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Real-Time Quantum Dynamics of a Single Spin 1/2 Coupled to a Spin Bath

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Abstract

We performed real-time dynamics of a spin $\frac{1}{2}$ quantum system that is coupled to a bath of N quantum spin $\frac{1}{2}$ particles. The quantities we study are the time dependence of the magnetization and of the quantum purity, $\mathcal{P}(t)$. If the spins that constitute the bath have no interactions with each other, the result is compared to a recent theoretical result. We also present simulations to study the effect of interactions between the bath spins. In particular, we analyze how $\mathcal{P}(t)$ approaches its asymptotic value for large t and N.

Keywords: Quantum Dynamics, Spin Bath, Quantum Purity, Decoherence

1. Introduction

Advances in quantum information processing and quantum computing have been steady for over a decade [1, 2]. However, additional theoretical understanding and improved physical implementations are necessary before a quantum computer becomes a practical device. At the simplest level a quantum computer can be viewed as a time development problem for a quantum spin system coupled to a bath that is its environment. At the computational level, the time development of the quantum system is in principle simple, since the underlying equation is just the time-dependent Schrödinger equation. However in practice there are two complications that make calculations of such quantum systems difficult. First, the precise nature of the environment must be taken into account quantum mechanically, and hence the system to be simulated is much larger than just the quantum system of the qubits of the quantum computer. Second, the development of real-time algorithms for the time-dependent Schrödinger equation are very difficult due to the imaginary phase in the propagator of the quantum system. In quantum statistical mechanics simulations this difficulty is referred to as the 'minus sign' problem. There has however been significant progress in simulation of quantum spin systems in real time and the physical understanding of these systems [3, 4, 5, 6].

Suppression of decoherence of spin systems is of fundamental importance for building quantum computers [2, 4]. A recent paper [7] calculated the quantum frustration of dissipation of a single spin $\frac{1}{2}$ coupled to one or two spin baths, with no interactions between the spins of the bath. They showed that the quantum purity, $\mathcal{P}(t)$, decayed as an exponential for coupling to one bath but as a power law for coupling to two baths. In this paper we describe our simulation to check their expressions for a spin $\frac{1}{2}$ coupled to one spin bath. Simulations are restricted by the largest number of spins that can be simulated on modern supercomputers, so we study the approach to the asymptotic result for a finite number of spins. Furthermore in our calculations we are not restricted to zero interactions between the bath spins, and therefore we address the question of whether a spin bath with random interactions will allow a faster approach to the asymptotic region for $\mathcal{P}(t)$.

2. Problem and Theory

We consider a quantum spin system coupled to a quantum spin bath. The Hamiltonian for the system+bath is

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_{SB} + \mathcal{H}_B \tag{1}$$

where $\mathcal{H}_S = \omega_0 S^z$ is the Hamiltonian of the system composed of a single spin $\frac{1}{2}$ interacting with an external magnetic field, $\mathcal{H}_{SB} = gS^x \sum_{k=1}^{N} I_k^x$ is the interactions of the system with the bath spins, $\mathcal{H}_B$ is the Hamiltonian for interactions among the bath spins. The spin operators are S and I, for example $S^z = \frac{1}{2}\sigma^z$ with σ^z the Pauli spin matrix.

For the case where $\mathcal{H}_B = 0$ the form of the interactions with the bath ensure that the total x component of the spins of I are a conserved quantity. We consider the case where the system spin is initially in the down state. Therefore the time dependence of the z component of the single spin that makes up the system is given by [7]

$$\left\langle \vec{S}(t) \right\rangle = \mathrm{Tr}\left(\rho(0)\vec{S}(t)\right) = \sum_{m=-\frac{N}{2}}^{\frac{N}{2}} \lambda_m \mathrm{Tr}\left(\vec{S}_m(t)\rho_m(0)\right) \tag{2}$$

where $\rho(0)$ is the initial quantum density matrix and

$$\lambda_m = \binom{N}{\frac{N}{2}-m} = \frac{N!}{\left(\frac{N}{2}-m\right)!\left(\frac{N}{2}+m\right)!}. \tag{3}$$

In addition $\langle S^x(t)\rangle = \langle S^y(t)\rangle = 0$. Define $\Omega_m = \sqrt{(mg)^2 + \omega_0^2}$. Then one obtains [7]

$$\langle S^z(t)\rangle = -\frac{1}{2^{N+1}} \sum_{m=-\frac{N}{2}}^{\frac{N}{2}} \frac{\lambda_m}{\Omega_m^2}\left[m^2g^2\cos(\Omega_m t) + \omega_0^2\right]. \tag{4}$$

Using the Laplace-de Moivre theorem

$$\frac{1}{2^N}\sum_m \lambda_m \approx \sqrt{\frac{2}{\pi N}}\int_{-\infty}^{\infty} dm\, \exp\left(-\frac{2m^2}{N}\right) \tag{5}$$

gives the asymptotic result for $\omega_0 = 0$ and large N, valid for all times t,

$$\langle S^z(t)\rangle = -\frac{1}{2}\exp\left(-\frac{Ng^2t^2}{8}\right). \tag{6}$$

The quantum purity in our case is defined as

$$\mathcal{P}(t) = \mathrm{Tr}\left(\rho^2\right) = \frac{1}{2} + 2\langle S^z\rangle^2 = \frac{1}{2} + \frac{1}{2}\exp\left(-\frac{Ng^2t^2}{4}\right). \tag{7}$$

Note the factor of $\frac{1}{4}$ in the exponential, compared to Eq. (27) of Ref. [7]. A rederivation of their result [8] gives the correct factor in Eq. 7. For a pure quantum state $\mathcal{P} = 1$, and hence the rate of decrease of the purity is a measure of the decoherence of the spin of the system.

3. Results

In Fig. (1a) we show results for $2\mathcal{P}(t) - 1$ as a function of $N t^2$. The quantum purity was calculated from Eq. (7) and Eq. (4), with $g{=}1$. To compare with the asymptotic form we have plotted $2\mathcal{P}(t) - 1$ versus $N t^2$ rather than as a function of either the number of spins N in the bath or the time t. Clearly to go to larger values of Nt^2 the number of spins in the bath, N, must increase. There is a limit to the number of bath spins which can be simulated, currently on

the largest supercomputers one is restricted to about $N \approx 40$. Our calculation results performed for $N = 8$ and $N = 16$ were indistinguishable from the results of Eq. (4), until numerical rounding error occurred for very small values of $2\mathcal{P}(t) - 1$. In Fig. (1b) we show results for the fractional error due to finite N in $2\mathcal{P}(t) - 1$ as a function of N. The fractional error is defined as

$$\text{fractional error} = \frac{[2\mathcal{P}(t) - 1]_{\text{asymptotic}} - [2\mathcal{P}(t) - 1]_{\text{calculated}}}{[2\mathcal{P}(t) - 1]_{\text{asymptotic}}}. \tag{8}$$

As long as N is large enough the fractional error for fixed Nt^2 approaches the exact result as a power law in N. The computer calculations are limited in the number of bath spins N, and hence can reach the power law approach to the asymptotic value only for small values of Nt^2.
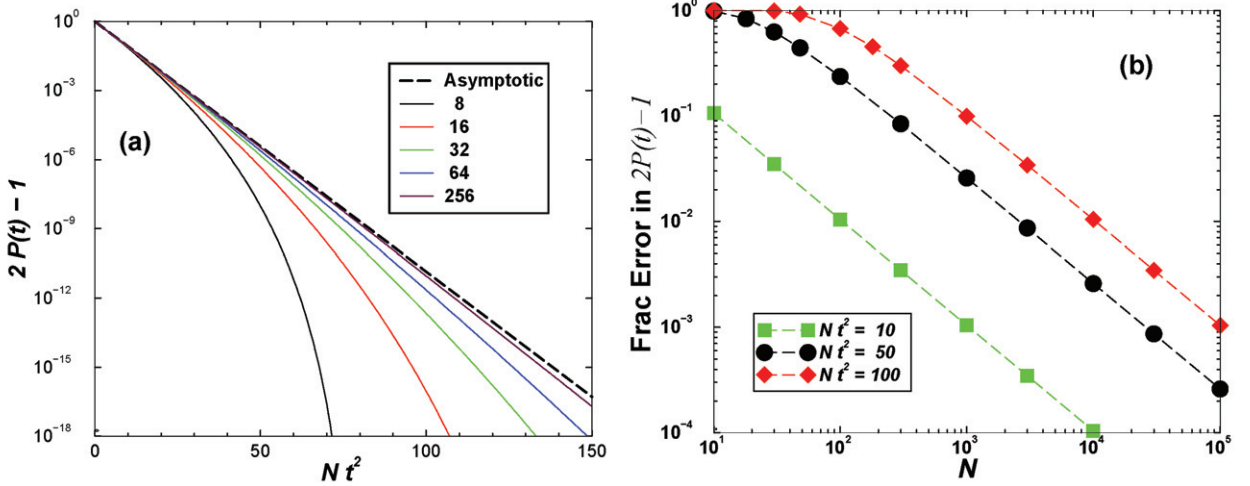

Figure 1: (a) The decay of the quantum purity as a function of the variable Nt^2. For $N = 8$ and $N = 16$ the results from the simulation are the same as the results shown here from Eq. (7). (b) The fractional error in $2\mathcal{P}(t) - 1$ as a function of N for three values of Nt^2.

The computer calculation is limited to values of N of less than about forty. However, unlike the exact calculation the computer calculations are not limited to the case $\mathcal{H}_{\text{B}} = 0$. Therefore it is natural to ask whether or not having interactions within the bath can allow a closer approach to the asymptotic limit. This is shown in Fig. (2) for $N = 10$, 20, and 30. The exact calculation is from Eq. (7) and Eq. (4). The label 'No BI' is from the program for $\mathcal{H}_{\text{B}} = 0$, and is indistinguishable on this scale from the exact results. For the case of interactions within the bath the bath Hamiltonian is

$$\mathcal{H}_{\text{B}} = \sum_{k=1}^{N} \sum_{j=1, j \neq k}^{N} \left(g_{kj,x} I_k^x I_j^x + g_{kj,y} I_k^y I_j^y + g_{kj,z} I_k^z I_j^z \right) \tag{9}$$

for the components of the spin $\frac{1}{2}$ operators I_k. Each component of the values of g_{kj} were chosen randomly from a distribution uniformly distributed between chosen bounds $[-g_{\text{max}}, g_{\text{max}}]$. Fig. (2) shows that there exists a value of g_{max} for a given value of Nt^2 that brings the value of the purity closer to the asymptotic value. However for a fixed value of Nt^2 making the random bath interactions too strong hinders the approach with N to the asymptotic limit.

4. Conclusions and Discussion

We presented results for a single quantum spin $\frac{1}{2}$ coupled to a bath of N quantum spin $\frac{1}{2}$ particles with a coupling g between the x-components of the spin operators. The comparison of the simulation results with the exact results for no interactions between the bath spins is excellent. Furthermore, for large enough N for a fixed value of Nt^2 the approach to the exact result is a power law in N. Adding random interactions among the bath spins changes the approach to the large N limit for a fixed value of Nt^2.
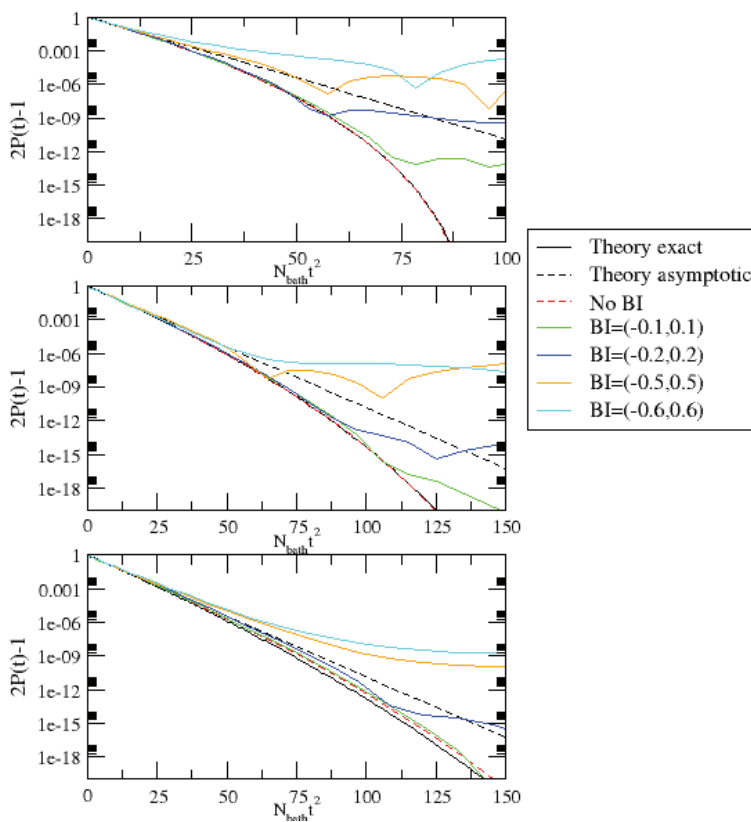
Figure 2: $2\mathcal{P}(t) - 1$ is shown as a function of Nt^2. The asymptotic result is shown, as is the theoretical and program result for no bath interaction (BI). Also shown are a single realization of the random bath interactions with different strengths g_{max}. The graphs are for $N = 10$, 20, and 30 from top to bottom.

A number of questions remain to be addressed. First, is there a mechanism to systematically pick the strength of the random bath interactions, g_{max}, to approach the asymptotic limit more quickly for fixed N? Second, can adding interactions among the bath spins also allow a faster approach to the asymptotic limit when there is more than one bath? Third, how can this approach improve on current simulations of quantum computers? Answers to these questions will hopefully be found in the near future.

Acknowledgements

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