Solving the time-dependent Schrödinger equation numerically

Toshiaki Iitaka*
Department of Solid State Physics, Weizmann Institute of Science, Rehovot 76100, Israel
and Department of Physics, Waseda University, Tokyo 169, Japan
(Received 11 October 1993)

We introduce an explicit scheme to solve the time-dependent Schrödinger equation. The scheme is a straightforward extension of the second order differencing scheme to the fourth, sixth, and higher order accuracy. The accuracy is remarkably improved with minor changes in the second order differencing program. This method is conditionally stable. There is a trade-off between the higher order accuracy and the condition of stability. The performance is evaluated and compared to the standard methods, such as the Crank-Nicholson scheme (CN) and the Chebyshev scheme (CH). The new scheme is much more accurate than CN, almost equal to CH.

PACS number(s): 02.70.−c

I. INTRODUCTION

With the increasing availability of high performance computers, the development of efficient integration methods of the time-dependent Schrödinger equation [1]

$$i\frac{d}{dt}|\phi,t\rangle = H|\phi,t\rangle \tag{1}$$

has become an important task in various fields of physics such as scattering theory [2], quantum chaos [3], quantum wire [4], tunneling time problem [5], laser-atom or laser-molecule interactions [6,7], etc. In this paper, we assume that H is a *time-independent* Hamiltonian represented by an $N \times N$ Hermitian matrix and $|\phi,t\rangle$ is a wave function represented by an N-dimensional complex vector. The atomic unit $\hbar = m_e = e = 1$ is used throughout this article. The eigenstates of the Hamiltonian are denoted as

$$H|E_m\rangle = E_m|E_m\rangle, \quad (m = 1,2,\ldots,N) \tag{2}$$

while the range of energy spectrum is defined as

$$\Delta E_{grid} = E_{max} - E_{min}, \tag{3}$$

where $E_{max} = \max[\{E_m\}]$ and $E_{min} = \min[\{E_m\}]$ are the largest and the smallest eigenvalues of the Hamiltonian.

The formal solution of (1) is expressed by the time evolution operator, which is represented by a matrix exponential function [1]

$$|\phi,t+\Delta t\rangle = \exp(-iH\Delta t)\,|\phi,t\rangle. \tag{4}$$

Various schemes have been proposed to approximate this exponential function [8–10]. The simplest Euler scheme (EU) expands the exponential function to the first order of $H\Delta t$

$$|\phi;t+\Delta t\rangle = (1-iH\Delta t)|\phi;t\rangle + O((H\Delta t)^2), \tag{5}$$

and uses (5) repeatedly to obtain $|\phi;t+n\Delta t\rangle$. This is an explicit scheme, that is, it does not need matrix inversion, but it is unstable due to the lack of the time symmetry $(t \to -t)$. Moreover it is not unitary.

To avoid this instability, the Crank-Nicholson scheme (CN) has been widely used in which the exponential function is approximated by Caley transform

$$|\phi,t+\Delta t\rangle = \frac{1-iH\Delta t/2}{1+iH\Delta t/2}|\phi,t\rangle + O((H\Delta t)^3). \tag{6}$$

This scheme is unitary, unconditionally stable, and accurate up to $(H\Delta t)^2$. However, this implicit method is prohibitive in more than two dimensions due to the large memory and CPU time required by the matrix inversion. Therefore, the development of explicit, stable integration methods has been desired.

One of these explicit methods is the product formula [9]. Another is the symmetrized version of the EU, which is called the second order differencing scheme (MSD2) [10],

$$\begin{aligned}|\phi,t+\Delta t\rangle - |\phi,t-\Delta t\rangle &= [\exp(-iH\Delta t) - \exp(+iH\Delta t)]\,|\phi,t\rangle \\ &= -2iH\Delta t|\phi,t\rangle + O((H\Delta t)^3).\end{aligned} \tag{7}$$

This scheme is symmetric in time and shown to be conditionally stable [10]. Furthermore the scheme is accurate up to $(H\Delta t)^2$.

The more accurate and stable method is the Chebyshev scheme (CH) [8]. This method is classified as a global propagator method. It uses very long time steps and sometimes completes the calculation with a single time step. The CH approximates the exponential function in (4) by a Chebyshev polynomial expansion

*Electronic address: iitaka@cfi.waseda.ac.jp

$$|\phi,t\rangle = \exp[-i(\Delta E_{grid}/2 + E_{min})t] \times \sum_{n=0}^{N_{CH}} a_n(\beta)\,\Phi_n(-iH_{norm})\,|\phi,t=0\rangle, \quad (8)$$

where the Φ_n are the Chebyshev polynomials, $\beta = \Delta E_{grid}t/2$, and $a_n(\beta) = 2J_n(\beta)$ with $a_0(\beta) = J_0(\beta)$. Here $J_n(x)$ is Bessel function of the first kind. The normalized Hamiltonian is defined as

$$H_{norm} = \frac{2}{\Delta E_{grid}}\left[H - I\left(\frac{\Delta E_{grid}}{2} + E_{min}\right)\right], \quad (9)$$

where I is the $N \times N$ identity matrix. The number of terms is taken as $N_{CH} > \beta$ to converge the sum, because the coefficient $J_n(\beta)$ decreases exponentially for $n > \beta$. The CH is very accurate and the error can be reduced up to the machine limit. The only shortcoming of the CH is that the intermediate wave functions are not available, while the stepwise methods, such as the CN and the MSD2, produce the wave function at each time step. The purpose of this paper is to develop improved versions of MSD2 that have both the advantages of the MSD2 and the accuracy of the CH.

II. MULTISTEP DIFFERENCING SCHEME

The extension of MSD2 (7) to the higher order accuracy forms, which we call the multistep differencing scheme (MSD), is straightforward. For example, the fourth and sixth order MSD (MSD4 and MSD6) are, respectively,

$$|\phi,t+2\Delta t\rangle = |\phi,t-2\Delta t\rangle - 4iH\Delta t\left[-\frac{1}{3}|\phi,t\rangle + \frac{2}{3}\left(|\phi,t+\Delta t\rangle + |\phi,t-\Delta t\rangle\right)\right] + O((H\Delta t)^5), \quad (10)$$

$$|\phi,t+3\Delta t\rangle = |\phi,t-3\Delta t\rangle - 6iH\Delta t\left[\frac{13}{10}|\phi,t\rangle - \frac{7}{10}\left(|\phi,t+\Delta t\rangle + |\phi,t-\Delta t\rangle\right) + \frac{11}{20}\left(|\phi,t+2\Delta t\rangle + |\phi,t-2\Delta t\rangle\right)\right] + O((H\Delta t)^7). \quad (11)$$

Equation (10) for the MSD4 is derived as follows. First, we expand the exponential functions

$$e^{-2iH\Delta t} - e^{+2iH\Delta t} = -4iH\Delta t - \frac{8}{3}(iH\Delta t)^3 + O((H\Delta t)^5) = -4iH\Delta t\left(1 + \frac{2}{3}(iH\Delta t)^2\right) + O((H\Delta t)^5), \quad (12)$$

$$e^{-iH\Delta t} + e^{+iH\Delta t} = 2 + (iH\Delta t)^2 + O((H\Delta t)^4). \quad (13)$$

Then, comparing (12) and (13), we obtain

$$e^{-2iH\Delta t} - e^{+2iH\Delta t} = -4iH\Delta t\left(-\frac{1}{3} + \frac{2}{3}(e^{-iH\Delta t} + e^{+iH\Delta t})\right) + O((H\Delta t)^5). \quad (14)$$

Finally, Eq. (10) is derived by multiplying (14) to $|\phi,t\rangle$. The sixth and the higher order MSD's are derived also in a similar way. Note that these schemes have symmetry in time as the MSD2.

III. STABILITY, ERROR, AND COST ANALYSIS

Let us study the time evolution of the eigenstates $|E_m\rangle$ in various schemes, i.e., the EU, CN, and MSD's. Note that (5)–(7), (10), and (11) contain only identity matrices and Hamiltonian matrices. Therefore the wave function remains in the same eigenstate during the time evolution if the initial wave functions are prepared in an eigenstate. Thus the growth factor g can be defined as

$$|E_m,t+\Delta t\rangle = g|E_m,t\rangle, \quad (15)$$

where g is a complex number. Here we ignored the possible t dependence of g as in Ref. [10]. If the scheme calculates the exact time evolution, the growth factor becomes

$$g = \exp(-iE_m\Delta t). \quad (16)$$

However, an approximate scheme gives the growth factor of general form

$$g = |g|\exp(-iE_m\Delta t + i\epsilon_{phase}). \quad (17)$$

If $|g| \neq 1$, then the error in norm grows exponentially as $|g|^{N_{step}} - 1$, where N_{step} is the number of time step. Thus the scheme becomes unstable. On the other hand, if $|g| = 1$, then the norm is conserved, and the accumulating error appears mainly in the phase error ϵ_{phase}. Note that phase error accumulates, after N_{step} time evolution, as

$$\epsilon_{phase}^{N_{step}} = \epsilon_{phase}N_{step}, \quad (18)$$

which grows not exponentially but linearly in time.

Introducing (15) into (5), we obtain the growth factor equation of the EU,

$$g + i\alpha - 1 = 0, \tag{19}$$

where α is the dimensionless time step

$$\alpha = E_m \Delta t. \tag{20}$$

Then, the scheme is found to be unconditionally unstable,

$$|g| = \sqrt{1+\alpha^2} > 1. \tag{21}$$

For the CN of (6), the growth factor equation becomes

$$g = \frac{1 - i\alpha/2}{1 + i\alpha/2}, \tag{22}$$

from which the unconditional stability of CN is shown as

$$|g| = \frac{|1 - i\alpha/2|}{|1 + i\alpha/2|} = 1. \tag{23}$$

For the MSD2 of (7), we obtain the growth factor equation

$$g^2 + 2i\alpha g - 1 = 0 \tag{24}$$

and its solutions

$$g_{1,2} = -i\alpha \pm \sqrt{1-\alpha^2}. \tag{25}$$

If the stability condition $\alpha \leq 1$ is satisfied, the absolute value of the growth factor becomes unity,

$$|g_1| = |g_2| = 1, \tag{26}$$

which shows that the MSD2 is conditionally stable.

In the same way, the growth factor equations are obtained for the MSD4 and MSD6, respectively,

$$g^4 + \frac{8}{3}i\alpha g^3 - \frac{4}{3}i\alpha g^2 + \frac{8}{3}i\alpha g - 1 = 0, \tag{27}$$

$$g^6 + \frac{33}{10}i\alpha g^5 - \frac{21}{5}i\alpha g^4 + \frac{39}{5}i\alpha g^3 - \frac{21}{5}i\alpha g^2 + \frac{33}{10}i\alpha g - 1 = 0. \tag{28}$$

The absolute value of the numerical solutions of (27) and (28) are plotted in Fig. 1 as a function of α. The graphs show that MSD4 is stable if $\alpha < 0.4$ and MSD6 is stable if $\alpha < 0.1$. There is a trade-off between the higher order accuracy and the condition of the stability.

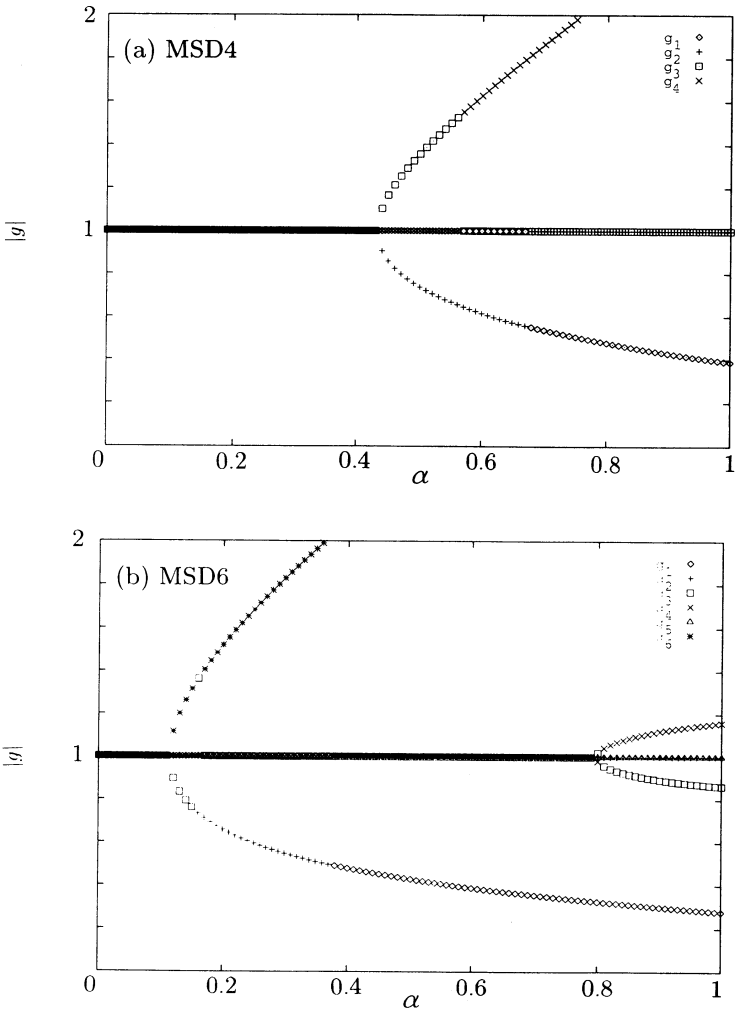

FIG. 1. The absolute value of the growth factors g_i as a function of the dimensionless time step $\alpha = E_m \Delta t$. (a) MSD4 and (b) MSD6.

The phase error under the stability condition can be estimated by the Taylor expansion of the time evolution operators in (6), (7), (10), and (11),

$$\epsilon_{phase}^{CN} = \frac{1}{12}\alpha^3 N_{step}, \tag{29}$$

$$\epsilon_{phase}^{MSD2} = -\frac{1}{6}\alpha^3 N_{step}, \tag{30}$$

$$\epsilon_{phase}^{MSD4} = \frac{7}{90}\alpha^5 N_{step}, \tag{31}$$

$$\epsilon_{phase}^{MSD6} = -\frac{41}{840}\alpha^7 N_{step}. \tag{32}$$

The above criteria about the stability and the errors can also be applied to a general wave function, which is a superimposition of many eigenstates, by redefining the parameter α as

$$\alpha = E_c \Delta t, \tag{33}$$

where

$$E_c = \max[|E_{max}|, |E_{min}|]. \tag{34}$$

Now let us study the computational cost of the MSD and the CH. The CPU time T_{CPU} can be estimated by the number of matrix multiplying operations. For MSD, it is equal to the number of time steps,

$$T_{CPU} = t/\Delta t = (E_c t)/\alpha \tag{35}$$

and, for the CH, it is equal to the number of Chebyshev polynomials N_{CH} in (8), which is estimated as

$$T_{CPU} = E_c t/2. \tag{36}$$

Thus the MSD costs $2/\alpha$ times more than the CH. However, the MSD produces $(E_c t)/\alpha$ intermediate wave functions, while the CH usually produces only one final wave function. Thus the CPU time per wave function becomes 1 for the MSD and $E_c t/2$ for the CH. Therefore the cost of MSD per wave function is less than that of the CH by the factor $2/E_c t$.

IV. NUMERICAL EXAMPLES

In this section, we study the Hamiltonian of an electron in one dimension,

$$H = \frac{p^2}{2} + V(x), \tag{37}$$

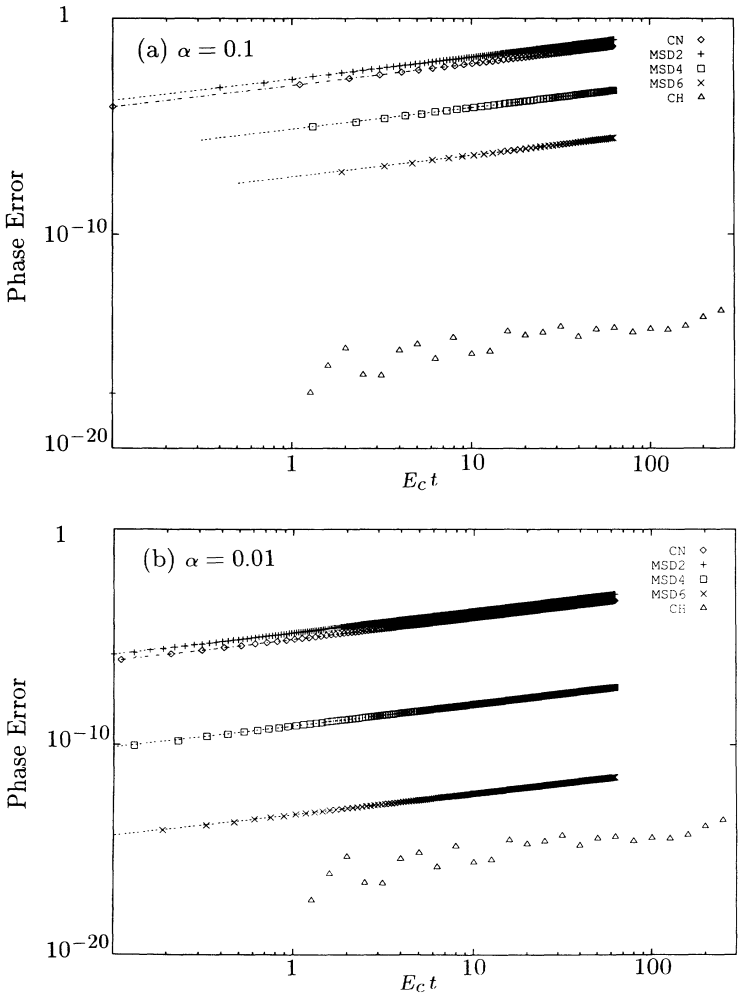

FIG. 2. Phase error in the time evolution of $|E_1\rangle$. The dimensionless time step is (a) $\alpha = 0.1$ and (b) $\alpha = 0.01$. The lines show the theoretical predictions.

TABLE I. Grid, potential, and wave function parameters (atomic units)

Grid	Potential	Wave function
$\Delta x = 1$	$V_0 = 0.2$	$\bar{x} = 25$
$N = 100$	$x_L = 45$	$k = 0.63$
	$x_R = 55$	$\sigma = 10$

where $V(x)$ is the static potential. After discretizing in space, the Hamiltonian is approximated by the tight binding form

$$H = \frac{-1}{2\Delta x^2} \sum_{i=0}^{N+1} \left(c_i^\dagger c_{i+1} + c_i c_{i+1}^\dagger \right) + \sum_{i=0}^{N+1} \epsilon_i c_i^\dagger c_i, \quad (38)$$

where $\epsilon_i = V(x_i)$ and $c_i^\dagger$ and c_i are the creation and annihilation operators of an electron at the site $x_i = i \times \Delta x (i = 0, 1, \ldots, N+1)$. The boundary condition is set as

$$\langle i = 0 | \phi \rangle = \langle i = N+1 | \phi \rangle = 0, \quad (39)$$

where $|i\rangle$ is the electron state at the ith site. Note that the energy is shifted by $-1/\Delta x^2$ so that E_c becomes smaller. The Hamiltonian (38) is represented by a symmetric tridiagonal matrix of N dimension.

In the following, we take (38) as the starting point of our study and do not discuss the errors caused by the space discretization from (37) to (38), since the aim of this paper is to evaluate the accuracy of the time evolution scheme but not of the space discretization scheme.

A. Eigenstates

In the case of $V(x) = 0$, the exact eigenstates and eigenvalues of the Hamiltonian (38) with the boundary conditions (39) are well known,

$$|E_m\rangle = A \sum_{i=0}^{N+1} \sin\left(\frac{mi}{N+1} \pi \right) |i\rangle, \quad (40)$$

$$E_m = \frac{-1}{\Delta x^2} \cos\left(\frac{m}{N+1} \pi \right), \quad (41)$$

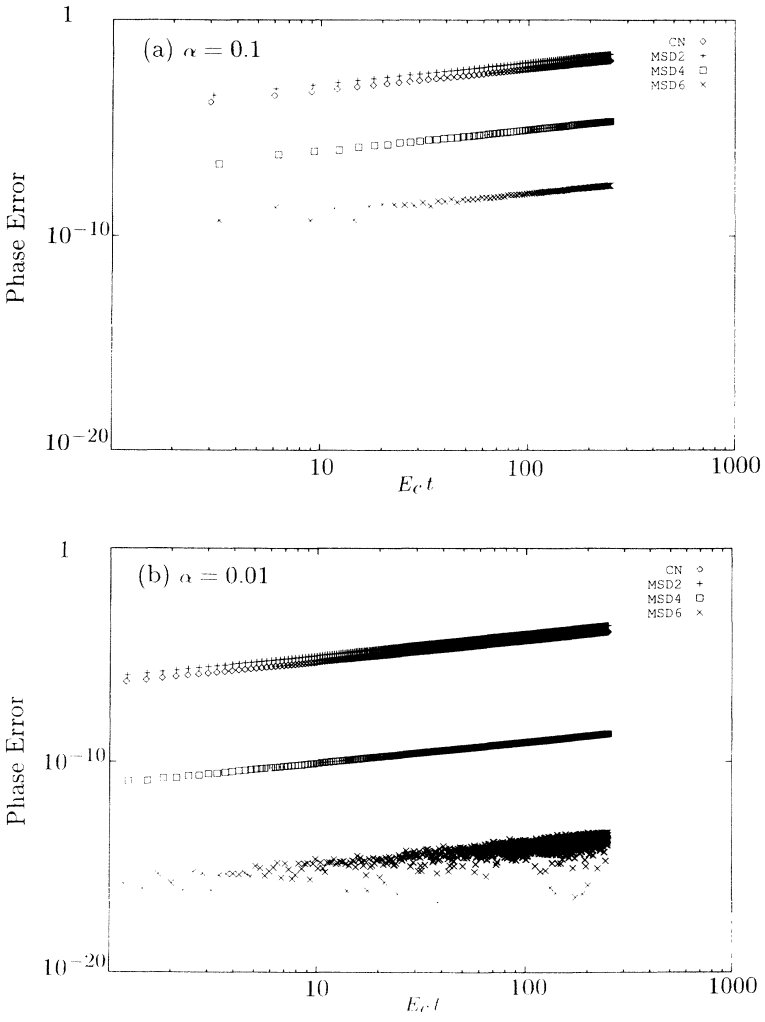

FIG. 3. Phase error in the scattering of a wave packet. The dimensionless time step is (a) $\alpha = 0.1$ and (b) $\alpha = 0.01$.

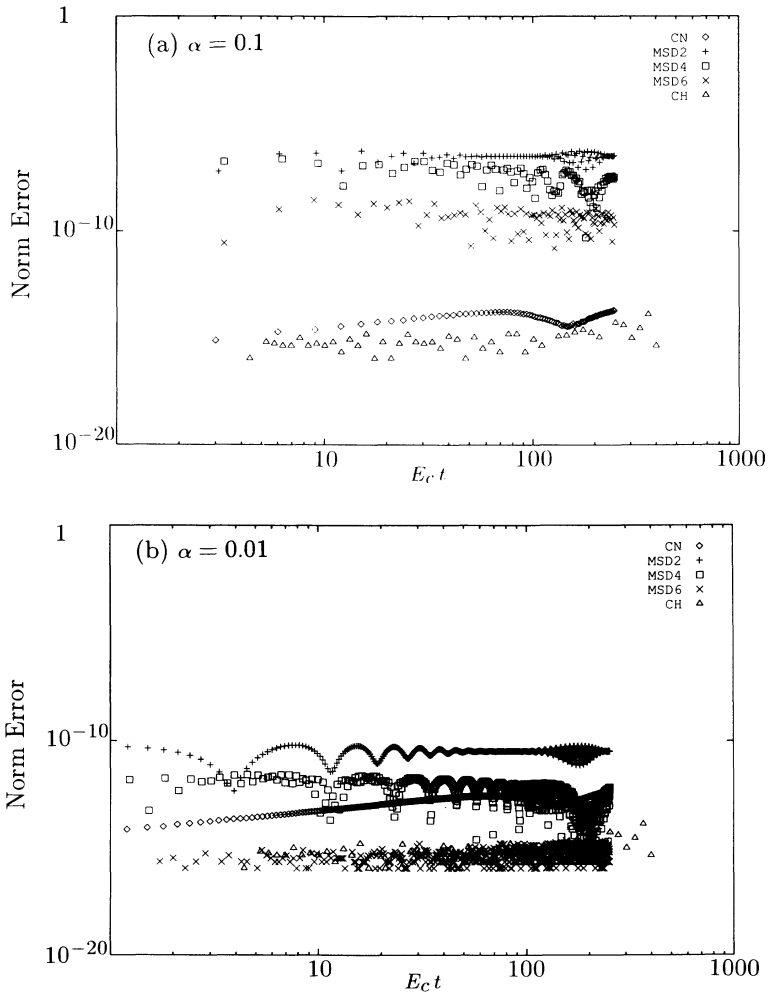

FIG. 4. Norm error in the scattering of a wave packet. The dimensionless time step is (a) $\alpha = 0.1$ and (b) $\alpha = 0.01$.

where A is a normalizing constant and m is an integer $m = 1, 2, \ldots, N$. Therefore, the exact time evolution of $|E_m\rangle$ is calculated from (40) and (41) as

$$|E_m, t\rangle_{exact} = \exp(-iE_m t)\,|E_m\rangle. \tag{42}$$

All numerical results in this article are calculated in the complex double precision of FORTRAN.

Figure 2 shows the phase error of $|E_1, t\rangle_{calc}$ calculated by the five schemes (CN, MSD2, MSD4, MSD6, and CH) as a function of the dimensionless time $E_m t$. The phase error is defined as

$$\epsilon_{phase} = |\arg[{}_{calc}\langle E_m, t|E_m, t\rangle_{exact}]|\,. \tag{43}$$

The auxiliary initial wave functions at $t = \Delta t, 2\Delta t, \ldots$, required by the MSD's are calculated directly from (42). The state $m = 1$ is chosen as an example since it has the largest $|E_m|$, forcing the severest condition of accuracy. Errors of other eigenstates are much smaller. The parameter α is 0.1 in Fig. 2(a) and 0.01 in Fig. 2(b). The error becomes smaller for higher order schemes and for smaller time step α. See Table I for other parameters. The theoretical predictions of the error (29)–(32), are also shown in the figures by lines, which agree with the calculated values. Note that the error of the CH is the smallest and does not depend on the value of α, as each plot of the CH is calculated from the initial state by a single global time step. Since the error of the MSD6 is proportional to α^7, it approaches to the accuracy of the CH when $\alpha = 0.01$.

B. Scattering of a wave packet

Figure 3 shows the phase error in the scattering of a wave packet as a function of the dimensionless time $E_c t$. Figure 3(a) is for $\alpha = 0.1$ and Fig. 3(b) is for $\alpha = 0.01$. Since we have no exact solution of this problem, we use the solution of the CH in place of the exact one. Thus the phase error is not available for the CH. See Table I for other parameters. Note that the time is taken sufficiently long so that the wave packet is scattered by the potential. The initial wave function is a Gaussian wave packet

$$\langle i|\phi\rangle = \frac{1}{\pi^{1/4}\sqrt{\sigma}} \exp\left(ik(x_i - \bar{x}) - \frac{(x_i - \bar{x})^2}{2\sigma^2}\right) \tag{44}$$

and the auxiliary initial wave functions at $t = \Delta t, 2\Delta t, \ldots$, which are necessary to start the MSD, are prepared by using the Taylor expansion of the time evolution operator

$$|\phi;t\rangle = \exp(-iHt)\,|\phi;t=0\rangle \approx \sum_{n=0}^{N_{order}} \frac{(-iHt)^n}{n!}|\phi;t=0\rangle, \quad (45)$$

where N_{order} is the order of the MSD. The scattering potential is a rectangular potential

$$V(x_i) = \begin{cases} V_0 & (x_L \le x_i \le x_R) \\ 0 & (\text{otherwise}). \end{cases} \quad (46)$$

Qualitatively, Fig. 3 shows the same features as Fig. 2, while the error is smaller than that of Fig. 2. The reason is because a wave packet is a superimposition of many eigenstates whose error is smaller than that of $|E_1\rangle$.

Figure 4 shows the norm error in the scattering of a wave packet as a function of the dimensionless time $E_c t$. The norm error

$$\epsilon_{norm} = |\,{}_{calc}\langle\phi,t|\phi,t\rangle_{calc} - 1| \quad (47)$$

is smaller than the phase error and does not increase monotonically as a function of time.

V. SUMMARY

In summary, we proposed an integration scheme of the time-dependent Schrödinger equation, which is a natural extension of the conventional second order differencing scheme. We compared the performance of the higher order MSD and that of the MSD2. If the stable condition is satisfied, the MSD2 can be replaced by the higher order MSD with a slight increase of CPU time and memory storage, but also with orders of improvement in accuracy. Therefore higher order MSD is superior to the MSD2 when the accuracy is important.

Comparing the higher order MSD with the CH, the MSD requires $2/\alpha$ times CPU time for the accuracy comparable to the CH, $\alpha = 0.01$ for the MSD6, but it produces $E_c t/\alpha$ times more intermediate wave functions, so that the cost per wave function becomes $2/E_c t$ of that of the CH. Therefore the higher order MSD is recommended rather than the CH when the intermediate wave functions are important.

ACKNOWLEDGMENTS

The author is grateful to Professor Y.H. Ohtsuki and Professor H. Fukuyama for their encouragement and to Professor Y. Imry for his hospitality at Weizmann Institute of Science. He wishes to thank Dr. H. Sakai for careful reading of the manuscript. This work was supported by the Japan Society for the Promotion of Science.

[1] J.J. Sakurai, *Modern Quantum Mechanics* (The Benjamin/Cummings Publishing Company, Redwood City, CA, 1985).
[2] H. Kröger, Phys. Rep. **210**, 45 (1992).
[3] S. Tomsovic and E.J. Heller, Phys. Rev. Lett. **67**, 664 (1991); Phys. Rev. E **47**, 282 (1993).
[4] J. Wang and H. Guo, Phys. Rev. B **48**, 12 072 (1993).
[5] C.R. Leavens, Solid State Commun. **85**, 115 (1993); N. Carjan, O. Serot, and D. Strottman, Proceedings of the 4th International Symposium on Foundations of Quantum Mechanics, Tokyo, 1992 [JJAP Ser. **9**, 86 (1993)].
[6] C. Cerjan and R. Kosloff, Phys. Rev. A **47**, 1852 (1993).
[7] B.M. Garraway and S. Stenholm, Phys. Rev. A **46**, 1413 (1992); K.A. Suominen, B.M. Garraway, and S. Stenholm, *ibid.* **45**, 3060 (1992).
[8] C. Leforestier, R.H. Bisseling, C. Cerjan, M.D. Feit, R. Friesner, A. Guldberg, A. Hammerich, G. Jolicard, W. Karrlein, H.-D. Meyer, N. Lipkin, O. Roncero, and R. Kosloff, J. Comput. Phys. **94**, 59 (1991).
[9] H.D. Raedt, Comput. Phys. Rep. **7**, 1 (1987).
[10] A. Askar and A.S. Cakmak, J. Chem. Phys. **68**(6), 2794 (1978).