introduction

The description of a quantum spin system (below referred to as a central spin system (CSS)) interacting with its quantum environment (bath) is among the most fundamental problems of theoretical physics. Even if the energy exchange between the CSS and the bath is absent (no dissipation), the system-bath interaction still strongly affects the motion of the CSS due to a loss of phase coherence between different eigenstates of the central system. This many-body quantum phenomenon is commonly called decoherence.

Decoherence is fundamental for quantum measurement theory [1–3] and for condensed matter physics; it can suppress the tunneling of defects in crystals [4], spin tunneling in magnetic molecules and nanoparticles [5], or can destroy the Kondo effect in a dissipationless manner [6]. Decoherence is of particular relevance for quantum computation since the loss of phase relations between different states of the quantum computer may result in an accumulation of errors and may prevent the computer from working correctly [7]. A detailed theoretical understanding of decoherence would definitely help to alleviate this fundamental problem.

Most theoretical studies of decoherence are based on a model of a single spin interacting with a bath of bosons [4]. This model is too simple in the context of e.g. quantum computation or tunneling in magnetic molecules. Extensive studies of many-spin central systems interacting with other types of environment, such as a bath of nuclear spins [5], are needed.

A many-spin system interacting with a bath of quantum spins presents a fairly complex many-body quantum problem, and numerical simulation is

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an indispensable tool for investigating the long-time dynamics of a decohered CSS. One of the most reliable approaches is to model directly the quantum motion of the whole system (CSS plus bath) by solving the corresponding time-dependent Schrödinger equation (TDSE). For such simulations, the numerical algorithms that solve the TDSE should be (1) numerically stable (i.e. conserve the norm of the wave function) for all integration times of interest, (2) sufficiently accurate and allow for controlled increase of the accuracy (e.g. to rule out that the loss of phase coherence is due to poor accuracy, rounding errors etc.), (3) efficient in terms of memory and CPU use, in particular for large spin systems. Below we compare three different numerical techniques that have the potential to meet these requirements: four Suzuki-formula algorithms [8–13], a Chebyshev polynomial technique [14–17], and the short-iterative-Lanczos method [15, 18–20].

10.2 Model and Algorithms

Consider the simple-looking but non-trivial model defined by the Hamiltonian

$$H = J_0(\boldsymbol{S}_1 + \boldsymbol{S}_2)^2 + \sum_{n=1}^{L} J_n \boldsymbol{I}_n \cdot (\boldsymbol{S}_1 + \boldsymbol{S}_2)\,. \tag{10.1}$$

The CSS $(\boldsymbol{S}_1, \boldsymbol{S}_2)$, where $S_1 = S_2 = 1/2$, is coupled to L bath spins $\{\boldsymbol{I}_n\}$ ($I_n = 1/2$) by a Heisenberg exchange interactions $\{J_n\}$. The initial states of the spins $\{\boldsymbol{I}_n\}$ are assumed to be random and uncorrelated. For the initial state of the CSS we take the state with one spin up and the other spin down. We are interested in the time evolution of the magnetization of one of the CSS spins, e.g. $\langle S_1^z(t)\rangle$.

A nice feature of the model (10.1) is that if all $J_n = J$ then, in the large L limit, $\langle S_1^z(t)\rangle$ can be calculated exactly [21]:

$$\langle S_1^z(t)\rangle = \frac{1}{6}[1 + 2(1 - LJ^2t^2)e^{-LJ^2t^2/2}]\cos 2(J_0 - J)t\,. \tag{10.2}$$

The result (10.2) exhibits an interesting feature: initially, the amplitude of the magnetization rapidly decays to zero, then increases again and becomes constant (1/6) as $t \to \infty$ [21]. This is similar to the two-step decoherence process discovered earlier [22] and can be understood from simple physical arguments [21]. The model (10.1) captures some non-trivial aspects of decoherence, and provides a simple test to compare various algorithms for solving the TDSE under conditions that are rather demanding from the point of view of algorithmic, memory and CPU requirements. We now discuss four different approaches to solve the TDSE for models such as (10.1).

Exact Diagonalization (ED) is the most straightforward approach. Standard library routines can be used to compute all eigenvalues and eigenvectors of the $D \times D$ matrix H ($D = 2^{L+2}$ denotes the dimension of the Hilbert space spanned by the states of the $L+2$ spins 1/2). The initial state is represented as a superposition of eigenvectors, and the wave function $\psi(t)$ is obtained by two matrix-vector multiplications of length D and a phase-shift operation on a vector. In practice, the amount of memory needed to store the $D \times D$ elements of the eigenvectors limits the application of this approach to problems with D of the order of 10 000, which corresponds to systems with about 14 $S = 1/2$ spins. Memory and CPU time of the ED algorithm scale as D^2 and D^3 respectively.

Suzuki Product-formula Algorithms (SP) are based on the approximation

$$e^{-i\tau H} \approx U_2(\tau) = e^{-i\tau H_1/2} \dots e^{-i\tau H_p/2} e^{-i\tau H_p/2} \dots e^{-i\tau H_1/2} ,$$

where

$$H = \sum_{j=1}^{p} H_j .$$

We consider two different decompositions that can be implemented efficiently: The original pair-product split-up [8, 11] in which H_j contains all contributions of a particular pair of spins, and a XYZ decomposition in which we break up the Hamiltonian according to the x, y and z components of the spin operators [13]. $U_2(\tau)$ is the building block for the fourth-order-in-time approximation

$$e^{-i\tau H} \approx U_4(\tau) = U_2(a\tau)U_2(a\tau)U_2((1-4a)\tau)U_2(a\tau)U_2(a\tau) ,$$

where $a = 1/(4 - 4^{1/3})$ [10]. The error on the wave function is bounded as

$$\| e^{-itH}\Psi(0) - U_n^m(\tau)\Psi(0) \| \le c_n t \tau^n ,$$

where $t = m\tau$ and c_n is positive constant. By construction, all these algorithms conserve the norm of the wave function and, as a consequence are unconditionally stable [9]. These time-stepping algorithms advance the state of the quantum system by small time steps τ ($\tau \|H\| \ll 1$) and work equally well if the Hamiltonian contains couplings to time-dependent external fields [13]. For a fixed accuracy, memory and CPU time of the n-th order SP algorithm scales as D and $nt^{(1+1/n)}D$ respectively

The Chebyshev Polynomial Algorithm (CP) [14–17] uses the identity

$$\Psi(t) = \lim_{K\to\infty} \left[J_0(t\|H\|)I + 2\sum_{k=1}^{K} J_k(t\|H\|)\hat{T}_k(H/\|H\|) \right] \Psi(0) .$$

The polynomials $\hat{T}_k(X)$ are defined by the recursion

$$\hat{T}_{k+1}(X)\Psi(0) = -2iX\hat{T}_k(X)\Psi(0) + \hat{T}_{k-1}(X)\Psi(0)$$

for

$$k \geq 1\,, \quad \hat{T}_0(X)\Psi(0) = \Psi(0) \quad \text{and} \quad \hat{T}_1(X)\Psi(0) = -iX\Psi(0)\,.$$

Using standard 14-digit arithmetic, all Bessel functions $|J_k(z)|$ are zero to machine precision if $k > K = |z| + 100 = |t|\|H\| + 100$ and therefore the Chebyshev polynomial approximation to $\Psi(t)$ is accurate to machine precision also (up to small rounding errors). Although the CP algorithm is not unconditionally stable, it is so accurate that it can safely be used for time stepping (also with very large time steps). Note that once t has been fixed, the CP algorithm cannot be used to generate reliable information for shorter times. As K is linear in t, the computation time required to reach a time t increases *linearly* with t (and D). This linear dependence on t (and the very high accuracy) suggests that the Chebyshev polynomial algorithm may be the method of choice if we want the solution of the TDSE for a few (very long) times [17]. Memory and CPU time of the CP algorithm scale as D and tD respectively ($K \ll D$ for most problems of interest).

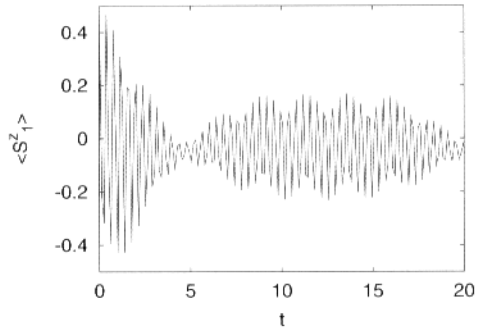
The Short Iterative Lanczos Algorithm (SIL) [15, 18–20] is based on the approximation

$$e^{-i\tau H}\Psi \approx e^{-i\tau P_N H P_N}\Psi\,,$$

where P_N is the projector on the N-dimensional subspace spanned by the vectors $\{\Psi, H\Psi, \ldots, H^{N-1}\Psi\}$. We calculate $e^{-i\tau P_N H P_N}\Psi$ by generating the orthogonal Lanczos vectors in the usual manner [23], and use exact diagonalization of the resulting $N \times N$ tri-diagonal matrix for time propagation [15, 18, 19]. Clearly $e^{-i\tau P_N H P_N}$ is unitary and hence the method is unconditionally stable. The accuracy of this algorithm depends both on the order N and the state Ψ [15, 18, 19]. In exact arithmetic,

$$e^{-i\tau H} = \lim_{N\to\infty} e^{-i\tau P_N H P_N}\Psi\,,$$

but in practice, the loss of orthogonality during the Lanczos procedure [23] limits the order N and the time step τ that can be used without introducing spurious eigenvalues [23]. Furthermore, we require $N \ll D$ because the memory needed to store the eigenvectors (and/or all Lanczos vectors) is proportional to N^2. In practice, the low-order SIL algorithm may not work well if Ψ contains contributions from many eigenstates of H with very different energies, because it is unlikely that all these eigenvalues will be present in $P_N H P_N$ (for small N). Memory and CPU time of the SIL algorithm scale as D and $N^2 Dt/\tau$ respectively. In general, N increases with τ in a non-trivial, problem dependent manner.



Method	Error	CPU-time (s)
ED	MP	6739.1
SP-Pair (U_2)	0.26×10^{-3}	2.6
SP-Pair (U_4)	0.42×10^{-8}	9.6
SP-XYZ (U_2)	0.97×10^{-1}	1.1
SP-XYZ (U_4)	0.23×10^{-4}	5.6
CP	MP	5.9
SIL (N=5)	0.29×10^{-5}	68.3
SIL (N=10)	MP	137.8

Fig. 10.1. Left: Magnetization $\langle S_1^z(t) \rangle$ as a function of time as obtained by numerical simulation of two central spins interacting with a bath of $L = 10$ spins. The parameters of model (10.1) are $J_0 = 8$, $J_k = 0.128$. Except for the CP algorithm, a time step $\tau = 0.05$ was used. Right: Comparison of the efficiency of various algorithms to solve the TDSE, for the case of the data shown at the left. The entry "MP" denotes "machine precision". CPU times as measured on a Windows 2000 Athlon XP 1900+ system

10.3 Numerical Tests

In Fig. 10.1, we show a typical simulation result for $\langle S_1^z(t) \rangle$, as obtained by the CP solution of the TDSE for model (10.1). The initial fast decay, and subsequent reappearance of the oscillations is clearly present. Qualitatively these results agree with the analytical (large L) solution (10.2). Also shown is the error

$$\| \Psi_{\mathrm{ED}}(t = 20) - \Psi_{\mathrm{X}}(t = 20) \| ,$$

where X is one of the seven algorithms used. It is clear that SIL is not competitive for this type of TDSE problem, as already anticipated above. The fourth-order pair-approximation is close but still less efficient than the CP algorithm, but the other SP algorithms are clearly not competitive. The reason that the pair-approximation is performing fairly well in this case is related to the form of the Hamiltonian (10.1). The present results support our earlier finding [17] that the numerical simulation of decoherence in spin systems is most efficiently done in a two-step process: the CP algorithm can be used to make a big leap in time, followed by the SP algorithm calculation to study the time dependence on a more detailed level. From a more general perspective, to increase the confidence in numerical simulation results, it is always good to have several different algorithms performing the same task.

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