An efficient Polynomial scheme for time evolution of quantum systems

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Orthogonal Polynomial Schemes

Two Examples

Conclusion

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Directory

1. Orthogonal Polynomial Schemes
   - Chebyshev and Hermite
   - Laguerre
2. Two Examples
   - a decoherence spin-model
   - A double well potential problem
3. Conclusion

time-Evolution of a quantum system

Time-dependent Schorödinger equation (differential equation group essentially):

$$i\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$$

$$\begin{cases} |\psi\rangle = U|\psi_0\rangle \\ U = \exp(-i\hat{H}t) \end{cases}$$

for quantum measurement hypothesis:

$$|\psi_0\rangle = \sum_n C_n|n\rangle|\chi\rangle \rightarrow \sum_n C_n(t)|n\rangle|\chi_n(t)\rangle$$

If $\langle\chi_n|\chi_m\rangle \approx \delta_{nm}$, then

$$\rho_s = \mathrm{T}r_E(\rho_{SE}) \approx \sum_n |C_n(t)|^2|n\rangle\langle n|$$

Chebyshev and Hermite polynomial schemes

We could expand the time-evolution operator by orthogonal polynomials:

$$1, \quad U(t) = \exp(-i\hat{H}t) \Rightarrow \exp(-i\tau\tilde{H}) = \sum_{k=0}^{\infty} c_k T_k(\tilde{H})$$

where $\tau = E_0 t/2$, $\tilde{H} = 2\hat{H}/E_0$, E_0 is a scale factor, $T_k(x) = \cos(k \arccos x)$ and $c_k = a_k(-i)^k J_k(\tau)$ with $J_k(\tau)$ the Bessel function of the kth order and $a_0 = 1$ as $k = 0$, $a_k = 2$ as $k \geqslant 1$.

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

Laguerre polynomial scheme

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

if $s = it/(\lambda+it)$, $x = \lambda\hat{H}$, then

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

and

$$\begin{aligned} \phi_0 &= \psi_0 \\ \phi_1 &= (\alpha+1-\hat{H})\psi_0 \\ (k+1)\phi_{k+1} &= (2k+\alpha+1-\hat{H})\phi_k - (k+\alpha)\phi_{k-1} \end{aligned}$$

Hamiltonian for a spin-bath model

Two-body open system in a bath of $m = N - 2$ spins without inner-coupling:

$$\hat{H} = 2J\vec{\sigma}_1 \cdot \vec{\sigma}_2 + \sum_{k=3}^{N} A_k(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{\sigma}_k.$$

where

$$\vec{\sigma} = \sigma_x \vec{i} + \sigma_y \vec{j} + \sigma_z \vec{k}$$

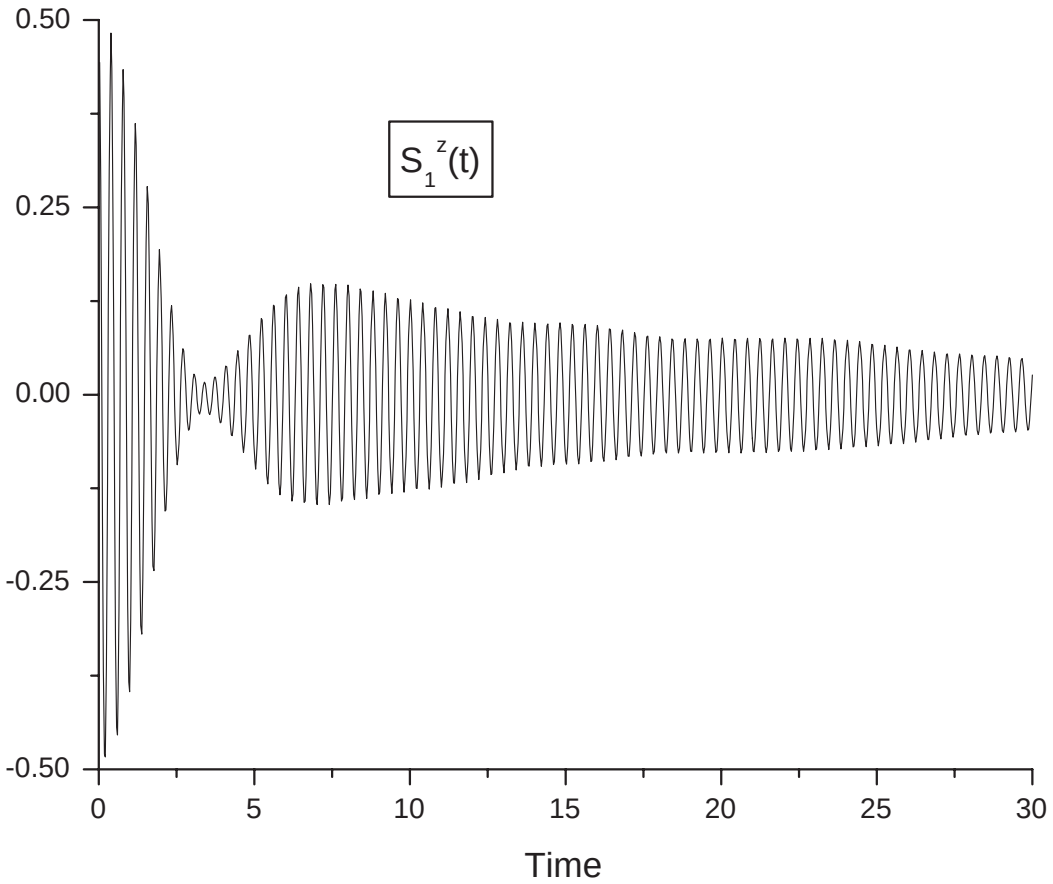
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and

$$A_k \ll J.$$

z-component oscillation

The z-component oscillation of any one of the center spins, i.e. $\langle s_i^z \rangle$, $i = 1$ or 2.



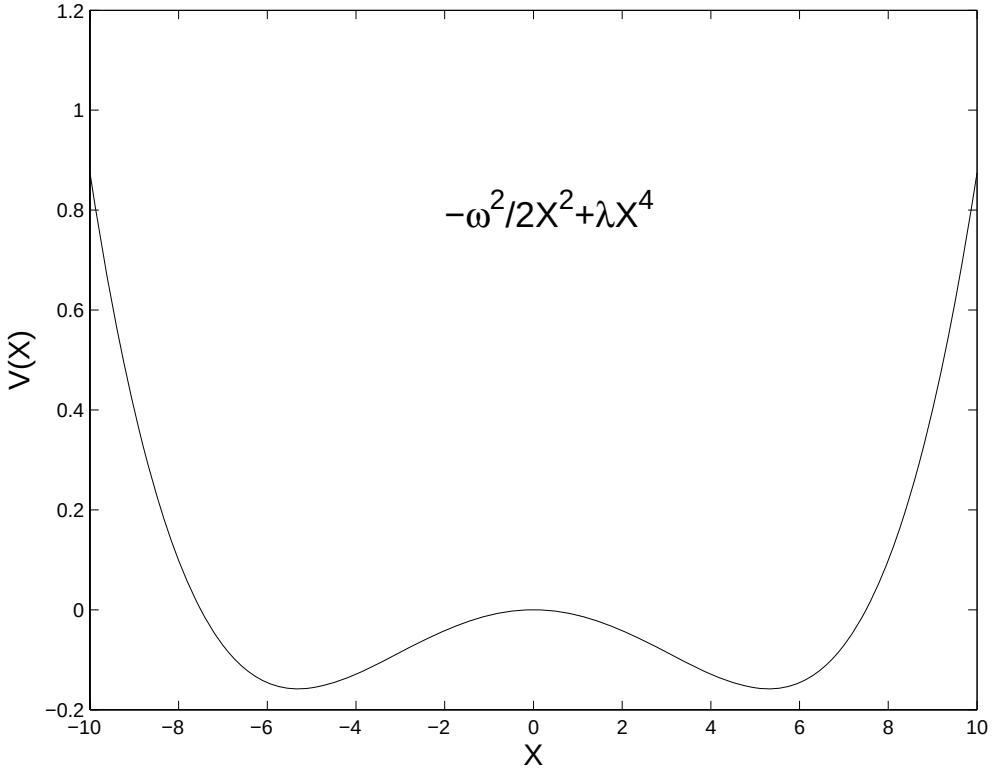
Comparison of the polynomial scheme with the Runge-Kutta method

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

Scheme	Δt	m	precision	t	CPU time
R-K	0.0036	4	10^{-6}	$9000\Delta t$	2
P-S	0.036	4	10^{-6}	$900\Delta t$	2
R-K	0.0036	8	10^{-6}	$9000\Delta t$	406
P-S	0.036	8	10^{-6}	$900\Delta t$	50
R-K	0.0036	10	10^{-6}	$9000\Delta t$	2065
P-S	0.036	10	10^{-6}	$900\Delta t$	242

Hamiltonian for a particle in double-well

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



The depth of the well is $\frac{\omega^4}{16\lambda}$, and the bottom is $|x_0| = \omega/\sqrt{4\lambda}$.

Initial condition

The initial state is:

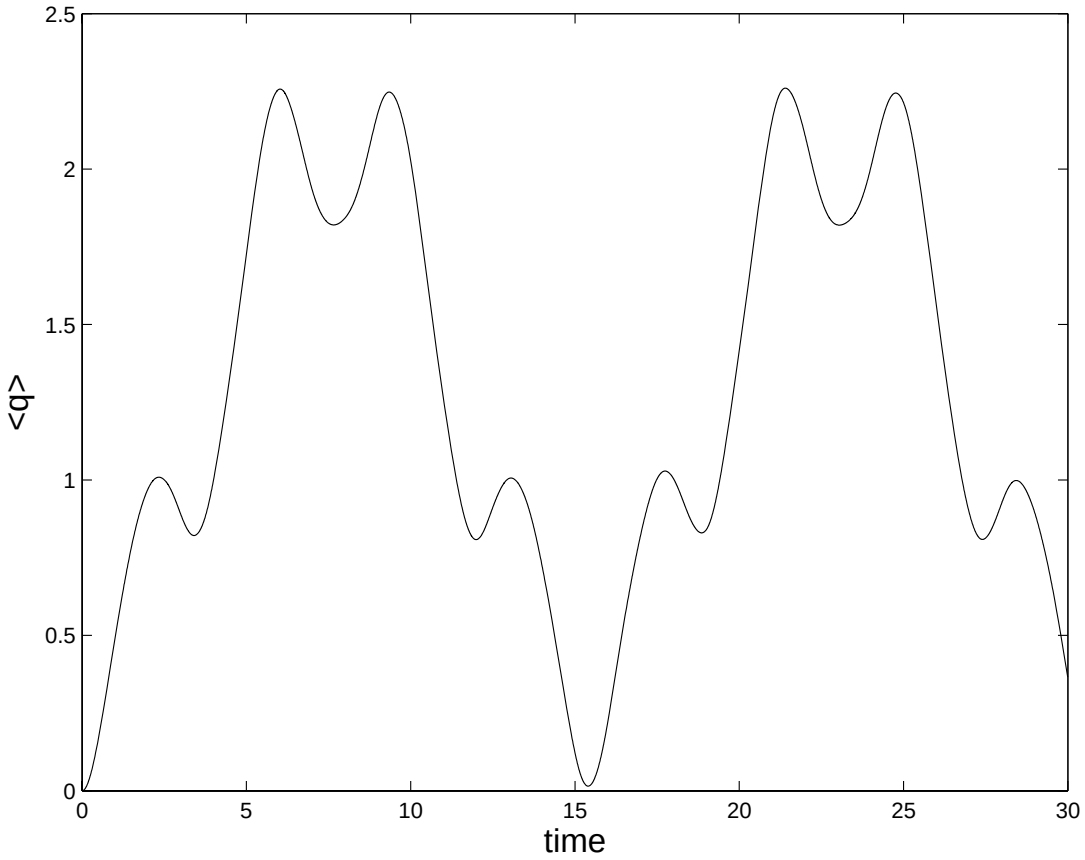
$$\psi(0) = \left(\frac{\omega}{\pi}\right)^{1/4} e^{-\omega(x-x_0)^2/2} = \phi_n(x - x_0)$$

$\phi_n(x) = |n\rangle$ is one eigenstate of $h = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2$, so

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

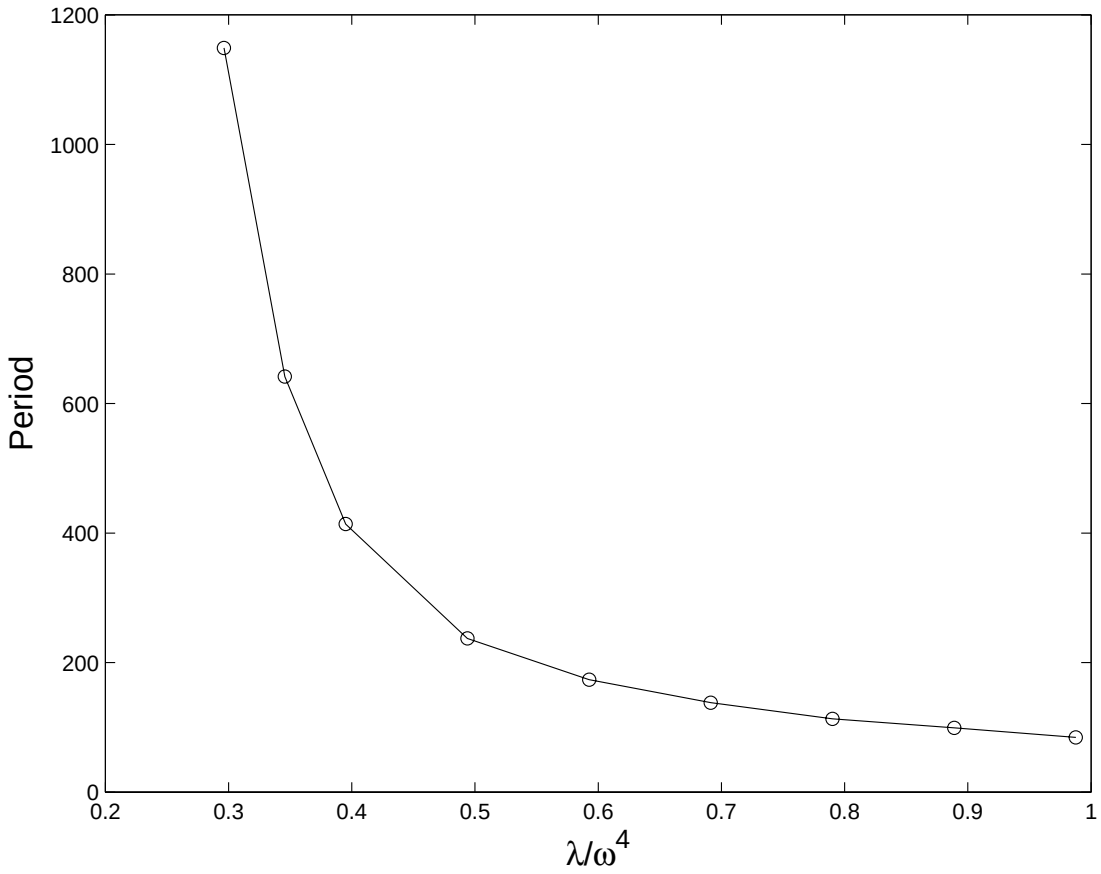
The average position of the particle

If the x coordinate is transformed to q by $q = x + x_0$, $\omega = \sqrt{8.0}$ and $\psi(0) = \phi_0(x - x_0)$, the average position of the particle is:



The relation between period with λ/ω^4

The period as a function of the ratio λ/ω^4 with $\psi(0) = \phi_0(x - x_0)$: it is decreasing monotonically as expected.



Remarks

- The obvious merit of the Laguerre and Hermite polynomial compared to the Chebyshev polynomial expansion scheme is that no scaling to Hamiltonian is required.
- The computation efficiency and accuracy of the method is much better than ordinary differential equation solver, the *predictor-corrector (P-C)* and *Runge-Kutta (R-K)* methods.
- The Laguerre scheme could be applied into the dynamics of other types of Quantum system with great suitability and efficiency.

Thank you!