Comparison of the Chebyshev Method and the Generalized Crank-Nicholson Method for time Propagation in Quantum Mechanics

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Abstract. We compare efficiency of two methods for numerical solution of the time-dependent Schrödinger equation, namely the Chebyshev method and the recently introduced generalized Crank-Nicholson method. As a testing system the free propagation of a particle in one dimension is used. The space discretization is based on the high-order finite diferences to approximate accurately the kinetic energy operator in the Hamiltonian. We show that the choice of the more effective method depends on how many wave functions must be calculated during the given time interval to obtain relevant and reasonably accurate information about the system, i.e. on the choice of the time step.

Keywords: time propagation, time-dependent problems, Chebyshev method, Crank-Nicholson method
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INTRODUCTION

In atomic, molecular, and nuclear physics many problems which are described within the quantum mechanics lead to a system of coupled time-dependent Schrödinger equations (see for example reviews [1]) which we write in a concise form as (for simplicity we use atomic units, i.e. we set $\hbar = 1$ and $m_e = 1$)

$$i\frac{\partial \Psi(t)}{\partial t} = H\Psi(t) \tag{1}$$

which describes the time evolution of a quantum-mechanical system from some initial state $\Psi(t = t_0) = \Psi_0$ whose dynamics is given by its Hamiltonian H. Once the wave function $\Psi(t)$ is obtained at all times of interest one can extract physically relevant quantities (such as transition probabilities) from it using e.g. the Fourier transform.

Because analytical solutions are not available for most of the systems, efficient and accurate numerical techniques of solving (1) are needed. Several efficient methods were proposed in the past (see [1, 2] and references therein) and still new methods are introduced as for example the generalization of the Crank-Nicholson method based on the Padé approximation of the evolution operator. In this paper we compare this generalized Crank-Nicholson method [3, 4, 5] with the Chebyshev method [6, 7, 8]. We apply them to propagation of a free particle and compare them with respect to efficiency.

CHEBYSHEV METHOD

Instead of solving directly the equation (1) we will use an equivalent approach and write the wave function at the time $t + \Delta t$ in the form

$$\Psi(x, t + \Delta t) = \exp(-iH\Delta t)\Psi(x, t) \tag{2}$$

where the time-evolution operator $\exp(-iH\Delta t)$ propagates the wave function from t to $t + \Delta t$.

The Chebyshev method (see [6] for details of the derivation) is based on the approximation of the evolution operator in Eq. (2) as

$$\exp(-iH\Delta t) \approx \sum_{k=0}^{M} a_k T_k(X) \tag{3}$$

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where $T_k(x)$ is the Chebyshev polynomial of the order k, X denotes the operator (scaled Hamiltonian)

$$X = \frac{2H - (E_{max} + E_{min})}{E_{max} - E_{min}}, \tag{4}$$

E_{max} and E_{min} being the largest and smallest eigenvalues of the Hamiltonian, and the coefficients a_k are given as

$$a_k = (-i)^k e^{R+G}(2 - \delta_{k0}) J_k(|R|) \tag{5}$$

where $J_k(x)$ is the Bessel function of the first kind and

$$R = -i\Delta t(E_{max} - E_{min})/2, \qquad G = -i\Delta t E_{min}. \tag{6}$$

For the given Hamiltonian with the highest and lowest eigenvalues E_{max} and E_{min} and for a given time step Δt, i.e. for a particular R one can always choose M large enough to have the coefficients a_k for $k > M$ negligible due to exponential decrease of the Bessel function $J_k(|R|)$ for a fixed $|R|$ as $k \to \infty$.

GENERALIZED CRANK-NICHOLSON METHOD

The generalized Crank-Nicholson method [3] for the time propagation of the wave function can be derived from (2) if the exponential function is approximated using the diagonal Padé I [N/N] rational function (see e.g. [10])

$$\exp(z) \approx \frac{1 + a_1 z + a_2 z^2 + \cdots + a_N z^N}{1 - a_1 z + a_2 z^2 - \cdots + (-1)^N a_N z^N} = \prod_{s=1}^{N} \left(\frac{1 - z/z_s^{(N)}}{1 + z/[z_s^{(N)}]^*} \right) \tag{7}$$

where $z_s^{(N)}$ are the roots of the polynomial in the numerator. The wave function at the time $t + \Delta t$ can be then calculated as

$$\Psi(x, t + \Delta t) \approx \prod_{s=1}^{N} K_s^{(N)} \Psi(x, t) \tag{8}$$

where the operators $K_s^{(N)}$ are defined as

$$K_s^{(N)} = \frac{1 + iH\Delta t/z_s^{(N)}}{1 - iH\Delta t/[z_s^{(N)}]^*} \tag{9}$$

and $z_s^{(N)}$ are the complex roots of the numerator in the Padé I [N/N] approximation of the exponential function.

The time propagation given by (8) is much more precise with less computational effort than the standard Crank-Nicholson method which is a special case of the described method for $N = 1$ as was demonstrated in [4, 5].

RESULTS FOR FREE PROPAGATION OF THE ONE-DIMENSIONAL GAUSSIAN WAVE-PACKET

To compare accuracy and efficiency of the Chebyshev and the generalized Crank-Nicholson method we have chosen the simplest system, free propagation of a particle of the mass μ in the one-dimension, for which the Hamiltonian operator is simply

$$H = -\frac{1}{2\mu} \frac{d^2}{dx^2}. \tag{10}$$

As the initial state we have used the Gaussian wave-packet of the width σ_0 localized at x_0 with the momentum p_0

$$\psi_0(x, t = 0) = \frac{1}{(2\pi\sigma_0^2)^{1/4}} e^{-\frac{(x - x_0)^2}{4\sigma_0^2}} e^{ip_0(x - x_0)}. \tag{11}$$

For this benchmark system there exists an analytical solution (see e.g. [9]) for all times t having also the shape of the Gaussian wave-packet

$$\psi(x,t) = \frac{1}{(2\pi\sigma^2(t))^{1/4}} e^{-\frac{(x-x_0(t))^2}{4\sigma^2(t)}} e^{i\varphi(x,t)} \tag{12}$$

where the mean position and width are given as

$$x_0(t) = x_0 + \frac{p_0 t}{\mu}, \qquad \sigma^2(t) = \sigma_0^2 + \frac{t^2}{4\mu^2\sigma_0^2} \tag{13}$$

and the phase changes with time as

$$\varphi(x,t) = p_0(x - x_0(t)) + \frac{(x-x_0(t))^2}{8\mu\sigma_0^2\sigma^2(t)} t + \frac{p_0^2}{2\mu} t + \mathrm{Arg}\left(\frac{1}{\sqrt{\mu + \frac{it}{2\sigma_0^2}}}\right). \tag{14}$$

The function Arg returns the argument of a complex number.

Both approximative methods for time evolution described above are more or less independent of the particular Hamiltonian if we would be able to represent Hamiltonian with high accuracy. In practical applications in quantum-mechanical problems one usually represents the Hamiltonian on a numerical grid discretizing the underlying configuration space or in some basis to which the wave function of the system is expanded. Here we discretize the one-dimensional space using equidistant grid and approximate the second order derivative in the Hamiltonian (10) using the high order $(2r+1)$-point finite-difference scheme.

In particular, the numerical values used in our calculations are summarized in the Table 1. The mass is close to proton mass and the space interval and grid have been chosen to be large and dense enough to provide sufficient accuracy during the whole propagation.

TABLE 1. Numerical values used in our calculations. All values are in atomic units ($\hbar = 1$ and $m_e = 1$).

Mass	Initial state			Space grid			
μ	x_0	p_0	σ	x_{min}	x_{max}	Δx	r
1836	-10	12	1/2	-30	30	0.02	8

In the Table 2, we compare effectiveness of the Chebyshev and generalized Crank-Nicholson method to propagate the free particle wave packet with a given accuracy for time interval from $t_0 = 0$ to $\tau = 4000$ a.u. The errors e_{Ch} and e_{CN} shown in the Table 2 are the errors of the wave function at the time $\tau = 4000$ a.u. defined for both methods as

$$e^2 = \int_{x_{min}}^{x_{max}} dx \left|\Psi(x,\tau) - \Psi^{exact}(x,\tau)\right|^2 \tag{15}$$

where the exact solution $\Psi^{exact}(x,\tau)$ is given by Eq. (14), i.e. $\Psi^{exact}(x,\tau) = \varphi(x,\tau)$. For each time step Δt we set up the parameters of both methods to get the accuracy of about 10^{-11} or better. The most relevant number characterizing the efficiency of the Chebyshev method is the number of multiplications of the wave function by the operator X and the efficiency of the generalized Crank-Nicholson method is the number of multiplications of the wave function by the operator $K_s^{(N)}$ which is equal to the number of the matrix inversions performed during the time propagation.

As the time step is increased we can see from the Table 2 that the number of applications of both operators X and $K_s^{(N)}$ on the wave function is rapidly decreasing while obtaining the same accuracy. A similar decrease we observe for the CPU time T. Though the Chebyshev method is 4 times faster than the generalized Crank-Nicholson method for the time step 0.02 a.u., for larger time steps we can see that both methods become equally efficient and for very large time steps the generalized Crank-Nicholson method is even faster because the number of applications of $K_s^{(N)}$ drops more rapidly than the number of applications of X.

Which method is finally more efficient for a given problem will, of course, depend on the used computer architecture and on the optimization of the numerical implementation of the matrix multiplication and matrix inversion. Even though we expect that in general a similar result would be obtained.

TABLE 2. Comparison of efficiency of the Chebyshev and generalized Crank-Nicholson methods: for each given time step (i.e. for a given number $n = \tau/\Delta t$ of wave function evaluations over the time $\tau = 4000$ a.u.) we determined the orders M (as one can observe it is always greater than $|R|$) and N needed to obtain the absolute error given by Eq. (15) of the order 10^{-11} or better, the corresponding number of applications of the operator X, see eq. (4), in the Chebyshev method and of the operator $K_s^{(N)}$, see eq. (9), in the generalized Crank-Nicholson method and the CPU time T for both methods are also shown.

		Chebyshev					generalized Crank-Nicholson			
Δt	n	$\|R\|$	M	$\#X$	e_{Ch}	T_{Ch}[s]	N	$\#K_s^{(N)}$	e_{CN}	T_{CN}[s]
0.02	200000	0.04	7	1600000	$8.4(-11)$	715.0	2	400000	$2.4(-12)$	2390.9
0.05	80000	0.1	8	720000	$3.9(-11)$	263.4	2	160000	$8.2(-12)$	975.3
0.1	40000	0.2	9	400000	$9.7(-12)$	142.9	3	120000	$2.3(-12)$	726.1
0.2	20000	0.4	11	240000	$5.2(-12)$	110.2	3	60000	$2.3(-12)$	390.0
0.5	8000	1.1	14	120000	$2.2(-12)$	44.6	3	24000	$2.6(-12)$	146.6
1	4000	2.2	17	72000	$5.7(-12)$	28.8	4	16000	$2.1(-12)$	103.3
2	2000	4.3	22	46000	$5.2(-12)$	17.1	4	8000	$2.2(-12)$	50.3
5	800	11	34	28000	$2.4(-12)$	10.2	5	4000	$2.3(-12)$	27.2
10	400	22	49	20000	$8.0(-12)$	7.3	6	2400	$2.4(-12)$	13.5
20	200	43	77	15600	$4.7(-12)$	5.8	8	1600	$2.3(-12)$	9.5
50	80	108	152	12240	$5.7(-12)$	5.0	10	800	$2.4(-12)$	4.7
100	40	215	270	10840	$5.1(-12)$	4.2	15	600	$2.5(-12)$	3.6
200	20	430	498	9980	$4.2(-12)$	3.8	20	400	$2.3(-12)$	2.5

CONCLUSIONS

Two efficient numerical techniques for solving the time-dependent Schrödinger equation were compared. It was shown that if the same accuracy is to be obtained the choice of the more effective method depends on a particular time step. For short time steps for which only small number of terms in the Chebyshev method is needed to get very accurate approximation of the evolution operator, the Chebyshev method is several times faster than the generalized Crank-Nicholson method. As the time step is increased the Crank-Nicholson method becomes more effective because of relatively small number of the matrix inversions needed to obtain high accuracy while the number of terms in the Chebyshev approximation grows rapidly for large time steps.

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