Numerical solutions of the Schrödinger equation with source terms or time-dependent potentials

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We develop an approach to solving numerically the time-dependent Schrödinger equation when it includes source terms and time-dependent potentials. The approach is based on the generalized Crank-Nicolson method supplemented with an Euler-MacLaurin expansion for the time-integrated nonhomogeneous term. By comparing the numerical results with exact solutions of analytically solvable models, we find that the method leads to precision comparable to that of the generalized Crank-Nicolson method applied to homogeneous equations. Furthermore, the systematic increase in precision generally permits making estimates of the error.

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I. INTRODUCTION

Recent interest in accurate numerical solutions of the time-dependent Schrödinger equation (TDSE) using a generalized Crank-Nicolson (CN) approach [1,2], suggests further study for cases where the Schrödinger equation has a nonhomogeneous term and where the Hamiltonian is time dependent. Over the years the method of choice for solving the homogeneous Schrödinger equation with time-independent interactions has been the Chebyshev expansion of the propagator introduced in 1984 by Talezer and Kosloff [3]. However, comparison of this method with the generalized CN approach, in which the time-evolution operator is expressed as a Padé approximant [4], demonstrates that the two approaches are similar in efficiency and accuracy. Under different circumstances either method may outperform the other [5]. One advantage of the Padé approach is that it is explicitly unitary, whereas the Chebyshev-expansion approach is not. Since the latter can give very precise wave functions, however, this does not seem to be an issue in practice.

The Chebyshev-propagator method has recently been applied to nonhomogeneous Schrödinger equations [6] and to time-dependent Hamiltonians [7]. Given that Padé-approximant expression of the propagator yields comparable results for homogeneous systems, this paper explores the extension of the Padé-approximant method to solving nonhomogeneous equations. A natural sequitur is an approach to solve equations in which the interaction is time dependent. For such a case the time-dependent interaction term can be considered to be the nonhomogenous term and the solution can be obtained by self-consistent iterations. We also discuss this approach. A decided advantage of the method discussed in this paper is that the basic calculations are unitary whereas the wave functions do not in general have time-independent normalization. The calculations with unitary operators places a strong constraint on the problem resulting in stable solutions.

Solutions of the TDSE form the basis of the study of a multitude of nonrelativistic quantum systems. For stationary states, such as bound states, one can reduce the problem to the determination of solutions of the time-independent Schrödinger equation. For detailed investigations of quasistable systems or more general time-dependent systems one needs to solve the TDSE. There are only a few analytically solvable models (see, e.g., Refs. [8,9] and references contained in them), but most realistic systems require numerical solutions. In an earlier paper [1] (hereafter referred to as I) we presented an accurate and efficient method for obtaining solutions of the homogeneous Schrödinger equation in one dimension and for uncoupled partial waves in three dimensions.

In some problems, however, it is necessary to solve the nonhomogeneous Schrödinger equation. Among others, two important classes of problems involve such equations. The first concerns systems in which the Hamiltonian can be split into parts, one of which leads to an exact analytic solution. Consider the Hamiltonian of a system $H = H_0 + V_1$. The wave function Ψ describing the system is the solution of

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)\Psi = 0. \tag{1.1}$$

If the wave function of the system with H_0 instead of H is Ψ_0, we can obtain Ψ through a correction Ψ_1, so that $\Psi = \Psi_0 + \Psi_1$, by solving

$$\left(i\hbar\frac{\partial}{\partial t} - H_0 - V_1\right)\Psi_1 = V_1\Psi_0, \tag{1.2}$$

where $(i\hbar\frac{\partial}{\partial t} - H_0)\Psi_0 = 0$. This formulation is exact and may also be useful when Ψ_0 is known analytically and V_1 not necessarily small.

The second class deals with problems associated with reactions in which particles are created or annihilated. The nonhomogeneity in the TDSE plays the role of a source or sink of these particles. The bremsstrahlung associated with α decay is an example of such a process [10,11].

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The interaction of particles with a strong radiation field can be formulated in terms of a TDSE in which the Hamiltonian is explicitly time-dependent [7,12]. Such systems can be formulated as nonhomogeneous equations where the wave function is a factor in the source term. The solution for the nonhomogeneous equation can be adapted to solve such equations.

In this paper we present a method of numerically obtaining solutions to the nonhomogeneous Schrödinger equation, which are accurate to an arbitrary order of the spatial and temporal step size. The method, like that for the homogeneous Schrödinger equation [1], proves to be capable of high precision and efficiency.

In Sec. II we derive the numerical solution to the nonhomogeneous equation. We do this in stages to develop the notation and eventually generalize the method to arbitrary order in time. The approach is evaluated by comparison to analytically known solutions in Sec. III. In Sec. IV the numerical solutions when the interaction depends on time is discussed and compared to known exact solutions. We conclude with summary comments in Sec. V.

II. GENERALIZED CRANK-NICOLSON METHOD IN THE PRESENCE OF A NONHOMOGENEOUS TERM

Let us consider the TDSE with a nonhomogeneous term. Suppressing the dependence on spatial coordinate(s) we write the equation as

$$\left(i\hbar\frac{\partial}{\partial t}-H\right)\psi(t)=N(t). \tag{2.1}$$

For now we assume that the Hamiltonian H is independent of time t. The homogeneous equation corresponding to Eq. (2.1) has a solution, which can be written in terms of the time-evolution operator, i.e.,

$$\psi_{\rm h}(t+\Delta t)=e^{-iH\Delta t/\hbar}\psi_{\rm h}(t). \tag{2.2}$$

The nonhomogeneous equation has a particular solution

$$\psi_{\rm nh}(t+\Delta t)=-\frac{i}{\hbar}e^{-iH(t+\Delta t)/\hbar}\int_t^{t+\Delta t}e^{iHt'/\hbar}N(t')\,dt'. \tag{2.3}$$

The general solution is

$$\psi(t)=\psi_{\rm h}(t)+\psi_{\rm nh}(t) \tag{2.4}$$

with the boundary condition value inserted such that $\psi(t_0)=\psi_{\rm h}(t_0)=\phi$ where ϕ is a normalized function of the spatial coordinate(s). Thus the solution with the appropriate boundary condition may be obtained by increasing t (starting at t_0) by steps equal to Δt using

$$\psi(t+\Delta t)=e^{-iH\Delta t/\hbar}\psi(t)-\frac{i}{\hbar}e^{-iH\Delta t/\hbar}\int_0^{\Delta t}e^{iH\theta/\hbar}N(t+\theta)\,d\theta. \tag{2.5}$$

A. Trapezoidal rule

Using the trapezoidal rule for the integral in Eq. (2.5), we obtain

$$\psi(t+\Delta t)=e^{-iH\Delta t/\hbar}\psi(t)-\frac{i}{\hbar}e^{-iH\Delta t/h}\frac{\Delta t}{2}[e^{iH\Delta t/\hbar}N(t+\Delta t)+N(t)]+O[(\Delta t)^3]. \tag{2.6}$$

In the spirit of Moyer [13], we write

$$\psi(t+\Delta t)+\frac{i\Delta t}{2\hbar}N(t+\Delta t)=e^{-iH\Delta t/\hbar}\left(\psi(t)-\frac{i\Delta t}{2\hbar}N(t)\right)+O[(\Delta t)^3]. \tag{2.7}$$

Expanding the time-evolution operator to the lowest-order unitary form, we obtain

$$\psi(t+\Delta t)+\frac{i\Delta t}{2\hbar}N(t+\Delta t)=\frac{1-\frac{i}{2\hbar}H\Delta t}{1+\frac{i}{2\hbar}H\Delta t}\left(\psi(t)-\frac{i\Delta t}{2\hbar}N(t)\right)+O[(\Delta t)^3]. \tag{2.8}$$

The expansion of the time-evolution operator and the trapezoidal rule both give an error term that is of third order in Δt. We rewrite this equation as

$$\left(1+\frac{i}{2\hbar}H\Delta t\right)\left[\psi(t+\Delta t)+\frac{i\Delta t}{2\hbar}N(t+\Delta t)\right]=\left(1-\frac{i}{2\hbar}H\Delta t\right)\left[\psi(t)-\frac{i\Delta t}{2\hbar}N(t)\right]+O[(\Delta t)^3]. \tag{2.9}$$

If we include the x dependence of $\psi(t)$ and $N(t)$ explicitly, the equation is

$$\left(1+\frac{i}{2\hbar}H\Delta t\right)\left[\psi(x,t+\Delta t)+\frac{i\Delta t}{2\hbar}N(x,t+\Delta t)\right]=\left(1-\frac{i}{2\hbar}H\Delta t\right)\left[\psi(x,t)-\frac{i\Delta t}{2\hbar}N(x,t)\right]+O[(\Delta t)^3], \tag{2.10}$$

and is similar to Eq. (2.5) of I. It can therefore be solved numerically as outlined in Sec. II of I to any order of accuracy in Δx. We define

$$\Psi^{(\pm)}(x,t)=\psi(x,t)\pm\frac{i\Delta t}{2\hbar}N(x,t). \tag{2.11}$$

The solution with a time advance of step Δt is found by solving the equivalent of Eq. (2.12) of I, i.e.,

$$A\Psi_{n+1}^{(+)}=A^*\Psi_n^{(-)}, \tag{2.12}$$

where the matrix A is defined in I and the vector $\Psi_n^{(\pm)}$ has components $\psi_{j,n}\pm(i\Delta t/2\hbar)N_{j,n}$. (As in I we use partitions of x: $x_0,x_1,\ldots,x_j,\ldots,x_J$ with $\Delta x=x_j-x_{j-1}$ and of t: $t=t_0,t_1,\ldots,t_n,\ldots$ with $\Delta t=t_n-t_{n-1}$.) Since $N(x,t)$ is a given known function for all x and t, and $\psi(x,t)$ is presumed known

from the calculation of the previous step, $\psi(x,t+\Delta t)$ can be determined from the calculated $\Psi_{n+1}^{(+)}$. Thus we obtain a solution, which has an error of $O[(\Delta x)^{2r}]$ for any integer $r>0$ in the x dependence and of $O[(\Delta t)^3]$ in the t dependence. (The parameter r determining the order of the spatial integration is defined in I.)

B. Improved integration over time

In order to obtain higher-order approximations to the time evolution of the solution of the nonhomogeneous TDSE, we use a quadrature of higher order than the trapezoidal rule in Eq. (2.5). Let us consider the Euler-MacLaurin formula [14, formula 23.1.31],

$$\int_0^{\Delta t} f(\theta)\,d\theta = \frac{\Delta t}{2}[f(\Delta t)+f(0)] - \sum_{k=1}^{M-1}\frac{B_{2k}}{(2k)!}(\Delta t)^{2k}[f^{(2k-1)}(\Delta t)-f^{(2k-1)}(0)] - \frac{(\Delta t)^{2M+1}}{(2M)!}B_{2M}f^{(2M)}(\eta\Delta t)$$

$$= \frac{\Delta t}{2}[f(\Delta t)+f(0)] - \sum_{k=1}^{M-1}\frac{B_{2k}}{(2k)!}(\Delta t)^{2k}[f^{(2k-1)}(\Delta t)-f^{(2k-1)}(0)] + O[(\Delta t)^{2M+1}], \tag{2.13}$$

where $0\leqslant\eta\leqslant 1$. The B_i, $i=1,2,\ldots$ are the Bernoulli numbers, i.e., $B_1=1/2, B_2=1/6, B_3=0, B_4=-1/30, B_5=0$, $B_6=1/42, B_7=0, B_8=-1/30,\ldots$. It should be noted that if $f(\theta)$ is not a polynomial, the Euler-MacLaurin formula is an asymptotic series [15, pg. 469].

The first term of the sum includes the next higher approximation compared to Eq. (2.6). We obtain

$$\psi(t+\Delta t) = e^{-iH\Delta t/\hbar}\psi(t) - \frac{i}{\hbar}e^{-iH\Delta t/\hbar}\frac{\Delta t}{2}[e^{iH\Delta t/\hbar}N(t+\Delta t)+N(t)]$$

$$+\frac{i}{\hbar}e^{-iH\Delta t/\hbar}\frac{(\Delta t)^2}{12}\left[\frac{i}{\hbar}He^{iH\Delta t/\hbar}N(t+\Delta t)+e^{iH\Delta t/\hbar}N'(t+\Delta t)-\frac{i}{\hbar}HN(t)-N'(t)\right]+O[(\Delta t)^5], \tag{2.14}$$

where the prime refers to differentiation with respect to t. Rearranging the equation we get

$$\psi(t+\Delta t)+\frac{i\Delta t}{2\hbar}N(t+\Delta t)-\frac{i(\Delta t)^2}{12\hbar}\left[\frac{i}{\hbar}HN(t+\Delta t)+N'(t+\Delta t)\right]$$

$$= K_2^{(2)}K_1^{(2)}\left\{\psi(t)-\frac{i\Delta t}{2\hbar}N(t)-\frac{i(\Delta t)^2}{12\hbar}\left[\frac{i}{\hbar}HN(t)+N'(t)\right]\right\}+O[(\Delta t)^5], \tag{2.15}$$

where $K_s^{(M)}$ is defined in I as [15]

$$K_s^{(M)} \equiv \frac{1+(iH\Delta t/\hbar)/z_s^{(M)}}{1-(iH\Delta t/\hbar)/\bar{z}_s^{(M)}}. \tag{2.16}$$

The order in which the operators $K_s^{(M)}$ are applied is not important since they commute. We define

$$\Psi^{(+)} \equiv \Psi_{n+1} = \psi_{n+1}+\frac{i\Delta t}{2\hbar}N_{n+1}-\frac{i(\Delta t)^2}{12\hbar}\left[\frac{i}{\hbar}HN_{n+1}+N'_{n+1}\right], \tag{2.17}$$

and

$$\Psi^{(-)} \equiv \Psi_n = \psi_n-\frac{i\Delta t}{2\hbar}N_n-\frac{i(\Delta t)^2}{12\hbar}\left[\frac{i}{\hbar}HN_n+N'_n\right]. \tag{2.18}$$

Thus

$$\Psi_{n+1} = K_2^{(2)}K_1^{(2)}\Psi_n. \tag{2.19}$$

We use the known $\psi_n\approx\psi(x,t)$ to calculate Ψ_n from Eq. (2.18). Then we iteratively obtain $\Psi^{(+)}$ from $\Psi^{(-)}$ *à la* the method described in I, i.e., $\Psi_{n+1/2}=K_1^{(2)}\Psi_n$ and $\Psi^{(+)}\equiv\Psi_{n+1}=K_2^{(2)}\Psi_{n+1/2}$. From Eq. (2.17) we obtain $\psi_{n+1}\approx\psi(x,t+\Delta t)$. The conversion from $\Psi^{(\pm)}$ to ψ and vice versa occurs before and after the sequence of the iterative applications of the $K_s^{(M)}$ operators.

For known $N(x,t)$ Eq. (2.15) can be solved in principle using the method described in I. Two new features are the operation of H on N and the time differentiation of $N(x,t)$. The function $N(x,t)$ can be discretized in the same way as $\psi(x,t)$ so that we form discrete elements $N_{n,j}\approx N(x_j,t_n)$. In the discretized form

$$(H\Psi_n)_j = -\frac{\hbar^2}{2m(\Delta x)^2}\sum_{k=-r}^{r}c_k^{(r)}\psi_{n,j+k}+V_j\psi_{n,j}, \tag{2.20}$$

where

$$e_k^{(r)} = -\frac{\hbar^2}{2m(\Delta x)^2}c_k^{(r)},$$

$$f_j^{(r)} = -\frac{\hbar^2}{2m(\Delta x)^2}c_0^{(r)}+V_j = e_0^{(r)}+V_j. \tag{2.21}$$

The coefficients $c_k^{(r)}$ are defined as in I. The matrix form of H is (suppressing the superscripts $^{(r)}$)

$$H = \begin{pmatrix} f_0 & e_1 & e_2 & \cdots & e_r & 0 & & & \\ e_1 & f_1 & e_1 & \cdots & e_{r-1} & e_r & & & \\ e_2 & e_1 & f_2 & \cdots & e_{r-2} & e_{r-1} & & & \\ \vdots & \vdots & \vdots & & \vdots & \vdots & & & \\ e_r & e_{r-1} & e_{r-2} & \cdots & f_r & e_1 & & & \\ 0 & e_r & e_{r-1} & \cdots & e_1 & f_{r+1} & & & \\ & & & & & & \ddots & & \\ & & & & & & & f_{J-1} & e_1 \\ & & & & & & & e_1 & f_J \end{pmatrix}. \tag{2.22}$$

The time partial derivative of $N(x,t)$ is straightforward if N is an analytically known function of x and t. If the function is given in a discretized form, say $N_{n,j}$, accurate time derivatives may pose a challenge, especially the higher-order ones.

C. Integration over time with arbitrary precision.

For the general case, we start again with Eq. (2.5),

$$\psi(t+\Delta t) = e^{-iH\Delta t/\hbar}\psi(t) - \frac{i}{\hbar}e^{-iH\Delta t/\hbar}\int_0^{\Delta t} e^{iH\theta/\hbar}N(t+\theta)\,d\theta. \tag{2.5}$$

Using the Euler-MacLaurin series (2.13), we obtain

$$\begin{aligned}\psi(t+\Delta t) = {} & e^{-iH\Delta t/\hbar}\psi(t) - \frac{i\Delta t}{2\hbar}e^{-iH\Delta t/\hbar}[e^{iH\Delta t/\hbar}N(t+\Delta t)+N(t)] \\ & + \frac{i}{\hbar}e^{-iH\Delta t/\hbar}\sum_{k=1}^{M-1}\frac{B_{2k}}{(2k)!}(\Delta t)^{2k}\left\{\frac{\partial^{2k-1}}{\partial\theta^{2k-1}}[e^{iH\theta/\hbar}N(t+\theta)]|_{\theta=\Delta t} - \frac{\partial^{2k-1}}{\partial\theta^{2k-1}}[e^{iH\theta/\hbar}N(t+\theta)]|_{\theta=0}\right\}\end{aligned} \tag{2.23}$$

We note that θ is a time so that $[H, \frac{\partial}{\partial\theta}] = 0$. We can simplify the partial derivatives,

$$\frac{\partial^{2k-1}}{\partial\theta^{2k-1}}e^{iH\theta/\hbar}N(t+\theta) = e^{iH\theta/\hbar}\left(\frac{i}{\hbar}H + \frac{\partial}{\partial\theta}\right)^{2k-1}N(t+\theta). \tag{2.24}$$

Using the binomial theorem, we obtain

$$\left.\frac{\partial^{2k-1}}{\partial\theta^{2k-1}}e^{iH\theta/\hbar}N(t+\theta)\right|_{\theta=\Delta t} = e^{iH\Delta t/\hbar}\sum_{l=0}^{2k-1}\binom{2k-1}{l}\left(\frac{i}{\hbar}H\right)^{2k-1-l}N^{(l)}(t+\Delta t)\,, \tag{2.25}$$

where $N^{(l)}$ is the lth partial derivative with respect to θ. Similarly

$$\left.\frac{\partial^{2k-1}}{\partial\theta^{2k-1}}e^{iH\theta/\hbar}N(t+\theta)\right|_{\theta=0} = \sum_{l=0}^{2k-1}\binom{2k-1}{l}\left(\frac{i}{\hbar}H\right)^{2k-1-l}N^{(l)}(t). \tag{2.26}$$

Inserting the last two equations in Eq. (2.23) we get

$$\begin{aligned}\psi(t+\Delta t) = {} & e^{-iH\Delta t/\hbar}\psi(t) - \frac{i\Delta t}{2\hbar}e^{-iH\Delta t/\hbar}[e^{iH\Delta t/\hbar}N(t+\Delta t)+N(t)] + \frac{i}{\hbar}e^{-iH\Delta t/\hbar}\sum_{k=1}^{M-1}\frac{B_{2k}}{(2k)!}(\Delta t)^{2k} \\ & \times\left\{e^{iH\Delta t/\hbar}\sum_{l=0}^{2k-1}\binom{2k-1}{l}\left(\frac{i}{\hbar}H\right)^{2k-1-l}N^{(l)}(t+\Delta t) - \sum_{l=0}^{2k-1}\binom{2k-1}{l}\left(\frac{i}{\hbar}H\right)^{2k-1-l}N^{(l)}(t)\right\}.\end{aligned} \tag{2.27}$$

We collect items evaluated at $t+\Delta t$ on the left side of the equation.

$$\begin{aligned}& \psi(t+\Delta t) + \frac{i\Delta t}{2\hbar}N(t+\Delta t) - \frac{i}{\hbar}\sum_{k=1}^{M-1}\frac{B_{2k}}{(2k)!}(\Delta t)^{2k}\sum_{l=0}^{2k-1}\binom{2k-1}{l}\left(\frac{i}{\hbar}H\right)^{2k-1-l}N^{(l)}(t+\Delta t) \\ & = e^{-iH\Delta t/\hbar}\left[\psi(t) - \frac{i\Delta t}{2\hbar}N(t) - \frac{i}{\hbar}\sum_{k=1}^{M-1}\frac{B_{2k}}{(2k)!}(\Delta t)^{2k}\sum_{l=0}^{2k-1}\binom{2k-1}{l}\left(\frac{i}{\hbar}H\right)^{2k-1-l}N^{(l)}(t)\right]\end{aligned} \tag{2.28}$$

We generalize the vector functions $\Psi_n^{(\pm)}$ by letting

$$\Psi^{(\pm)}(x,t) = \psi(x,t) \pm \frac{i\Delta t}{2\hbar} N(x,t) - \frac{i}{\hbar} \sum_{k=1}^{M-1} \frac{B_{2k}}{(2k)!} (\Delta t)^{2k} \sum_{l=0}^{2k-1} \binom{2k-1}{l} \left(\frac{i}{\hbar} H\right)^{2k-1-l} N^{(l)}(x,t) + O[(\Delta t)^{(2M+1)}]. \tag{2.29}$$

With $M = 2$, Eq. (2.28) and following are consistent with Eq. (19) of Ref. [16] with error of $O[(\Delta t)^5]$.

We now express the time-evolution operator as (see Ref. [1])

$$e^{-iH\Delta t/\hbar} = \prod_{s=1}^{M} K_s^{(M)} + O[(\Delta t)^{2M+1}]. \tag{2.30}$$

Since Eq. (2.28) is equivalent to

$$\Psi^{(+)} \equiv \Psi_{n+1} = e^{-iH\Delta t/\hbar} \Psi_n, \tag{2.31}$$

where $\Psi_n \equiv \Psi^{(-)}$, we write the relation as

$$\Psi_{n+1} = \prod_{s=1}^{M} K_s^{(M)} \Psi_n. \tag{2.32}$$

Defining

$$\Psi_{n+s/M} \equiv K_s^{(M)} \Psi_{n+(s-1)/M}, \tag{2.33}$$

we solve for Ψ_{n+1} recursively, starting from

$$\Psi_{n+1/M} = K_1^{(M)} \Psi_n. \tag{2.34}$$

Assuming that $\Psi^{(-)} \equiv \Psi_n$ is known from $\psi(x,t)$ and $N(x,t)$, we determine $\Psi_{n+1/M}$ from Eq. (2.34), which has a form similar to that of Eq. (2.12). This is repeated to obtain in succession $\Psi_{n+2/M}, \Psi_{n+3/M}, \ldots, \Psi_{n+(M-1)/M}, \Psi_{n+1} \equiv \Psi^{(+)}$. Since the operators $K_s^{(M)}$ commute, they can be applied in any order. Note that $\psi_{n+1,j}$ can be extracted from Ψ_{n+1} and Ψ_n can be constructed from $\psi_{n,j}$. In each case it is assumed that $N(x,t)$ and its time derivatives are known. The $\Psi_{n+1}^{(+)}$ is obtained from $\Psi_n^{(-)}$ by means of a unitary operator. Hence the normalization of the two functions is the same, although this is in general not so for ψ. Nevertheless the integration process is stable.

Let us return to the time evolution within a step Δt,

$$\Psi_{n+s/M} = K_s^{(M)} \Psi_{n+(s-1)/M} = \prod_{s'=1}^{s} K_{s'}^{(M)} \Psi_n. \tag{2.35}$$

The form of the operator is[1]

$$K_s^{(M)} = \frac{1 + (iH\Delta t/\hbar)/z_s^{(M)}}{1 - (iH\Delta t/\hbar)/\bar{z}_s^{(M)}} \tag{2.36}$$

with $z_s^{(M)}$ a root of the numerator of the $[M/M]$ Padé approximant of e^z. In general $z_s^{(M)}$ is a complex number. Nevertheless $K_s^{(M)}$ is a unitary operator. In effect $K_s^{(M)}$ increases the time by a complex increment $-2\Delta t/z_s^{(M)}$. As a check on the time increment formula one can show that the roots $z_s^{(M)}$ for a particular M obey the relationship

$$\sum_{s=1}^{M} \frac{1}{z_s^{(M)}} = -\frac{1}{2}. \tag{2.37}$$

It is interesting to note that the times t_n, $t_{n+1} = t_n + \Delta t$, $t_{n+2} = t_n + 2\Delta t$, etc., are real, but the intermediate times $t_n - 2\Delta t \sum_{s'=1}^{s} (1/z_{s'}^{(M)})$ are complex. The times between t_n and t_{n+1} can be denoted as

$$t_{n+s/M} = t_n - 2\Delta t \sum_{s'=1}^{s} \frac{1}{z_s^{(M)}}, \quad s = 1,2,\ldots,M. \tag{2.38}$$

We define the dimensionless time increment

$$\Delta\tau_s^{(M)} \equiv \frac{t_{n+s/M} - t_n}{\Delta t} = -2 \sum_{s'=1}^{s} \frac{1}{z_{s'}^{(M)}}. \tag{2.39}$$

In Fig. 1 we plot $\Delta\tau_s$ on the complex time plane.

The recursion (2.33) effectively gives us functions $\Psi_{n+s/M}$, which are related to the wave function at complex times; these wave functions need not be calculated since the iteration only involves the $\Psi_{n+s/M}$. As we go through the M operations of the $K_s^{(M)}$ we make, as it were, an excursion away from the real axis in the complex-time plane, but after the Mth operation we are back on the real axis. By placing the $z_s^{(M)}$ in different order we can follow different paths from the initial to final points; those paths however are not all as smooth. One possible path is one which involves complex conjugates next to each other; then every other point lies on the real axis and points in between make excursions off the real axis. However, since the operators $K_s^{(M)}$ commute the final point and time advance will be the same after completing a full time step Δt. The significance of this comment is that even when $N(x,t)$ is a real

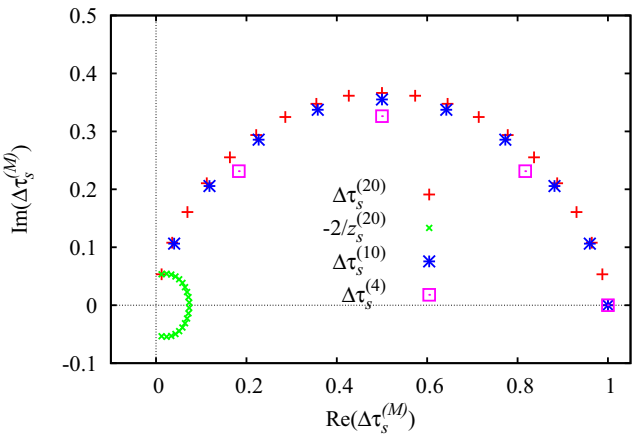

FIG. 1. (Color online) The $\Delta\tau_s^{(M)}$ for each $s = 1,\ldots,M$ from left to right plotted as dots on the complex plane. In this graph $M = 20$, 10, and 4. The individual contributions for $M = 20$, namely $-2/z_s^{(20)}$, are plotted as green dots.

[1]There is an error in Ref. [1]. The plus and minus signs in Eq. (3.4) of that paper should be interchanged.

quantity with real arguments, in the calculation N and t need to be complex [see Eq. (2.29)].

As a final task we need to evaluate $N(x,t)$ and its partial time derivatives. Even if $N(x,t)$ is known analytically, only for the simplest form can one write down the time derivative of arbitrary order. There may be problem-specific ways in which any-order time derivative can be obtained in a straightforward manner for more complex situations.

D. Evaluation of the Bernoulli numbers

The Bernoulli polynomials $B_n(x)$ are defined through the generating function [14, formula 23.1.1]

$$\frac{te^{xt}}{e^t-1}=\sum_{n=0}^{\infty}B_n(x)\frac{t^n}{n!}. \tag{2.40}$$

The Bernoulli numbers are $B_n=B_n(0)$. Some special values are $B_0=1$, $B_1=-\frac{1}{2}$, and $B_{2n+1}=0$ for $n=1,2,\ldots$. The remaining Bernoulli numbers can calculated using the Fourier expansion for the Bernoulli polynomial [14, formula 23.1.16]

$$B_n(x)=-2\frac{n!}{(2\pi)^n}\sum_{k=1}^{\infty}\frac{\cos\left(2\pi kx-\frac{1}{2}\pi n\right)}{k^n}, \tag{2.41}$$

which converges when $n>1$, $0\leqslant x\leqslant 1$. The Bernoulli numbers occur when $x=0$ so that

$$B_{2n}=-2(-1)^n\frac{(2n)!}{(2\pi)^{2n}}\sum_{k=1}^{\infty}\frac{1}{k^{2n}}. \tag{2.42}$$

The following relations, due to Ramanujan, provide an efficient method for calculating Bernoulli numbers for even m:
for $m\equiv 0 \mod 6$,

$$\binom{m+3}{m}B_m=\frac{m+3}{3}-\sum_{j=1}^{m/6}\binom{m+3}{m-6j}B_{m-6j}; \tag{2.43}$$

for $m\equiv 2 \mod 6$,

$$\binom{m+3}{m}B_m=\frac{m+3}{3}-\sum_{j=1}^{(m-2)/6}\binom{m+3}{m-6j}B_{m-6j}; \tag{2.44}$$

and for $m\equiv 4 \mod 6$,

$$\binom{m+3}{m}B_m=-\frac{m+3}{6}-\sum_{j=1}^{(m-4)/6}\binom{m+3}{m-6j}B_{m-6j}. \tag{2.45}$$

As we observe from Table I, the Bernoulli numbers are increasing in magnitude with n. This is a manifestation of the asymptotic nature of the Euler-MacLaurin series. One expects the convergence of the series in Eq. (2.29) to depend on the magnitude of Δt.

E. Errors

In Ref. [1] we analyze truncation errors in the solution wave function obtained from the homogeneous equations. These are expressed as

$$e^{(r)}=C^{(r)}(\Delta x)^{2r} \quad \text{and} \quad e^{(M)}=C^{(M)}(\Delta t)^{2M+1}, \tag{2.46}$$

TABLE I. The Bernoulli coefficients B_n.

n	B_n	n	B_n
0	$1.00000\times10^{+00}$	18	$5.49712\times10^{+01}$
2	1.66667×10^{-01}	20	$-5.29124\times10^{+02}$
4	-3.33333×10^{-02}	22	$6.19212\times10^{+03}$
6	2.38095×10^{-02}	24	$-8.65803\times10^{+04}$
8	-3.33333×10^{-02}	26	$1.42552\times10^{+06}$
10	7.57576×10^{-02}	28	$-2.72982\times10^{+07}$
12	-2.53114×10^{-01}	30	$6.01581\times10^{+08}$
14	$1.16667\times10^{+00}$	32	$-1.51163\times10^{+10}$
16	$-7.09216\times10^{+00}$	34	$4.29615\times10^{+11}$

for the spatial and temporal dependencies. The constants $C^{(r)}$ and $C^{(M)}$ are expected to be slowly varying functions of r and M, respectively. The variables x and t are independent. When a particular precision of the wave function has been achieved in one variable, we can increase the order of approximation for the other variable and will reach that precision, saturating the process; the results will continue to be identical regardless how much more the order of the second variable is increased. This is shown in Refs. [4,17].

For the solutions of the nonhomogeneous equations we have taken the same orders of approximation for the wave function and for the Euler-MacLaurin expansion. Depending on the particular equation, it may be more efficient to consider different orders. For instance, if $N(x,t)$ is much slower varying function of x and t than $\psi(x,t)$, lower orders in the Euler-MacLaurin expansion may be appropriate. In our examples we do not know that ahead of time, so we use the same orders. We do emphasize, however, that the constants $C^{(M)}$ and $C^{(r)}$ depend on the higher-order partial derivatives of the wave function and the source term, and hence are model dependent.

When the exact solution is known the error of the numerical calculation at final time t_1 can be obtained using the formula

$$(e_2)^2=\int_{x_0}^{x_J}dx\ |\psi(x,t_1)-\psi_{\text{exact}}(x,t_1)|^2. \tag{2.47}$$

A small value of e_2 is indicative of near equality of both the modulus and the phase of ψ and ψ_{exact}. For this integral, and other integrals such as the normalization, we use the formula

$$\int_{x_0}^{x_J}dx\ f(x)=\Delta x\sum_{j=0}^{J}f(x_j). \tag{2.48}$$

Peters and Maley [18] have shown that this formula is an approximation to the integral to $O[(\Delta x)^{(2r+1)}]$ provided one includes correction terms, which involve $f(x_i)$ where $i=0,1,\ldots,r$ and $i=J-r,J-r+1,\ldots,J$. Since the correction terms depend only on the wave function near the extreme ends of the spatial range, they do not contribute significantly in our examples since the wave function is (nearly) zero there.

In cases for which the exact solution is not known we can estimate the error by comparing the results for M and r with those for $M+1$ and $r+1$. To that end we define the quantity

$$(\eta_{M,r})^2=\int_{x_0}^{x_J}dx|\psi^{(M,r)}(x,t_1)-\psi^{(M+1,r+1)}(x,t_1)|^2. \tag{2.49}$$

Here the exact solution in Eq. (2.47) is approximated by $\psi^{(M+1,r+1)}(x,t)$.

III. NUMERICAL STUDIES

A. Example 1: Nonspreading wave packet

The examples for the numerical studies are chosen so that they have exact analytic solutions to which the numerical solutions can be compared. They do not correspond in detail to actual physical systems. Hopefully once the numerical method is validated, the method can be used for realistic systems.

Nonspreading or nondispersive wave packets have been discussed and observed recently [19]. Such Michelangelo packets rely on an absorption process that removes the unwanted spreading part of the wave function so that the packet retains its width and shape in coordinate space. Earlier nonspreading wave packets in free space, that are expressed in terms of Airy functions, were discussed by Berry and Balazs [20,21]. Somewhat related are the diffraction-free beams of particles for which there is no spreading in the transverse direction [22,23].

Given the results of our calculations, the stationary nonspreading wave packet provides as rigorous a test for the method as the traveling free (spreading) wave packet. Thus in order to test the numerical procedure we consider the stationary nonspreading wave packet,

$$\phi(x,t) = (2\pi\sigma^2)^{-1/4}\exp\left[-\frac{(x-x_{\rm init})^2}{(2\sigma)^2} + ik_0(x-x_{\rm init}) - \frac{i\hbar}{2m}k_0^2 t\right], \tag{3.1}$$

where $x_{\rm init}$ is the expectation value of the position of the wave packet at time zero. This wave packet is a solution of

$$\left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\phi(x,t) = N(x,t) \tag{3.2}$$

when

$$N(x,t) = \frac{\hbar^2\{(x-x_{\rm init})^2 - 2\sigma^2[1+2ik_0(x-x_{\rm init})]\}}{8m\sigma^4}\phi(x,t). \tag{3.3}$$

This nonspreading wave packet is also a solution of the time-dependent homogeneous Schrödinger equation with the potential function

$$V(x) = \frac{\hbar^2}{8m\sigma^4}\{(x-x_{\rm init})^2 - 2\sigma^2[1+2ik_0(x-x_{\rm init})]\}. \tag{3.4}$$

In the example we used the same parameters as for the free traveling wave packet studied in I, and earlier in Ref. [24], i.e., $\sigma = 1/20$, $k_0 = 50\pi$, $x_0 = -0.5$, $x_J = 1.5$, and $x_{\rm init} = 0.25$ with the units chosen so that $\hbar = 2m = 1$. We set $\Delta t = 2(\Delta x)^2$ and allow as much time as would be required for the free traveling packet to move from $x_{\rm init} = 0.25$ to around 0.75. In our case the packet does not move at all, but that does not detract from the validity of the test, since inaccurate calculations show definite movement of the packet. The results are tabulated in Table II. The CPU time is the approximate time of computation and depends on the computer. For the same computer the CPU times indicate relative times of computation. We used two different computers, labeled as processor A (default, double precision) or B. Times for different computers should not be compared.

TABLE II. Summary of computational parameters and errors for example 1 with $k_0 = 50\pi$. The quantity τ is the CPU time (processor A) in seconds and $\nu = (\Delta x)^2$.

M	r	J	Δt	e_2	$\eta_{M,r}$	τ
1	1	2000	2ν	5.83×10^{-2}	5.82×10^{-2}	4.5
2	2	2000		1.76×10^{-4}	1.75×10^{-4}	15
3	3	2000		7.10×10^{-7}	7.06×10^{-7}	44
4	4	2000		3.19×10^{-9}	3.18×10^{-9}	110
5	5	2000		1.59×10^{-11}	1.54×10^{-11}	238
6	6	2000		5.66×10^{-13}	9.35×10^{-14}	457
2	19	260	2ν	1.98×10^{0}	1.95×10^{0}	.20
4	19	260		5.13×10^{-3}	4.99×10^{-3}	.86
6	19	260		2.90×10^{-6}	2.85×10^{-6}	2.5
8	19	260		1.71×10^{-9}	1.39×10^{-9}	5.7
10	19	260		9.54×10^{-10}	6.54×10^{-10}	.44 K[a]
12	19	260		9.55×10^{-10}	6.54×10^{-10}	.75 K[a]
14	19	260		9.55×10^{-10}	6.55×10^{-10}	1.2 K[a]
18	19	260	ν	9.55×10^{-10}	5.96×10^{-10}	134

[a]Calculation done in quadruple precision with processor B.

We graph the errors as a function of M for given values of r in Fig. 2. For this graph we use the parameters of Table II with 2ν and $J = 200$. The plateaus in the graph indicate a convergence of the error to a limit value. The estimated error in this region tends to be smaller than the exact error. However the two are of the same order of magnitude and, for the cases shown, the estimated error is no smaller than one third the exact error. This graph also indicates an approach to estimating the error when the exact solution is not known. If one is in the region of the plateaus, increasing M will not change the error, but increasing r will move one to a lower plateau. In a subsequent section we see similar plateaus for constant M as r is varied. So to estimate the error by increasing both M and r covers both instances.

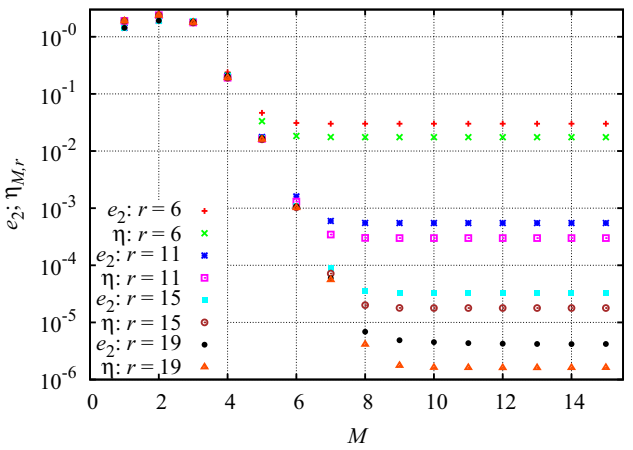

FIG. 2. (Color online) The errors (exact and estimated) for the calculations with the parameters of Table II including $\Delta t = 2\nu$ and $J = 200$. The η in the legend of the graph refers to $\eta_{M,r}$.

TABLE III. Same calculation as of Table II with $k_0 = 1$.

M	r	J	Δt	e_2	$\eta_{M,r}$	τ
1	1	2000	2ν	1.25×10^{-5}	1.25×10^{-5}	4.5
2	2	2000		1.53×10^{-9}	1.53×10^{-9}	15
3	3	2000		3.04×10^{-13}	3.04×10^{-13}	2.3 K[a]
4	19	260	2ν	1.90×10^{-13}	1.90×10^{-13}	43[a]
6	19	260		6.38×10^{-18}	6.38×10^{-18}	.11 K[a]
8	19	260		1.01×10^{-21}	1.89×10^{-21}	.24 K[a]
10	19	260		1.16×10^{-20}	6.39×10^{-20}	.44 K[a]

[a]Calculation done in quadruple precision with processor B.

We also considered a case with $k_0 = 1$, since that involves a smaller kinetic energy and a smaller (more reasonable) time derivative of $N(x,t)$. The results are given in Table III.

We expect the same qualitative behavior for smaller values of k_0. Such values of k_0 may make the differential equation less stiff and thus provide precise results with less effort. By judicious choice of the time and space discretization and orders of approximation one can obtain extremely accurate results. For this example one needs values of $M > 4$, whereas the traditional CN approach corresponds to $M = 1$. We note, however, that to obtain good results when $M \gtrsim 8$ the calculation need to be done in quadruple precision indicating that a substantial loss of significant figures in the computation occurs. The likely reason for this is the need to raise the Hamiltonian matrix to higher powers.

B. Example 2: Coherent oscillations

In this example we construct a nonhomogeneous Schrödinger equation from the one-dimensional harmonic oscillator,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi_{\rm nh}(x,t) + \frac{1}{2}Kx^2\phi_{\rm nh}(x,t) = i\hbar\frac{\partial}{\partial t}\phi_{\rm nh}(x,t). \tag{3.5}$$

The coherent oscillating wave packet, that is an exact solution, is

$$\phi_{\rm nh}(x,t) = \frac{\alpha^{1/2}}{\pi^{1/4}}\exp\left[-\frac{1}{2}[\xi - \xi_0\cos(\omega t)]^2 - i\left(\frac{1}{2}\omega t + \xi\xi_0\sin(\omega t) - \frac{1}{4}\xi_0^2\sin(2\omega t)\right)\right], \tag{3.6}$$

where $\omega = \sqrt{K/m}$, $\alpha = (mK/\hbar^2)^{1/4}$, $\xi = \alpha x$, and $\xi_0 = \alpha a$. The quantity a is the initial position of the wave packet. We can also consider $\phi_{\rm nh}(x,t)$ to be a particular solution of the nonhomogeneous Schrödinger equation

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right]\phi(x,t) = N(x,t) \tag{3.7}$$

where

$$N(x,t) = \tfrac{1}{2}Kx^2\phi_{\rm nh}(x,t). \tag{3.8}$$

The general solution of Eq. (3.7) is the general solution of the associated homogeneous equation plus a particular solution of the nonhomogeneous equation. The associated homogeneous equation is the free-particle equation which has as solution the free-particle wave packet

$$\phi_{\rm h}(x,t) = (2\pi\sigma^2)^{-1/4}[1 + i\hbar t/(2m\sigma^2)]^{-1/2}\exp\left\{\frac{-(x - x_{\rm init})^2/(2\sigma)^2 + ik_0(x - x_{\rm init}) - i\hbar k_0^2 t/(2m)}{1 + i\hbar t/(2m\sigma^2)}\right\}. \tag{3.9}$$

Thus a solution of Eq. (3.7) is the superposition of the traveling free wave packet and oscillating coherent wave packet, i.e.,

$$\phi(x,t) = \phi_{\rm h}(x,t) + \phi_{\rm nh}(x,t). \tag{3.10}$$

An important consideration is the fact that we need to calculate the partial time derivative of various orders of the function $N(x,t)$. Whereas in principle function (3.8) can be differentiated in closed form with respect to time an arbitrary number of times, such repeated differentiation is not practical because of the complexity of the dependence of $\phi_{\rm nh}$ as a function of time. Numerical differentiation becomes inaccurate quickly as the order increases. However, $\phi_{\rm nh}(x,t)$ satisfies Eq. (3.5), which we can write as

$$H_{\rm nh}\phi_{\rm nh}(x,t) = i\hbar\frac{\partial}{\partial t}\phi_{\rm nh}(x,t). \tag{3.11}$$

Thus we obtain the lth time derivative of N as

$$\frac{\partial^l}{\partial t^l}N(x,t) = \frac{1}{2}Kx^2\frac{\partial^l}{\partial t^l}\phi_{\rm nh}(x,t) = \frac{1}{2}Kx^2\left(\frac{-i}{\hbar}\right)^l H_{\rm nh}^l\phi_{\rm nh}(x,t). \tag{3.12}$$

The lth partial derivative obtained in this way is quite accurate and is (can be) obtained from the numerical wave function.

For the initial test we choose the parameters of I: $\omega = 0.2$, $a = 10, x_0 = -80, x_J = 80$ and final time $t_1 = 10\pi$, where the units are chosen such that $\hbar = m = 1$. From these parameters we determine K and α. For the free wave packet we choose $\sigma = 1/\alpha$, $k_0 = 0$ and $x_{\rm init} = 0$. Thus the free wave packet part of the wave function is stationary but is dispersing. The interference of the two wave packets can create significant oscillations in the overall wave function. Figure 3 shows the components and the total wave function at $t = 0$ and at $t = 2.5\pi$.

The results of the comparison of the exact and the numerical solutions are displayed in Table IV.

IV. TIME-DEPENDENT HAMILTONIAN

In this section we examine time-dependent Hamiltonians, or rather time-dependent potential functions. The method of I does not apply since it was assumed that the operators $K_s^{(M)}$ for different values of s commute. That is no longer the case if $H = H(t)$ is a function of time. A more fundamental way of

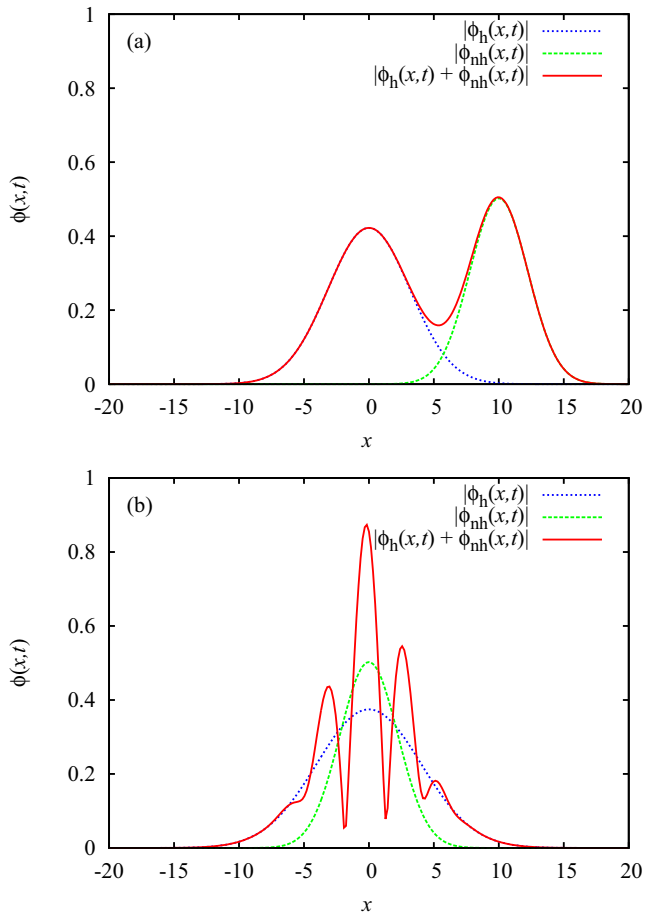

FIG. 3. (Color online) The wave functions of example 2 at (a) $t = 0$ and at (b) $t = 2.5\pi$. The units used are such that $\hbar = m = 1$.

seeing that is that H in the time-evolution operator is a function of time. Successive operations of the evolution operators at different times introduce nonzero commutators of the Hamiltonian at different times. In Ref. [16] the authors suggest an approach based on the Magnus expansion (see Ref. [25] for a review), where one can in principle systematically obtain solutions with an error to $O[(\Delta t)^{2M}]$, but beyond $M = 2$ the method becomes cumbersome (see also Ref. [26]). Our attempt involves considering the time-dependent potential term as the nonhomogeneous term in the equation, and then extract the wave function at the end of the time step from $\Psi^{(+)}$ by iteration.

TABLE IV. The computational parameters and errors for example 2. The common parameters are $\omega = 0.2, a = 10, x_0 = -80, x_J = 80, t_1 = 10\pi, dt = \pi/20, \sigma = 1/\alpha, k_0 = 0$, and $x_{\text{init}} = 0$. The units used are such that $\hbar = m = 1$.

M	r	J	e_2	$\eta_{M,r}$	τ
1	1	8000	1.67×10^{-1}	2.04×10^{-1}	5.7
2	2	4000	7.21×10^{-4}	8.78×10^{-4}	10
2	2	2000	8.54×10^{-4}	1.04×10^{-3}	3.7
2	2	1000	3.08×10^{-3}	3.69×10^{-3}	1.7
4	4	1000	1.79×10^{-6}	2.17×10^{-6}	14
6	6	1000	2.34×10^{-9}	2.74×10^{-9}	58
8	8	1000	4.40×10^{-12}	5.11×10^{-12}	6.9 K[a]
10	10	1000	3.33×10^{-14}	1.26×10^{-14}	16 K[a]
12	12	1000	3.11×10^{-14}	4.30×10^{-17}	32 K[a]
10	10	800	8.57×10^{-13}	9.59×10^{-13}	12 k[a]
10	10	300	5.69×10^{-5}	3.80×10^{-5}	110
15	15	300	1.59×10^{-6}	9.17×10^{-7}	560
19	19	300	1.44×10^{-7}	7.54×10^{-8}	1400

[a]Calculation done in quadruple precision with a different CPU, i.e., processor B.

We proceed as follows. Suppose the equation to be solved is

$$\left[i\hbar\frac{\partial}{\partial t} - H_0 - V(x,t)\right]\psi(x,t) = 0, \tag{4.1}$$

where H_0 could include another potential term which is independent of t. We can rewrite the equation as

$$\left(i\hbar\frac{\partial}{\partial t} - H_0\right)\psi(x,t) = V(x,t)\psi(x,t) \equiv N[x,t;\psi(x,t)]. \tag{4.2}$$

We explicitly indicate the dependence of N on ψ. At the beginning of a time interval $\psi(x,t)$ is known and we construct $\Psi^{(-)}(x,t)$ using Eq. (2.29). In the process we need the time derivatives of $N[x,t;\psi(x,t)] = V(x,t)\psi(x,t)$. We obtain them from

$$\frac{\partial^l}{\partial t^l}N[x,t;\psi(x,t)] = \sum_{l'=0}^{l}\binom{l}{l'}\frac{\partial^{l-l'}V}{\partial t^{l-l'}}\frac{\partial^{l'}\psi}{\partial t^{l'}}. \tag{4.3}$$

The partial time derivatives of $V(x,t)$ need to be calculated analytically, but those of ψ can be obtained using the following approach. We rewrite Eq. (4.1)

$$\frac{\partial}{\partial t}\psi(x,t) = A(x,t)\psi(x,t), \tag{4.4}$$

where $A(x,t) = (-\frac{i}{\hbar})[H_0(x) + V(x,t)]$. We form a recursion to obtain the lth partial derivative with respect to t, i.e.,

$$\frac{\partial^l}{\partial t^l}\psi(x,t) = f_l(A)\psi(x,t) \tag{4.5}$$

with

$$f_0 = 1 \quad \text{and} \quad f_l(A) = \frac{\partial f_{l-1}}{\partial t} + f_{l-1}(A)A, \tag{4.6}$$

for $l = 1,2,3,\ldots$. The first five functions $f_l(A)$ are

$$f_1(A) = A$$

$$f_2(A) = A^2 + \frac{\partial A}{\partial t}$$

$$f_3(A) = A^3 + A\frac{\partial A}{\partial t} + 2\frac{\partial A}{\partial t}A + \frac{\partial^2 A}{\partial t^2}$$

$$f_4(A) = A^4 + A^2\frac{\partial A}{\partial t} + 2A\frac{\partial A}{\partial t}A + 3\frac{\partial A}{\partial t}A^2 + A\frac{\partial^2 A}{\partial t^2} + 3\left(\frac{\partial A}{\partial t}\right)^2 + 3\frac{\partial^2 A}{\partial t^2}A + \frac{\partial^3 A}{\partial t^3}$$

$$f_5(A) = A^5 + A^3\frac{\partial A}{\partial t} + 2A^2\frac{\partial A}{\partial t}A + 3A\frac{\partial A}{\partial t}A^2 + 4\frac{\partial A}{\partial t}A^3 + A^2\frac{\partial^2 A}{\partial t^2} + 3A\frac{\partial^2 A}{\partial t^2}A + 3A\left(\frac{\partial A}{\partial t}\right)^2 + 4\frac{\partial A}{\partial t}A\frac{\partial A}{\partial t}$$

$$+8\left(\frac{\partial A}{\partial t}\right)^2 A + 6\frac{\partial^2 A}{\partial t^2}A^2 + A\frac{\partial^3 A}{\partial t^3} + 4\frac{\partial A}{\partial t}\frac{\partial^2 A}{\partial t^2}$$
$$+6\frac{\partial^2 A}{\partial t^2}\frac{\partial A}{\partial t} + 4\frac{\partial^3 A}{\partial t^3}A + \frac{\partial^4 A}{\partial t^4}. \quad (4.7)$$

Any order of the derivative of the wave function can be obtained, but in practice the formulas become increasingly more onerous to work with as l increases.

After one time increment we obtain $\Psi^{(+)}(x,t)$ at the incremented time. From it we extract the new $\psi(x,t)$. (Note that $t \to t + \Delta t$, but for convenience we write t.) Thus

$$\psi(x,t) = \Psi^{(+)}(x,t) - \frac{i\Delta t}{2\hbar}N[x,t;\psi(x,t)] + F[x,t;\psi(x,t)], \quad (4.8)$$

where

$$F(x,t;\psi(x,t)) = \sum_{k=1}^{M-1}\frac{B_{2k}}{2k}(\Delta t)^{2k}\sum_{l=0}^{2k-1}\frac{1}{(2k-1-l)!l!}\left(\frac{i}{\hbar}\right)^{2k-l} \times H_0^{2k-1-l}N^{(l)}[x,t;\psi(x,t)] \quad (4.9)$$

for $M \geqslant 2$. Note that $F[x,t;\psi(x,t)]$ is at least $O[(\Delta t)^2]$. Thus we can write

$$\psi(x,t) = \frac{\Psi^{(+)}(x,t) + F[x,t;\psi(x,t)]}{1 + \frac{i\Delta t}{2\hbar}V(x,t)}. \quad (4.10)$$

We solve this equation iteratively by making an initial approximation

$$\psi^{(0)}(x,t) = \frac{\Psi^{(+)}(x,t) + F[x,t;\psi(x,t-\Delta t)]}{1 + \frac{i\Delta t}{2\hbar}V(x,t)}, \quad (4.11)$$

and evaluating successively

$$\psi^{(i+1)}(x,t) = \frac{\Psi^{(+)}(x,t) + F[x,t;\psi^{(i)}(x,t)]}{1 + \frac{i\Delta t}{2\hbar}V(x,t)}, \quad i = 0,1,\ldots. \quad (4.12)$$

We continue the process until $e^{(i)}$ defined as

$$(e^{(i)})^2 = \int_{x_0}^{x_J} dx\, |\psi^{(i+1)}(x,t) - \psi^{(i)}(x,t)|^2 \quad (4.13)$$

is smaller than a prescribed amount. In other words we look for the convergence

$$\lim_{i\to\infty}\psi^{(i)}(x,t) = \psi(x,t). \quad (4.14)$$

Example 3: Time-dependent oscillator

As a last example we will consider the harmonic oscillator with time-dependent frequency [27] (see also Ref. [28] and references contained in it). The potential has the form

$$V(x,t) = \tfrac{1}{2}m\omega^2(t)x^2 \quad (4.15)$$

with $\omega^2(t) = \omega_0^2(1 - fe^{-\mu t})$ where f is a positive proper fraction and μ a positive number. Systems with such potentials are known to have analytic solutions and we will compare the numerical solution to the analytical one. The time dependence of $V(x,t)$ is of such a nature that partial derivatives with respect to time can easily be obtained. On the other hand by choosing different values of μ we can make the potential term vary slowly or rapidly with time.

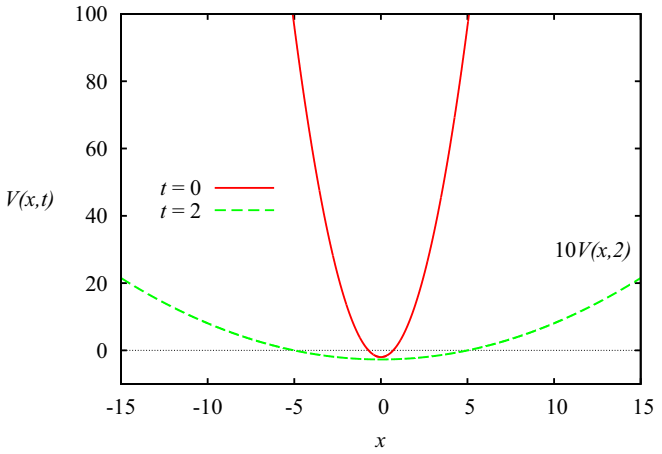

FIG. 4. (Color online) The potential of Eq. (4.16) as a function of x at $t = 0$ and $t = 2$. Since $V(x,2)$ is relative small, the curve plotted is magnified by a factor of ten. The units used are such that $\hbar = 2m = 1$.

A simpler potential can be obtained using the method of Fityo and Tkachuk [29]. When $\hbar = 1$ and $m = 1/2$ the potential

$$V(x,t) = \left(4e^{-2t} - \tfrac{1}{16}\right)x^2 - 2e^{-t} \quad (4.16)$$

yields a normalized wave function

$$\psi(x,t) = \left(\frac{2}{\pi}\right)^{1/4}\exp\left(-x^2e^{-t} - \frac{1}{4}t + \frac{i}{8}x^2\right). \quad (4.17)$$

The advantage of this potential as a test case is that it is easily differentiable with respect to time to any order. In order to obtain the derivatives of $N(x,t)$ we use Eqs. (4.3) and (4.6) with

$$\frac{\partial^l V}{\partial t^l} = (-1)^l(2^{l+2}e^{-2t}x^2 - 2e^{-t}) \quad (4.18)$$

for $l \geqslant 1$. To obtain a feel for the potential and the wave function they are plotted in Figs. 4 and 5 respectively.

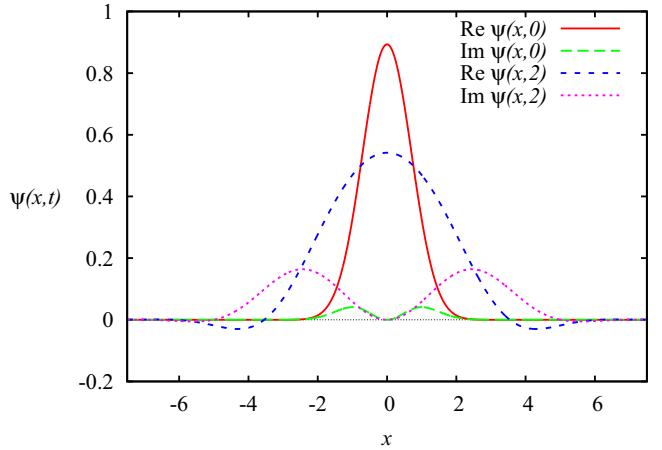

FIG. 5. (Color online) The wave functions Eq. (4.17) as a function of x at $t = 0$ and $t = 2$. The units used are such that $\hbar = 2m = 1$.

TABLE V. Parameters and errors for example 3.

M	r	J	Δt	e_2	$\eta_{M,r}$	τ[a]
1	19	200	0.0075	3.22035×10^{-5}	3.22173×10^{-5}	27
			0.0010	5.72355×10^{-7}	5.72353×10^{-7}	210
			0.0001	5.72356×10^{-9}		1.9 K
2			0.0075	7.60367×10^{-9}	7.60056×10^{-9}	91
			0.0010	2.40331×10^{-12}	2.40328×10^{-12}	590
3			0.0075	3.85317×10^{-12}	3.84974×10^{-12}	310
			0.0010	7.16318×10^{-15}	2.20551×10^{-17}	1.8 K
4			0.0075	8.77841×10^{-15}		1.2 K
			0.0010	7.16561×10^{-15}		6.5 K

[a]Time to calculate e_2 in quadruple precision with processor B.

The sample calculations were done with $-15 \leqslant x \leqslant 15$ and a final time of $t = 2$. The initial wave function was that of Eq. (4.17) with $t = 0$. The results are tabulated in Table V.

We observe an increase in efficiency and precision of the calculation with increasing values of M for relatively small M. When M is larger than 3 or 4, increasing the size of Δt gives unstable solutions in the sense that the convergence of the fixed point iteration (4.12) does not occur. The criterion of convergence that we used is that the iterative procedure is terminated when $e^{(i)} < 10^{-20}$.

In Fig. 6 we show the deviations from the exact solutions e_2 and the deviations from the next higher order approximation $\eta_{M,r}$. We obtain plateaus on which the values are very nearly the same. For instance for $M = 2$ for the six highest values of r each of the two errors are identical to seven significant figures and $e_2 = \eta_{M,r}$ to three significant figures. On the graph all the values of e_2 and $\eta_{M,r}$ for the same parameters are indistinguishable.

(As an aside, another candidate to test the method for time-dependent potentials is the linear time-dependent potential discussed by Guedes [30].)

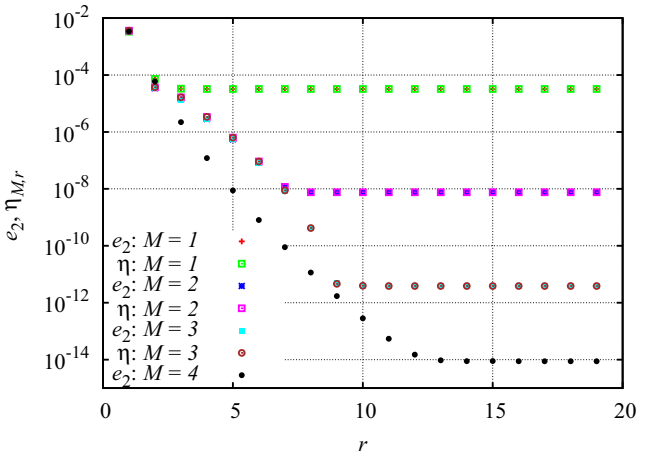

FIG. 6. (Color online) The errors (exact and estimated) for the calculations with the parameters $x_0 = -15, x_J = 15, J = 200, \Delta t = 0.0075$. The units used are such that $\hbar = 1, m = 1/2$. For the $M = 3$ case we terminate iteration for i when $e^{(i)} < 10^{-19}$. The η in the legend of the graph refers to $\eta_{M,r}$.

V. CONCLUDING REMARKS

We have developed accurate numerical methods for solving the TDSE with sources and/or time-dependent potentials. Since the function that is evaluated numerically, i.e., $\Psi^{(+)}$, from which the solution is extracted, is a normalized function the generalized CN method provides for a stable procedure. The examples of exactly solvable systems indicate that extremely accurate numerical solutions can be obtained. We employed double precision in the initial calculations, but with quadruple precision truncation errors could be driven down further (see Ref. [4]). There is a caveat, however, since the Euler-MacLaurin series is an asymptotic series; for a given Δt increasing the order of the approximation will eventually cause the precision to decrease.

The method allows for a calculation to arbitrary order of Δt and of Δx. In the calculations of the examples we calculate an error, which corresponds to the deviation from the exact solution. However, considering the difference of the numerical solution with one that is one order higher in both variables, we have an estimate of the error, which is of the same order of magnitude as the actual error. This permits one to estimate errors when no exact analytic solution is available.

The calculations were done in one dimension. They would be similar for partial wave calculations as was done in I. A natural extension is to consider systems of coupled equations as in Ref. [31]. Two- or three-dimensional calculations are a subject for future work.

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APPENDIX: HARMONIC OSCILLATOR WITH TIME-DEPENDENT FREQUENCY

To obtain potential (4.16) we use the method of Fityo and Tkachuk [29].[2] Using their notation, we choose

$$\tilde{f}(x,t) = x^2 e^{-t}. \tag{A1}$$

Thus we obtain

$$F(t) = \int_{-\infty}^{\infty} e^{-2\tilde{f}(x,t)}\, dx = \sqrt{\frac{\pi}{2}} e^{t/2}, \tag{A2}$$

which leads to

$$f(x,t) = \tilde{f} + \tfrac{1}{2}\ln F = x^2 e^{-t} + \tfrac{1}{4}t + \tfrac{1}{4}\ln \pi/2. \tag{A3}$$

We generate $g(x,t)$ from Eq. (5) of Ref. [29]

$$g(x,t) = \frac{1}{2}\int_0^x e^{2f(y,t)} \frac{\partial}{\partial t} \int_{-\infty}^{y} e^{-2f(z,t)}\, dz dy = -\frac{1}{8}x^2. \tag{A4}$$

[2]Equation (16) of Ref. [29] has a typo: the 3 should be replaced by 2.

Note that we remove a (constant) additive infinity from $g(x,t)$ by integrating over y from 0 to x rather than from $-\infty$ to x as in Ref. [29]. This has no consequence for the potential, but eliminates a (constant) infinite phase from the wave function.

The potential is obtained from

$$V(x,t) = g_t + f_x^2 - g_x^2 - f_{xx} \tag{A5}$$

and the normalized wave function is

$$\psi(x,t) = e^{-f(x,t)-ig(x,t)}. \tag{A6}$$

It is straightforward to verify that this wave function satisfies the time-dependent Schrödinger equation with potential (A5).

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