An efficient Polynomial scheme for time evolution of quantum systems

Jun Jing*, H. R. Ma

Institute of Theoretical Physics, Shanghai Jiao Tong University

800 DongChuan Road, MinHang, Shanghai 200240, China

(Dated: October 2, 2006)

Abstract

Based on the generation function of Laguerre polynomials, We proposed a new Laguerre polynomial expansion scheme in the calculation of evolution of time dependent Schrödinger equation. Theoretical analysis and numerical test show that the method is equally as good as Chebyshev polynomial expansion method in efficiency and accuracy, with extra merits that no scaling to Hamiltonian is needed and wider suitability.

PACS numbers: 03.65.-w, 03.67.-a, 05.30.Jp

* Email: jingjun@sjtu.edu.cn

I. INTRODUCTION

The studies of open quantum systems have a long history [1]. There has been renewed interest in recent years due to the developments of the conception and possible realization of quantum communication and quantum computation [2, 3]. A key concept in the open quantum system study is the decoherence of a quantum system interacting with environments, which plays a very important rule in almost all phenomena in the quantum devices used in quantum computation and quantum communication [4, 5, 6]. It has been shown that the states of an open quantum system will finally relax into a set of "pointer states" in the Hilbert space [5] by decoherence, i.e. for a quantum system prepared in a linear superposition of its eigenstates, interaction of the system with its environment results in a decay from the system's initial pure state, $\rho_s(t=0) = |\psi_0\rangle\langle\psi_0|$, to a mixed state, $\rho_s(t>0) = \sum_i p_i\rho_i$, $\sum_i p_i = 1$. To be specific, an arbitrary initial state of the system plus the environment may be written as:

$$|\psi(t=0)\rangle = (\sum_n C_n|n\rangle) \otimes |\psi_e\rangle, \tag{1}$$

where the set $|n\rangle$ stands for the eigenstates of the system and $|\psi_e\rangle$ is the initial state of the environment. This state at time t larger than the decoherence time τ_d evolved to a mixed state, which may be expanded as:

$$|\psi(t)\rangle = \sum_m C_m(t)(|m\rangle \otimes |e_m\rangle). \tag{2}$$

Here, the set of states $|m\rangle$ are the so-called pointer states of the system [7, 8, 9], and $|e_m\rangle$ are the corresponding states of the environment that entangled with $|m\rangle$[10]. A convenient way to represent the system interacting with the environment is the reduced density matrix, defined as

$$\rho_s = \mathrm{T}r_e\left(|\psi(t)\rangle\langle\psi(t)|\right),$$

where $\mathrm{T}r_e$ means tracing over the environment degrees of freedom. The evolution from (1) to (2) may be rewritten as:

$$\rho_s(0) \;\Rightarrow\; \rho_s(t) = \sum_m |C_m(t)|^2|m\rangle\langle m|. \tag{3}$$

When the time $t \gg \tau_d$, the non-diagonal elements of the reduced density matrix $\rho_s(t)$ vanish and the diagonal elements achieve their equilibrium values. This effect of decoherence is

typical for all known quantum systems that induces an increase of the system's entropy and the damping of quantum oscillations with time [11, 12].

A theoretical description of the evolution of the system from $\psi(0)$ to $\psi(t)$ driven externally by the environment is generally a very difficult problem. The case that the environment is described by Boson fields has been extensively studied in the context of Master equation approach, both with Markovian [7] or non-Markovian [13] approximations. Although the master equation scheme can be used for a large number of environments of possible types (phonon, photons, etc.) [12], however, the Master equation description is not universally valid for all the models of environment and fragile in some systems[14].

Generally, if the Hamiltonian of the compound system is known, the direct way to solve the decoherence problem is to follow the evolution of the compound system over a substantial period of time. By setting $\hbar = 1$, the time dependent Schrödinger equation is:

$$i\frac{\partial \psi(t)}{\partial\, t} = \hat{H}\psi(t). \tag{4}$$

Here $\hat{H}$ is the total Hamiltonian of the system plus the environment. The equation (4) can be decomposed into a set of first-order ordinary differential equations with the initial condition $\psi(0)$, and the total number of equations is the dimension of the Hilbert space of the whole system, which is usually very large. In principle, the set of equations can be solved by convenient methods of ordinary differential equations such as Predictor-Corrector method or Runge-Kutta method. However, direct solution of the equations will cost too much computer resource due to the large number of equations involved. Another scheme for propagating equation (4) is to expand the evolution operator $U(t) = \exp(-i\hat{H}\Delta t)$ in a Taylor series, where Δt is the time step.

$$\exp(-i\hat{H}\Delta t) = 1 - i\hat{H}\Delta t + \cdots . \tag{5}$$

It has been stated in Ref. [15] that a numerical scheme based on this expansion is not stable, because it does not conserve the time reversal symmetry of Schrödinger equation. Variations of the Taylor series have been proposed and used in calculations of evolution of quantum systems [16, 17]. Efficient and stable simulation methods are needed to reduce the computation load and to increase the simulation speed.

The polynomial expansion method has been used in the calculation of dynamics and/or spectral properties of large quantum systems with great success [15, 18, 19, 20], Tal-Ezer and Kosloff proposed the expansion in terms of the Chebyshev polynomials and tested the method with the simple harmonic oscillator and the problem of scattering from a surface, high accurate results were obtained with an efficiency six times higher compared to the conventional scheme [15, 19]. Silver and Röder used the Chebyshev polynomial expansion in the calculation of density of states of large sparse Hamiltonian matrix [20]. A fast evolution method based on the expansion of Chebyshev polynomial for dynamical quantum systems was proposed and checked by Loh et al [21]. Dobrovitski et al extended the Chebyshev polynomial expansion method in the study of a spin system interacting with a spin-bath [9], obtained the decoherence properties of the system and showed the efficiency and accuracy of the method. Since the Chebyshev polynomial is the most frequently used orthogonal polynomial in most numerical approximation theories [22], other kinds of orthogonal polynomials should also be applicable in the evolution problems. The argument of Chebyshev polynomial is bounded to the interval $[-1, +1]$, which is suitable for systems with a bounded Hamiltonian, and for systems that only bounded below, a cut off to the energy spectrum is inevitable in order to use the method. However, it is well known that some of the orthogonal polynomials, like Hermite polynomial and Laguerre polynomial, do not limit their arguments to finite intervals. Expansion in terms of these kinds of orthogonal polynomials may have the merit in the unbounded systems. In this paper, we will explore the efficiency and accuracy of methods based on all these orthogonal polynomials. We constructed methods based on the Hermite and Laguerre polynomials and found that the above two mentioned orthogonal polynomials do have the required properties. The rest of the paper is organized as follows. In Section II, we briefly review the spin-bath model and the difficulty on getting its exact solution; In Section III, three kinds of polynomial scheme will be described for the expansion of the evolution operator; In Section IV, we present the results of our numerical simulation; Finally, A brief summary is given in the Section V.

II. HAMILTONIAN

Two systems are used in this study to test the numerical methods. The first is a two spin-1/2 system coupled to a spin environment and the second is a particle moving in a

double well potential.

The spin Hamiltonian we used in testing our numerical schemes is the one that used in reference [9, 23, 24]. The system consists of two spins-1/2 interacting antiferromagneticly, and the system coupled to a bath of non-interacting spins-1/2. The Hamiltonian can be written as:

$$H = 2J\mathbf{s}_1 \cdot \mathbf{s}_2 + \sum_k A_k(\mathbf{s}_1 + \mathbf{s}_2) \cdot \mathbf{I}_k. \tag{6}$$

Here $\mathbf{s}_1$ and $\mathbf{s}_2$ are two spins with spin half coupled by the coupling constant J, favoring the antiparallel alignment, which constitute the system. The spins $\mathbf{I}_k$, $k = 1, 2, \cdots, N$ are N spin half environment spins, interacting with the system by Heisenberg coupling A_k, and do not interact with each other. The coupling constant between the two system spins is much larger than the couplings to the environment spins, $J \gg A_k$. The couplings A_k are uniformly distributed in an interval. Both of the system spins and the environment spins can be represented by Pauli matrices.

The Hilbert space of the whole system is 2^{N+2} dimensional when the environment consists of N spins. The basis state of the environment can be chosen as the direct product of the single states $|\uparrow\rangle$ or $|\downarrow\rangle$ for each spin $\vec{I}_k$, here $|\uparrow\rangle$ and $|\downarrow\rangle$ are eigenstates of the square and z components of each spin. For a moderate size of the environment, say, $N = 18$, we have to find an exact solution to about 10^6 differential equations. And when N is increased by one, the number of equations is doubled. For this reason efficient algorithms are needed in the studies of the evolution of this kind of problems, especially in the case of decoherence where long time simulation is required to reach the pointer state. The polynomial expansions based on both Chebyshev polynomial [9] and Hermite polynomial [25] are very successful in this case.

The Hamiltonian for the double well potential is given by:

$$H = \frac{p^2}{2} - \frac{1}{2}\omega^2 x^2 + \lambda x^4. \tag{7}$$

where we set $m = \hbar = 1$. This model is very important in the studies of critical phenomena and in the standard model of particle physics when the variable x is a scalar field. Here we take it to be a simple yet non trivial model to test our numerical method.

III. POLYNOMIAL SCHEME

The formal solution of the equation (4) is:

$$\psi(t) = e^{-i\hat{H}t}\psi(0) = U(t)\psi(0). \tag{8}$$

The evolution operator $U(t)$ is an exponential functional of the Hamiltonian operator $\hat{H}$ which is represented as a matrix in the Hilbert space of ψ. The method of polynomial expansion is to expand the evolution operator $U(t)$ in terms of the orthogonal polynomials of Hamiltonian $\hat{H}$. The expansions in Chebyshev polynomial and Hermite polynomial are presented in [9] and [25] respectively. We will briefly introduce the Chebyshev and Hermite polynomial expansion and give detailed derivation of expansion in terms of Laguerre polynomials and check the efficiency of the method numerically.

A. Chebyshev polynomial

The Chebyshev expansion of $U(t)$ given by Dobrovitski et al is:

$$U(t) = \exp(-i\tau\tilde{H}) = \sum_{k=0}^{\infty} c_k T_k(\tilde{H}), \tag{9}$$

where $\tau = E_0 t/2$ and $\tilde{H} = 2\hat{H}/E_0$, E_0 is a scale factor, T_k are the Chebyshev polynomials: $T_k(x) = \cos(k \arccos x)$. The reason that we change $\hat{H}$ into $\tilde{H}$ comes from the argument domain of $T_k(x)$, that is $x \in [-1, 1]$. For our spins system, $\hat{H}$ is bounded above and below, so that the scale factor E_0 can be determined in the following way:

$$\begin{aligned} E_{\max} &= \max\langle\psi|\hat{H}|\psi\rangle, \\ E_{\min} &= \min\langle\psi|\hat{H}|\psi\rangle, \\ E_0 &= 2\max(|E_{\max}, E_{\min}|). \end{aligned}$$

Using the orthogonal property of T_k, the expansion coefficients c_k of equation (9) can be calculated as:

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

where $J_k(\tau)$ is the Bessel function of the kth order, and $a_0 = 1$ when $k = 0$ and $a_k = 2$ when $k \geqslant 1$. The series of Chebyshev polynomials of Hamiltonian $\hat{H}$ can be calculated by

the recursion process:

$$\begin{aligned} T_0(\tilde{H}) &= 1, \\ T_1(\tilde{H}) &= \tilde{H}, \\ T_{k+1}(\tilde{H}) &= 2\tilde{H}T_k(\tilde{H}) - T_{k-1}(\tilde{H}). \end{aligned}$$

B. Hermite polynomial

In order to obtain the expansion in terms of Hermite polynomials, we start from its generating function [26]

$$e^{-s^2+2sx} = \sum_{k=0}^{\infty} \frac{s^k}{k!} H_k(x). \tag{10}$$

Where $H_k(x)$ denotes the Hermite polynomial of order k. The evolution operator (8) can be rearranged as

$$e^{-i\hat{H}t} = e^{-(t/2\lambda)^2} e^{-(-it/2\lambda)^2 + 2\lambda\hat{H}(-it/2\lambda)}. \tag{11}$$

The second part of the right hand side of equation (11) is identified to be the generating function of Hermit polynomial by setting $x = \lambda\hat{H}$ and $s = -it/2\lambda$ in equation (10), where λ is introduced for convenience. From equation (10) and (11) we obtain the Hermite expansion form of the exponential operator $U(t)$:

$$e^{-i\hat{H}t} = e^{-(t/2\lambda)^2} \sum_{k=0}^{\infty} \frac{(-i)^k}{k!} (t/2\lambda)^k H_k(\lambda\hat{H}). \tag{12}$$

The formal solution $\psi(t) = \exp(-i\hat{H}t)\psi(0)$ then becomes:

$$\begin{aligned} \psi(t) &= e^{-(t/2\lambda)^2} \sum_{k=0}^{\infty} \frac{(-i)^k}{k!} (t/2\lambda)^k \phi_k, \\ \phi_k &= H_k(\lambda\hat{H})\psi(0). \end{aligned} \tag{13}$$

The Hermite polynomial of H can be obtained by the following recursive algorithm:

$$\begin{aligned} \phi_0 &= \psi_0, \\ \phi_1 &= 2\lambda\hat{H}\psi_0, \\ \phi_{k+1} &= 2\lambda\hat{H}\phi_k - 2k\phi_{k-1}. \end{aligned}$$

To discuss the convergence of the expansion, we consider the term when k is large. The Hermite polynomial may be replaced by its asymptotical expression [26]:

$$H_k(x) \approx 2^{\frac{k+1}{2}} k^{\frac{k}{2}} e^{-\frac{k}{2}+\frac{x^2}{2}}, \cos\left(\sqrt{2k+1}x - \frac{k\pi}{2}\right). \tag{14}$$

Substitute this into equation (12) and using the Stirling's formula for the factorial,

$$k! \approx \exp[k(\ln k - 1)], \quad k \gg 1, \tag{15}$$

the magnitude of the kth term in the expansion of equation (12) for large k is:

$$\frac{(t/2\lambda)^k}{k!} H_k(\lambda \hat{H}) \approx \frac{(t/\lambda)^k}{2^k e^{k(\ln k - 1)}} 2^{\frac{k+1}{2}} k^{\frac{k}{2}} e^{-\frac{k}{2}+\frac{\lambda^2 \hat{H}^2}{2}} \cos\left(\sqrt{2k+1}\lambda \hat{H} - \frac{k\pi}{2}\right). \tag{16}$$

The physically meaningful Hamiltonian should always be bounded below, and for every evolution problem, the spectrum of the system has a maximum value determined by the initial state, which is in the order of the total energy of the initial state. If we set a maximum energy E_m, a few times of the total energy, then the states with energy larger than this maximum will not enter the calculation, and we have a natural energy cut off of the problem, the E_m. Then we can replace $\hat{H}$ in equation (16) with E_m to estimate the condition of the convergence of the expansion.

$$\begin{aligned}
\frac{(t/2\lambda)^k}{k!} H_k(\lambda E_m) &\leq 2^{-\frac{k-1}{2}} \exp\left[-\frac{k}{2}\ln k + \frac{k}{2} + \frac{\lambda^2 E_m^2}{2} + k \ln\left(\frac{t}{\lambda}\right)\right] \\
&= 2^{-\frac{k-1}{2}} \exp\left\{-\frac{k}{2}\left[\ln k - \ln e + \ln\left(\frac{t}{\lambda}\right)^{-2} - \frac{\lambda^2 E_m^2}{k}\right]\right\} \\
&= 2^{-\frac{k-1}{2}} \exp\left\{-\frac{k}{2}\left[\ln\left(\frac{k\lambda^2}{et^2}\right) - \frac{\lambda^2 E_m^2}{k}\right]\right\}.
\end{aligned}$$

From this expression we see that if

$$\ln\left(\frac{k\lambda^2}{et^2}\right) - \frac{\lambda^2 E_m^2}{k} \geq 0,$$

or the time step t satisfies

$$t \leq \sqrt{\frac{k}{e}} \lambda \exp\left(-\frac{\lambda^2 E_m^2}{2k}\right). \tag{17}$$

The kth term is not larger than $2^{-\frac{k-1}{2}}$, then the summation is convergent. In the numerical calculation given below, we set $\lambda = 1/2$.

C. Laguerre polynomial

The expansion in terms of Laguerre polynomials can also be derived from its generating function [26]:

$$(1-s)^{-\alpha-1}e^{xs/(s-1)} = \sum_{k=0}^{\infty} L_k^{\alpha}(x)s^k, \quad (|s|<1). \tag{18}$$

where α distinguishes different types of Laguerre polynomials. By setting $s = it/(\lambda+it)$ and $x = \lambda\hat{H}$, we get the Laguerre polynomial expansion as:

$$\begin{aligned} \psi(t) &= \left(\frac{\lambda}{\lambda+it}\right)^{\alpha+1}, \sum_{k=0}^{\infty}\left(\frac{it}{\lambda+it}\right)^k \phi_k, \\ \phi_k &= L_k^{\alpha}(\lambda\hat{H})\psi(0). \end{aligned} \tag{19}$$

The recursion relation of Laguerre polynomials are

$$\begin{aligned} L_0^{\alpha}(x) &= 1 \\ L_1^{\alpha}(x) &= \alpha+1-x \\ (k+1)L_{k+1}^{\alpha}(x) &= (2k+\alpha+1-x)L_k^{\alpha}(x) - (k+\alpha)L_{k-1}^{\alpha}(x). \end{aligned} \tag{20}$$

From the relation we obtain the Laguerre polynomial expansion of Hamiltonian $\hat{H}$ as:

$$\begin{aligned} \phi_0^{\alpha} &= \psi(0) \\ \phi_1^{\alpha} &= (\alpha+1-\lambda\hat{H})\psi(0) \\ (k+1)\phi_{k+1}^{\alpha} &= (2k+\alpha+1-\lambda\hat{H})\phi_k^{\alpha} - (k+\alpha)\phi_{k-1}^{\alpha}. \end{aligned} \tag{21}$$

Different α gives different choice of the algorithms, the domain of α is in the interval of $(-1,\infty)$. In the calculation of the spin bath Hamiltonian we use $\alpha = -1/2$ and set the parameter $\lambda = 1$ for convenience. For other kinds of Hamiltonian different values of α may be used to attain higher efficiency and accuracy.

The convergency of the expansion of equation (19) is guaranteed by the relationship between Laguerre polynomial and Hermite polynomial [26]:

$$L_k^{-\frac{1}{2}}(x) = \frac{(-1)^k}{2^{2k}k!}H_{2k}(\sqrt{x}). \tag{22}$$

Substituting equation (14), (15) and (22) into the expansion term $\left(\frac{it}{1+it}\right)^k L_k^{-\frac{1}{2}}(\hat{H})$ and replacing $\hat{H}$ with E_m, the total energy of the initial state, we could estimate its asymptotical

absolute value by such a procedure:

$$\begin{aligned}\left|\left(\frac{it}{1+it}\right)^k L_k^{-\frac{1}{2}}(E_m)\right| &\approx \left(\frac{t^2}{\lambda^2+t^2}\right)^{k/2} \frac{1}{2^{2k}e^{k(\ln k-1)}} 2^{\frac{2k+1}{2}} 2^k k^k e^{-k+\frac{E_m}{2}} \cos\left(\sqrt{2k+1}E_m - \frac{k\pi}{2}\right) \\ &\leq 2^{\frac{1}{2}} \left(\frac{t^2}{\lambda^2+t^2}\right)^{k/2} e^{\frac{E_m}{2}} \\ &= \exp\left\{-k/2\left[\ln\left(\frac{1+t^2}{t^2}\right) - \frac{E_m+\ln 2}{k}\right]\right\}\end{aligned}$$

For large k, and the suitably chosen time step

$$t < \left[\exp\left(\frac{E_m+\ln 2}{k}\right) - 1\right]^{-\frac{1}{2}}, \tag{23}$$

the terms approach to zero exponentially.

It should be noted that the energy cut off E_m is only used here for convergence proof. In practical calculations, we do not need to specify this cut off and the time step is chosen by test and error.

Comparing to the Chebyshev expansion, the methods of Hermite polynomial and Laguerre polynomial have an obvious advantage that no scaling to the Hamiltonian is needed. So that these expansions may have wider applications. On the other hand, the recurrence relation for both Hermite polynomial and Laguerre polynomial is not numerically absolute stable as compared to the recurrence relation of Chebyshev polynomial, which is marginal stable [27]. This fact limits the number of terms in the expansion to some value $k_{\max}$, the effect of numerical instability has little effect for $k < k_{\max}$ and the effect starts to show up beyond this cut off. In the practical calculations the $k_{\max}$ may be chosen to be 30, and the time step is set up accordingly with a specified error tolerance to get convergent results. The calculation schemes presented here are very general and are not dependent on the specific form of the Hamiltonian, however, the applicability should be tested for each kind of Hamiltonian before it can be used in practical simulations. The efficiencies of the three kinds of polynomial expansion are almost the same from our numerical calculation, careful comparison reveals that for the current models the Laguerre expansion with $\alpha = 1/2$ is a little bit faster than the others.

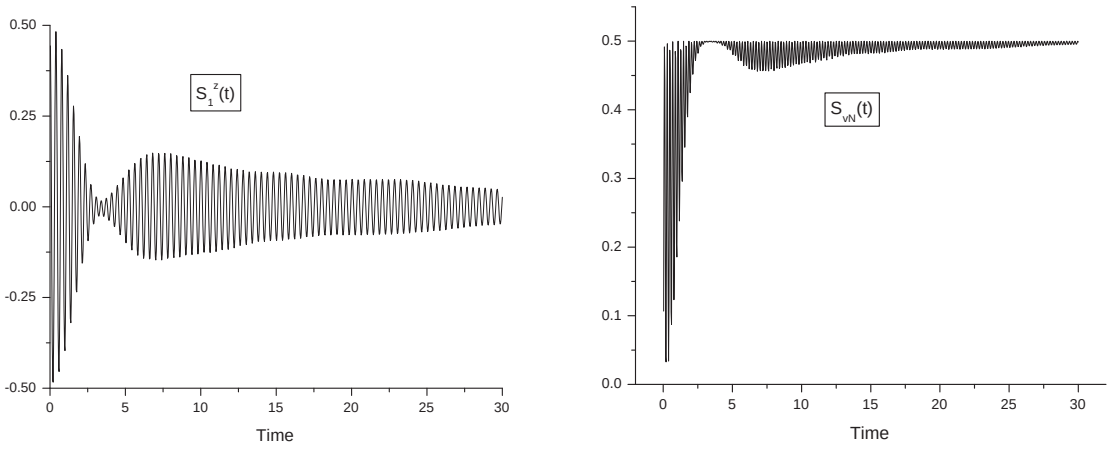
IV. NUMERICAL SIMULATION

A. Test of the spin model

The efficiency of the Chebyshev expansion over conventional method of calculation has already given by [9, 23]. In this section we checked numerically the efficiency of three kinds of polynomial expansions by comparing the performance among the three expansions as well as with the *predictor-corrector (P-C)* and *Runge-Kutta (R-K)* methods to the spin bath Hamiltonian given in section II. We calculated two particular variables using the Hamiltonian: (i) the z-component oscillation of any one of the center spins, i.e. s_i^z, $i = 1$ or 2, which demonstrated the decoherence rate of the system; (ii) the time dependence of von Neumann's entropy, i.e. $S_{vN} = -Tr\rho \ln \rho$, which characterizes the entanglement degree of the state of the system [5]. We use the same parameters as used in [9, 23], the exchange strength $J = 16.0$, A_k are uniformly distributed between 0 and 0.5; The initial condition of the system is $|\psi(0)\rangle = |\uparrow\downarrow\rangle$ or written as $|10\rangle$, and the environment is a normalized linear superposition of the product states of N spins with random coefficients. The time step is chosen as $\Delta t = 0.036$, which is determined by the compromise of convergence requirement, $\mathrm{T}r(\rho) = 1$, and the speed of computation. All of the three schemes are implemented and tested, the results are consistent with those given by [9, 23]. We also did the calculation with the two widely used ordinary differential equation solver, the *predictor-corrector (P-C)* and *Runge-Kutta (R-K)* methods. At the request of stability and speed, the time step in these two methods is almost 1/10 of that in polynomial scheme. We found that the calculation cost of the three polynomial expansion schemes are very close to each other, with the Laguerre polynomial expansion is slightly faster, and the results are practically the same. So we only give the datum thereinafter obtained by Laguerre polynomial expansion in the following.

Figure 1 are results of the oscillation of $s_1^z(t)$ and von Neumann's entropy $S_{vN}(t)$ of the spin-bath Hamiltonian with parameters given in the figure caption. The results are obtained by the Laguerre polynomial expansion method and are consistent with results by other methods we tested and those reported in literature [9, 23].

The comparison between computation costs of different methods with the same error



(a)Oscillation of $s_1^z(t)$ (b)Evolution of entropy $S_{vN}(t)$

FIG. 1: Decoherence of two coupled spins by a spin bath calculated by Laguerre method, the parameters are: $J = 16$, $N = 12$, the tolerance in obtained this figure is set to be 10^{-6}.

TABLE I: Comparison of the **R-K** method with the polynomial scheme (abbreviated as **P-S**)for the problem of decoherence of spin-bath

Scheme	Δt	*No. of bath-spin*	precision	t	CPU time
R-K	0.0036	4	10^{-6}	$9000\Delta t$	2 sec
P-S	0.036	4	10^{-6}	$900\Delta t$	2 sec
R-K	0.0036	8	10^{-6}	$9000\Delta t$	406 sec
P-S	0.036	8	10^{-6}	$900\Delta t$	50 sec
R-K	0.0036	10	10^{-6}	$9000\Delta t$	2065 sec
P-S	0.036	10	10^{-6}	$900\Delta t$	242 sec

tolerance listed in Table I. From the table we see that: (i) When N is very small, it is hard to distinguish the calculation speed of the two kinds of numerical computation methods; (ii) In general, the speed of polynomial scheme is about 8 times as fast as that of the direct solution methods, i.e, the Runge-Kutta (R-K) methods (the corresponding datum of predictor-corrector method are almost the same as R-K); (iii) With increasing N, the speed advantage becomes more evident. All the data reported here are obtained by a micro

computer with Intel Pentium M Banias Processor 1400MHz, Memory 256M.

B. The double well model with Laguerre polynomial scheme

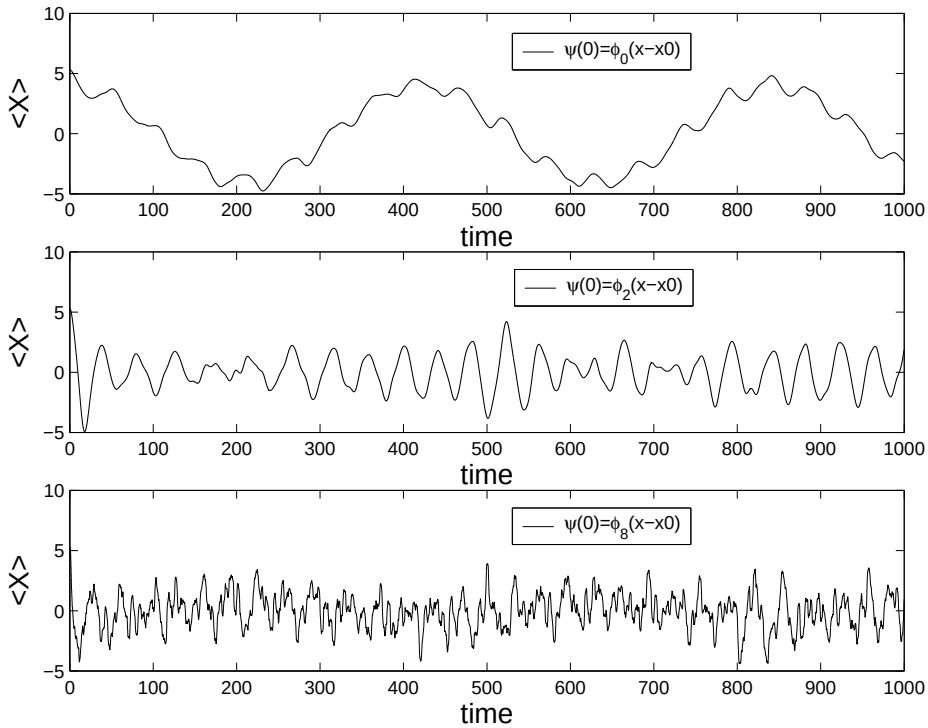


FIG. 2: The time evolution of $\langle x \rangle$ of three cases: (a), $\psi(0) = \phi_0(x - x_0)$; (b), $\psi(0) = \phi_2(x - x_0)$; (c), $\psi(0) = \phi_8(x - x_0)$. All of them are calculated in the condition of $\lambda/\omega = 0.0013$.

The Laguerre polynomial expansion scheme can easily be extended into the studies of continuous quantum systems. As an illustration, we used it in the calculation of the time-evolution of a given wave function packet in the double well system. The initial state prepared as one of the eigenstates of a harmonic oscillator with unit mass and frequency ω, centered at the bottom of the right well, $x_0 = \omega/\sqrt{4\lambda}$. That is:

$$\psi(0) = \left(\frac{\sqrt{\omega}}{\sqrt{\pi}2^m m!}\right)^{1/2} H_m(\sqrt{\omega}(x - x_0)) \exp[-\omega(x - x_0)^2/2]. \tag{24}$$

$H_m(x)$ is the Hermite polynomial of the mth order.

In order to use the Laguerre polynomial expansion scheme in the evaluation of the time evolution, we expand the state of the system by a complete basis state. In principle, any

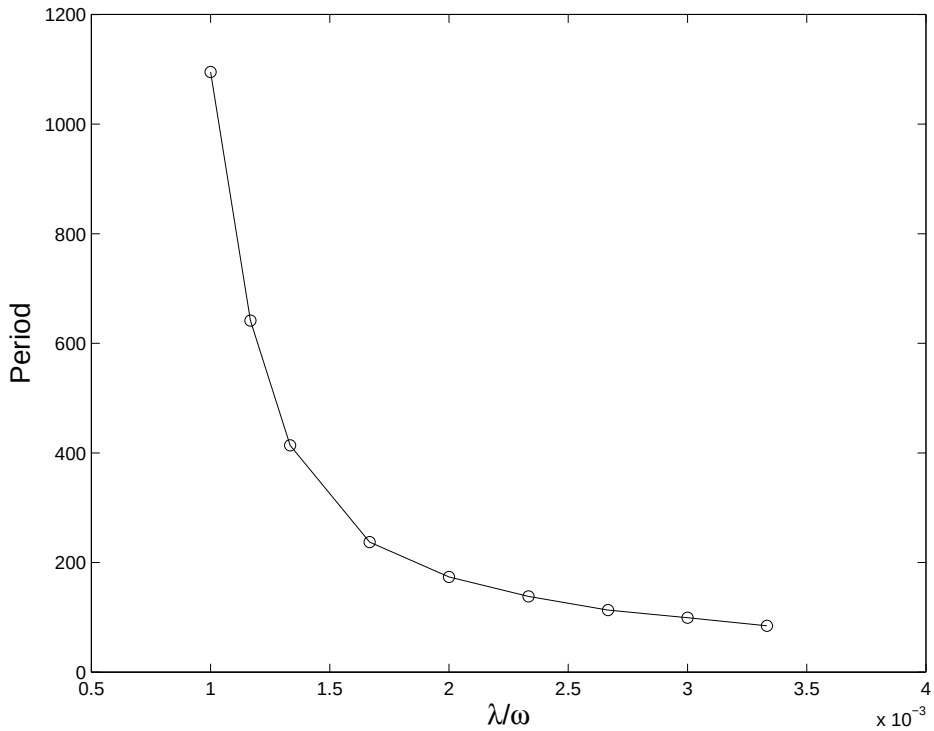


FIG. 3: The period of different λ/ω with the same initial state $\psi(0) = \phi_0(x - x0)$

complete basis can be used in this calculation, however, a better choice of the basis will greatly reduce the computation efforts and obtain high accuracy results. In this study we use the eigenstates of a simple harmonic oscillator, $\phi_n(x)$, $n = 0, 1, \cdots \infty$, abbreviated as $|n\rangle$ as as the expansion basis. The Hamiltonian of the simple harmonic oscillator that defines the basis is

$$h = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2. \tag{25}$$

This is not necessarily the optimized basis, however, calculation shows that it is pretty good in this problem.

By introduction of the creation operator a^+ and annihilation operator a, the matrix elements of the double-well Hamiltonian can easily be evaluated. The coordinate x and momentum p can be represented in terms of the operator a^+ and a:

$$\begin{aligned} x &= \sqrt{\frac{1}{2\omega}}(a^+ + a), \\ p &= i\sqrt{\frac{\omega}{2}}(a^+ - a). \end{aligned} \tag{26}$$

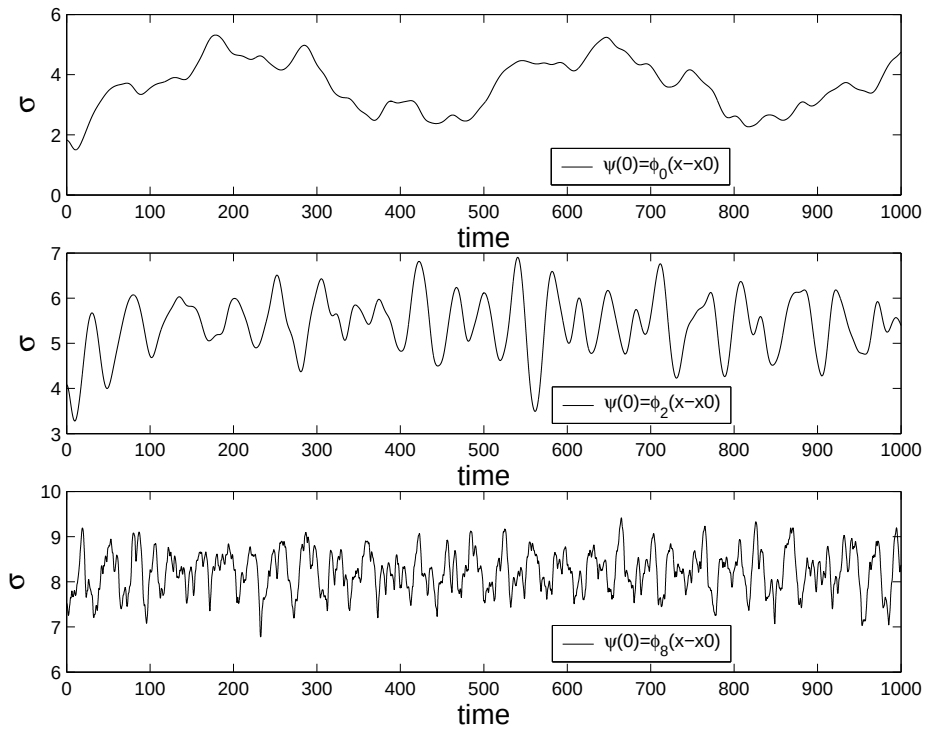


FIG. 4: The time evolution of Standard deviation of coordinate $\sigma = (\langle x^2\rangle - \langle x\rangle^2)^{1/2}$ of three cases: (a), $\psi(0) = \phi_0(x - x_0)$; (b), $\psi(0) = \phi_2(x - x_0)$; (c), $\psi(0) = \phi_8(x - x_0)$. All of them are calculated in the condition of $\lambda/\omega = 0.0013$.

The action of a^+ and a on $|n\rangle$ are:

$$a|n\rangle = \sqrt{n}|n-1\rangle, \tag{27}$$

$$a^+|n\rangle = \sqrt{n+1}|n+1\rangle, \tag{28}$$

$$h|n\rangle = \omega\left(n + \frac{1}{2}\right)|n\rangle.$$

In the a^+ and a representation, the double-well Hamiltonian (7) becomes:

$$H = -\frac{1}{2}\omega[(a^+)^2 + a^2] + \frac{\lambda}{4\omega^2}(a^+ + a)^4. \tag{29}$$

By using (27), the matrix elements of (29) can easily be obtained. And the matrix form of the Hamitonian can be substituted directly in the Laguerre polynomial expansion scheme providing a suitable cut off of the states is specified. In our calculation, we cut off the states at $n = 49$, at which in all cases we studied are already convergent. The initial state $\psi(0)$ in

the calculation is also expanded in terms of the $|n\rangle$. When $m = 0$ in (24), the expansion is:

$$\begin{aligned}\psi(0) &= \exp\left(-\frac{1}{2}\alpha_0^2\right)\sum_{n=0}^{N}\frac{\alpha_0^n}{\sqrt{n!}}|n\rangle, \\ \alpha_0 &= x_0\sqrt{\frac{\omega}{2}}.\end{aligned}$$

For other value of m in (24), the coefficients of the expansion can easily be evaluated numerically.

Using the Laguerre polynomial scheme, we calculated the average position $\langle x\rangle$ and the variation $\sigma = \left(\langle x^2\rangle - \langle x\rangle^2\right)^{1/2}$. Figure 2 plotted the evolution of the average position $\langle x\rangle$ with time. The initial states are the eigenstates of simple harmonic centered at the right well of the double well potential. For the state of $\phi_0(x - x_0)$, which is located at the x_0 initially, it oscillates back and forth with time. From figure 2(a) we see clearly the periodic motion and the period can easily be identified. The period depends on the value of λ/ω. Smaller λ/ω corresponding to a deeper well and thus a longer period. Figure 3 plots the period as a function of the ratio λ/ω, which is decreasing monotonically as expected. For the states of higher energies, though the initial state is also localized at the right potential well, the average position no longer follows a periodic oscillation between the two wells, instead, the particle spends most of the time moving around the center of the potential. Figure 4 are plots of the variation of the position, $\sigma = \left(\langle x^2\rangle - \langle x\rangle^2\right)^{1/2}$, as a function of time, which represents the width of the corresponding wave pocket. From the figure, we see that for the low energy state $\phi_0(x - x_0)$, the width is typically 4 as can be seen in the figure, smaller than the total width of the potential at the average energy of $\phi_0(x - x_0)$, which is about 10, and it looks like a wave pocket bouncing about. The energy of the state $\phi_0(x - x_0)$ for the parameters chosen is -0.0390, slightly lower than the height of the middle peak of the potential. The movement of the center of the particle between the two wells is a case of quantum tunneling. In the higher energy cases, the wave pocket spends most of the time oscillating around the center of the potential well and there is no well defined period can be found.

A similar problem was studied by Bender et al many years ago [28]. If we transform the x coordinate to q according to $q = x + \beta/2$ and set $\omega = \sqrt{8.0}$, the equation (7) is changed

into

$$H = \frac{1}{2}p^2 + 4q^2(q-\beta)^2/\beta^2 \tag{30}$$

which is exactly the equation (1) in reference [28]. We use the same initial conditions as used in [28] to calculate $\langle q \rangle$ by our scheme (Here the number of energy eigenstates N is truncated to 32, which is sufficient for convergent). The result is given in figure 5, which is the same as figure 1 in [28]. The calculation time for this figure is only about 4 seconds in a personal computer of Pentium(R) 4 CPU 2.60GHz, Memory 512M.

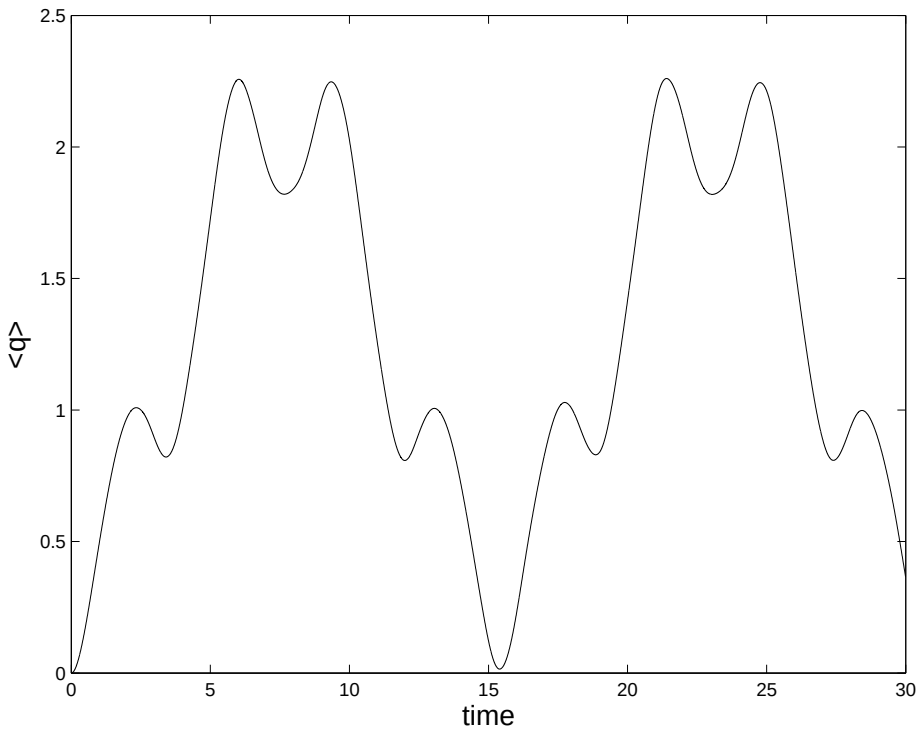


FIG. 5: Time dependence of $\langle q \rangle$ with $\beta = 2.5$

V. SUMMARY

In summary, we proposed a new polynomial scheme, the Laguerre polynomial expansion scheme, and tested its validity and efficiency by means of the spin bath model and a continuous double-well model. The obvious merit of this scheme compared to the Chebyshev polynomial expansion scheme is that no scaling to Hamiltonian is required, which means that a priori knowledge of the lower and upper bounds of the Hamiltonian is not needed. On the other hand, the computation efficiency and accuracy of the method are basically

the same as the Chebyshev polynomial expansion scheme.

We have also made use of the Laguerre expansion scheme in other kinds of model systems to study the affection of the intra-bath entanglement on the decoherence of the center spins. The method is also as efficient and accurate in those models as it was in the current spin bath model. The results will be reported in separate publications.

This work is supported by the National Nature Science Foundation of China under grant #10334020 and #90103035 and in part by the National Minister of Education Program for Changjiang Scholars and Innovative Research Team in University.

---

[1] Ulrich Weiss, *Quantum Dissipative Systems* (2nd edition), World Scientific 1999.

[2] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002).

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

[4] E. Joos, H.D. Zeh, et al *Decoherence and the Appearance of a Classical World in Quantum Theory* Springer-Verlag (2003)

[5] W.H. Zurek, Phys. Rev. D **24**, 1516 (1981)

[6] W.H, Zurek, Rev. Mod. Phys **75**, 715 (2003)

[7] C.W. Gardiner, *Quantum Noise* Springer-Verlag, Berlin, Heidelberg, New York (1991)

[8] K. Gottfried, Nature(London) **405**, 533 (2000)

[9] V.V. Dobrovitski, H.A. De Raedt Phys. Rev. E **67**, 056702 (2003)

[10] V. Braginsky and Khalili, *Quantum Measurement*, Cambridge University Press, London (1992)

[11] 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, Heidelberg, New York, (1996)

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

[13] S. Shresta, C. Anastopoulos, A. Dragulescu, and B.L. Hu, arXiv:quant-ph/0408084 v1 13 Aug

(2004)

[14] M. Frasca, arXiv:cond-mat/0303655 v2 24 Aug (2003)

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

[16] A. Askar and S. Cakmak, J. Chem. Phys. **68**,2794 (1978).

[17] D. Kosloff and R. Kosloff, J. Comp. Phys. **52**, 35(1983).

[18] A. Weiße, G. Wellein, A. Alvermann and H. Fehske, Rev. Mod. Phys. **78**, 275 (2006).

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

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

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

[22] E.W. Cheney *Introduction to Approximation Theory* McGraw Hill, New York, (1966)

[23] V.V. Dobrovitski, H.A. Raedt, M.I. Katsnelson, and B.N. Harmon, Phys. Rev. Lett. **90**, 210401 (2003)

[24] N.V. Prokofev, P.C.E. Stamp, Rep. Prog. Phys. **63**, 669 (2000)

[25] X.G. Hu, Phys. Rev. E **59**, 2471 (1999)

[26] G. Arfken, *Mathematical Methods of Physicists*, 3rd ed Academic, New York, (1985)

[27] W. H. Press, B. P. Flannery, S. A. Teukolsky and W. T. Vetterling, *Numerical Recipes*, Chapter 5, Cambridge University Press, Cambridge, (1986).

[28] C.M. Bender and F. Cooper, J.E. O'Dell, L.M. Simmons.Jr, Phys. Rev. Lett. **55**, 901 (1985)