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An Alternative Numerical Method for Initial Value Problems Involving the Contact Nonlinear Hamiltonians

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We suggest a new difference scheme for dealing with contact nonlinear Hamiltonians. The scheme has two parts. First, the system is transformed to the interaction picture of quantum mechanics using the time-independent Hamiltonian H_0. This reduces the problem to a system of ordinary differential equations in time. Subsequently, the system is integrated in time for a time step Δt and then transformed back to the initial representation. Standard time integration schemes make it possible to eliminate explicit use of transformation operators, thus significantly reducing the number of calculations. We give explicit expressions for integration using the Runge–Kutta scheme. We consider three applications of the method and illustrate the behavior of the norms of the resulting wave functions after many time steps. The method is compared to the standard split-step method, and we show that our method has five $N(u_0(\tau))$ more calculations in a single step of the scheme, for the simplest case of one time and one spatial dimension. Here $N(u_0(\tau))$ is the number of calculations needed to apply the evolution operator $u_0(\tau)$ to the wave function, where u_0 is defined in terms of the (time-independent) Hamiltonian. This increase in the number of steps is offset by at least one order higher accuracy of the method. Its implementation is straightforward. It uses a unique arrangement of the steps of the split-step method.

Key Words: partial differential equations; difference methods; nonlinear Hamiltonians; Bose–Einstein condensation.

1. INTRODUCTION

Numerical methods have been widely applied to many different types of problems in quantum mechanics. Some of the more complex problems involve partial differential equations in time and at least one spatial dimension. In order to solve these problems, a standard

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approach is to discretize the wave functions, i.e., to replace them by a vector of values at particularly chosen points in time and space, and to use the difference approximation to construct the operators; see [1, 2]. In one spatial dimension, if the wave function has been sampled at $N+1$ equidistant points $\{x_j\}_{j=0..N}$, at the given time t, then

$$\varphi(t,x) \to [\varphi(t,x_0), \varphi(t,x_1), \ldots, \varphi(t,x_N)]. \tag{1}$$

The kinetic and potential energy are the most often encountered operators in quantum mechanics. Discretization diagonalizes the potential operator $V(x)$ making it local. The operators that incorporate spatial partial derivatives of any order, such as momentum or kinetic energy become nonlocal; i.e., their value at a given point depends not only on the values of the wave function at that point, but also on its neighboring values. The kinetic energy T, which contains the second-order spatial derivatives, when discretized to the second-order in h (h being the distance between the two successive points) becomes

$$T\varphi(t,x_j) \propto \frac{\partial^2\varphi}{\partial x^2}(t,x_j) = \frac{\varphi(t,x_{j+1}) - 2\varphi(t,x_j) + \varphi(t,x_{j-1})}{h^2} + O(h^2). \tag{2}$$

The form of these operators depends on the choice of boundary conditions; one can keep the value of the wave function at the boundaries fixed (usually zero), or one can impose periodicity. If the wave functions are localized far from the boundaries, these approaches are equivalent.

In one spatial dimension, for fixed values of the wave function at the boundaries, the kinetic energy operator becomes a $(N+1)$-dimensional tridiagonal square matrix. We thus obtain a discretized version of the operator H_0. The evolution of the initial wave function is found by applying the operator

$$u_0(\tau) = e^{-iH_0\tau}. \tag{3}$$

However, to obtain a numerically stable $u_0(\tau)$, one has to use the well-known approximation [2, 5]

$$u_0(\tau) \simeq \left(1 + i\frac{\tau}{2}H_0\right)^{-1}\left(1 - i\frac{\tau}{2}H_0\right), \tag{4}$$

which is correct up to the order $O(\tau^2)$ in time. To circumvent the problems of storing the matrix and calculating the inverse of such a large sparse matrix, this operator is not calculated at all. Instead, for any given vector $f(0)$, the result after applying the operator $u_0(\tau)$ is given as the solution of the linear system

$$\left(1 + i\frac{\tau}{2}H_0\right) f(\tau) = \left(1 - i\frac{\tau}{2}H_0\right) f(0). \tag{5}$$

This simplifies the evaluation of the vector $f(\tau)$ because the storage requirement for the operator u_0 is $O(N)$ and the evolution of the vector $f(0)$ is also obtained in $O(N)$ steps.

For more than one interacting field or a nonlinear interaction, this straightforward integration becomes impractical if not impossible. One example of such systems is the Bose condensate, whose starting point is one or more Gross–Pitaevskii equations, e.g., [6] and references therein. Analytical solutions of these equations exist only for the case of no external potential. Thus, one relies heavily on numerics in investigations of such systems.

The methods most often used belong to the class of so-called split-step methods. Recall the split-step method in [3] and let us consider the one-dimensional initial value problem

$$\begin{aligned} i\frac{\partial \varphi}{\partial t} &= H_0\varphi + W[t,\varphi], \\ \varphi(0,x) &= f(x), \quad x \in \langle -L, L\rangle. \end{aligned} \tag{6}$$

Here, L represents the relevant size of the physical system and is usually a result of a truncation of the domain of the original problem (because the functions and the operators may have been defined over the whole $\langle -\infty, \infty\rangle$ range). Numerical integration using the split-step method starts with the following integration:

$$\begin{aligned} &\varphi_1(t_k) = \varphi(t_k), \\ &t_k \le t \le t_k + \Delta t, \quad i\frac{\partial \varphi_1}{\partial t} = H_0\varphi_1. \end{aligned} \tag{7}$$

This solution is used for the second step, where

$$\begin{aligned} &\varphi_2(t_k) = \varphi_1(t_k + \Delta t), \\ &t_k \le t \le t_k + \Delta t, \quad i\frac{\partial \varphi_2}{\partial t} = W[t,\varphi_2]. \end{aligned} \tag{8}$$

At the end, the so-calculated $\varphi_2(t_k + \Delta t)$ is used as $\varphi(t_k + \Delta t)$. This effectively reduces to propagating the wave function over the same time interval Δt, while neglecting one or the other operator, H_0 or W. This heuristic approach has the inherent problem that the splitting of the evolution into two parts introduces an error of the order of $O(\Delta t^2)$, the long-term effects of which are hard to evaluate a priori. Calculations have to be repeated for a variety of Δx and Δt values in search of satisfactory convergence.

The question of whether it is possible to improve this basic split-step scheme without introducing additional steps was what led us to the development of the numerical method which we present here. Our method is based on the interaction picture of quantum mechanics. In Section II we give a brief exposition of the interaction picture followed by a derivation of method in the single field case. These concepts are then extended to more interacting fields and more dimensions. Subsequently, we give three examples of the successful application of the method. Section III is a discussion of the method and its comparison to the split-step method as well as a discussion of the numerical properties of the method.

2. THE INTERACTION PICTURE IN QUANTUM MECHANICS AND ITS NUMERICAL IMPLEMENTATION

Consider the initial value problem in one spatial dimension, involving a time-independent Hamiltonian H_0 acting on field $\varphi(t,x)$, together with some contact interaction operator W, which is nonlinear in the field $\varphi(t,x)$:[1]

$$\begin{aligned} i\frac{\partial \varphi}{\partial t} &= H_0\varphi + W[t,\varphi], \\ \varphi(0,x) &= f(x), x \in \langle -L, L\rangle. \end{aligned} \tag{9}$$

[1] If W is linear in the field $\varphi(t,x)$, i.e., $W[t,\varphi] = W[t,x]\varphi(t,x)$, the interaction picture is not needed, at least from the numerical point of view.

Here by the term contact (interaction) operator it is assumed that the result of the action of the operator at a particular point $(\vec{x}, t)$ on a wave function φ depends only on the value of the same wave function at that particular point. For example, differential operators or nonlocal potentials are excluded from this set of operators. We eliminate H_0 in Eq. (9) via a transformation of the wave function $\varphi(t)$,

$$\varphi(t) = e^{-iH_0t}\tilde{\varphi}(t), \tag{10}$$

so that the equation for the transformed wave function $\tilde{\varphi}(t, x)$ becomes

$$i\frac{\partial\tilde{\varphi}}{\partial t} = e^{iH_0t}W[t, e^{-iH_0t}\tilde{\varphi}]. \tag{11}$$

This transformation of the Eq. (9) corresponds to what is known as the interaction picture in quantum mechanics; see, e.g., [7]. We now examine how we can utilize this formula in a numerical scheme.

2.1. *Derivation of the Method*

Let us first examine the equation of propagation of a wave function over the time interval $[t_k, t_{k+1}]$, for some $k \in N$. For $0 \le \tau \le \Delta t$, we have

$$i\frac{\partial\tilde{\varphi}(t_k+\tau)}{\partial\tau} = e^{iH_0(t_k+\tau)}W\left[t_k+\tau, e^{-iH_0(t_k+\tau)}\tilde{\varphi}(t_k+\tau)\right]. \tag{12}$$

We introduce a new wave function $\hat{\varphi}(\tau)$ which serves as a dummy variable[2] for the time integration. It is defined by

$$\hat{\varphi}(\tau) = e^{-iH_0t_k}\tilde{\varphi}(t_k+\tau), \tag{13}$$

whose evolution is described by

$$i\frac{\partial\hat{\varphi}(\tau)}{\partial\tau} = e^{iH_0\tau}W[t_k+\tau, e^{-iH_0\tau}\hat{\varphi}], \tag{14}$$

with the initial conditions

$$\hat{\varphi}(0) = e^{-iH_0t_k}\tilde{\varphi}(t_k) = \varphi(t_k). \tag{15}$$

The operator W is a contact operator, in the sense described earlier, so the time integration of the Eq. (14) can be performed using a standard ODE integration method [4].

This applied to the array of functions $\hat{\varphi}(\tau) = \{\hat{\varphi}(\tau, x_j)\}_{j=0\ldots N}$ yields the array $\hat{\varphi}(\Delta t) = \{\hat{\varphi}(\Delta t, x_j)\}_{j=0\ldots N}$. Let us see how this solution is related to the solution we are interested in (in the Schroedinger picture); i.e., $\varphi(t_k+\Delta t) = \varphi(t_{k+1})$.

First observe

$$\hat{\varphi}(\Delta t) = e^{-iH_0t_k}\tilde{\varphi}(\Delta t) = e^{-iH_0t_k}e^{iH_0(t_k+\Delta t)}\varphi(t_k+\Delta t). \tag{16}$$

[2] Using this function as the dummy variable renders its indexing with respect to the absolute time t_j, $j = 1\ldots M$ unnecessary. As it follows from the scheme, its values are discarded at the end of the evolution by Δt once the wave function $\varphi(t_k+\Delta t)$ is calculated.

then

$$\varphi(t_{k+1}) = \varphi(t_k + \Delta t) = e^{-iH_0\Delta t}\hat{\varphi}(\Delta t). \tag{17}$$

This is our final result. Let us summarize it.

The numerical solution of the initial value problem

$$\begin{aligned} i\frac{\partial\varphi}{\partial t} &= H_0\varphi + W[t,\varphi], \\ \varphi(0,x) &= f(x), x \in \langle -L, L\rangle, \end{aligned} \tag{18}$$

for time $[t_k, t_k + \Delta t]$ is thus equal to the solution of the following initial value problem

$$\begin{aligned} i\frac{\partial\hat{\varphi}(\tau)}{\partial\tau} &= e^{iH_0\tau}W[t_k+\tau, e^{-iH_0\tau}\hat{\varphi}(\tau)] \\ & 0 \le \tau \le \Delta t, \end{aligned} \tag{19}$$

for

$$\hat{\varphi}(0) = \varphi(t_k), \tag{20}$$

yielding

$$\varphi(t_{k+1}) = \varphi(t_k + \Delta t) = e^{-iH_0\Delta t}\hat{\varphi}(\Delta t). \tag{21}$$

This concludes the derivation of the method. We now proceed to the question of the choice of time integration scheme and its effects.

2.2. *Implementation of the Method*

We apply the standard Runge–Kutta fourth-order scheme for the time integration of Eq. (19). We use u_0 from Eq. (3). This yields

$$\begin{aligned} y_1' &= -iW[t_k, \varphi(t_k)], \\ y_2' &= -iu_0^{-1}\left(\frac{\Delta t}{2}\right)W\left[t_k + \frac{\Delta t}{2}, u_0\left(\frac{\Delta t}{2}\right)\left(\varphi(t_k) + \frac{\Delta t}{2}y_1'\right)\right], \\ y_3' &= -iu_0^{-1}\left(\frac{\Delta t}{2}\right)W\left[t_k + \frac{\Delta t}{2}, u_0\left(\frac{\Delta t}{2}\right)\left(\varphi(t_k) + \frac{\Delta t}{2}y_2'\right)\right], \\ y_4' &= -iu_0^{-1}(\Delta t)W[t_k + \Delta t, u_0(\Delta t)(\varphi(t_k) + \Delta t y_3')]. \end{aligned} \tag{22}$$

The final result of the time evolution becomes

$$\varphi(t_k + \Delta t) = u_0(\Delta t)\left(\varphi(t_k) + \frac{\Delta t}{6}(y_1' + 2y_2' + 2y_3' + y_4')\right). \tag{23}$$

The problem with Eq. (22) is that both operators, u_0 and u_0^{-1}, are present. This can be avoided if one examines more carefuly Eq.(23). There is a multiplication by $u_0(\Delta t)$ of all parts that come from the Runge–Kutta scheme that cancels the inverse of u_0. Taking

this into account before applying the Runge–Kutta scheme yields computationally simpler equations:

$$\begin{aligned}
Y_1' &= -iW[t_k, \varphi(t_k)],\\
Y_2' &= -iW\left[t_k + \frac{\Delta t}{2}, u_0\left(\frac{\Delta t}{2}\right)\left(\varphi(t_k) + \frac{\Delta t}{2}Y_1'\right)\right],\\
Y_3' &= -iW\left[t_k + \frac{\Delta t}{2}, u_0\left(\frac{\Delta t}{2}\right)\varphi(t_k) + \frac{\Delta t}{2}Y_2'\right],\\
Y_4' &= -iW\left[t_k + \Delta t, u_0\left(\frac{\Delta t}{2}\right)\left(u_0\left(\frac{\Delta t}{2}\right)\varphi(t_k) + \Delta t Y_3'\right)\right].
\end{aligned} \tag{24}$$

Using this in Eq. (23) yields

$$\varphi(t_k + \Delta t) = u_0(\Delta t)\left(\varphi(t_k) + \frac{\Delta t}{6}Y_1'\right) + \frac{\Delta t}{3}u_0\left(\frac{\Delta t}{2}\right)(Y_2' + Y_3') + \frac{\Delta t}{6}Y_4'. \tag{25}$$

This formula is the final result of this paper.

The error order of the method is the smaller of the error orders of Runge–Kutta, $O(\Delta t^5)$, and the error in the numerical approximation of u_0. If finite differences are used for the u_0, which was the case in this paper, then the error order is $O(\Delta t^3, \Delta h^2)$. Observe, however, that this can be improved by using alternative approaches, like spectral method or FFT. This is considered a technical detail that does not change the nature of the method, as presented in this paper, and can be the topic of further research.

2.3. *More Interacting Fields, More Dimensions*

Consider the case of N interacting fields, $\{\varphi_i\}_{i=1}^N$ and their Hamiltonians $H_{0,i} + W_i$. The contact interaction between the fields can generally be written as

$$W_i = W_i\left[x, t; \{\varphi k(x,t)\}_{k=1}^N\right]. \tag{26}$$

The equations are written in the same manner as for the single field. This time, though, each field has its own "interaction picture" operator $H_{0,i}$. The system of equations we solve is thus

$$\begin{gathered}
i\frac{\partial\hat{\varphi}_j(\tau)}{\partial\tau} = e^{iH_{0,j}\tau}W_j\left[t_k + \tau, \{e^{-iH_{0,k}\tau}\hat{\varphi}_k(\tau)\}_{k=1}^N\right], \quad j = 1\ldots N\\
0 \le \tau \le \Delta t,
\end{gathered} \tag{27}$$

where the initial conditions are the same

$$\hat{\varphi}_j(0) = \varphi_j(t_k), \quad j = 1\ldots N, \tag{28}$$

and

$$\varphi_j(t_{k+1}) = \varphi_j(t_k + \Delta t) = e^{-iH_{0,j}\Delta t}\hat{\varphi}_j(\Delta t), \quad j = 1\ldots N. \tag{29}$$

After the time integration scheme is chosen, each step in the time evolution scheme is evaluated for all fields at once, and then these results are used for the next step.

The method has a very simple extension to more dimensions if the operator W is a contact operator, in the sense defined earlier, and if the Hamiltonian H_0 is separable coordinatewise.

Coordinate separability of the H_0 means the operator H_0 can be written as a sum of coordinate pieces; i.e., $H_0 = H_0(\partial_{\vec{x}}, \vec{x}) = \sum_j H_{0,j}(\partial_j, x_j)$. This separability implies that the evolution operator due to H_0, $u_0(\Delta t) = \exp(-\frac{i}{\hbar} H_0 \Delta t)$ can be factorized into the product of coordinate evolution operators; i.e., $u_0(\Delta t) = \prod_j u_{0,j}(\Delta t)$. However, when applying this mathematical identity to a particular matrix representation of the operator, some caution is due. For example, if a finite difference method is used for a two-dimensional calculation, then the matrices $u_{0,x}$ and $u_{0,y}$ do not commute, except in a special case of a spherically symmetric potential. To remedy this lack of commutation the following can be done: (i) the operator u_0 can be symmetrized, e.g., in two dimensions $u_{0,(x,y)} = \frac{1}{2}(u_{0,x}u_{0,y} + u_{0,y}u_{0,x})$ or (ii) the Hamiltonian H_0 can be conveniently chosen so that its coordinate pieces, $H_{0,j}$'s, do commute even when discretized and written in matrix form. As an example of the latter one may use only the kinetic (energy) part as the operator H_0, while adding the potential $V(\vec{x})$ to the operator W.

2.4. *Examples*

We give three examples of the use of the method to point out its advantages and indicate possible problems. We have chosen examples from our numerical research in the field of Bose–Einstein condensation. Throughout we use the Runge–Kutta fourth-order method for time integration.

Example I is the calculation of the ground state of the Bose condensed system in one spatial dimension. Our method is modified in such a way that the evolution occurs in complex time instead of real time. To compensate for the loss of norm at every step the wave function is normalized. We solve

$$\begin{aligned} H_0 &= -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2, \\ W[\varphi] &= 4\pi a_0 |\varphi|^2 \varphi. \end{aligned} \tag{30}$$

The initial density, given by the ground state of the harmonic oscillator, and the final density of the field $\varphi(x)$ are given in Fig. 1. The values of the parameters are $a_0 = 5$, $L = 28.5$, $N = 1024$, $\Delta t = 0.01$.

Examples II and III demonstrate the behavior of the most common error in this type of calculation, preservation of the norm of the wave function. In Example II, the wave function found in Example I is propagated 500,000 steps. Figure 2 shows the dependence of the norm on the number of steps. Example III is the most intricate. Here we show the solution to a system of coupled harmonic oscillators with nonlinear second harmonic generation. The operators for the field $\varphi(x)$are

$$\begin{aligned} H_{0,\varphi} &= -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2, \\ W_\varphi &= -K\varphi^*\psi, \end{aligned} \tag{31}$$

and the field $\psi(x, t)$

$$\begin{aligned} H_{0,\psi} &= -\frac{1}{4}\frac{\partial^2}{\partial x^2} + x^2 - \delta, \\ W_\psi &= -K\varphi^2. \end{aligned} \tag{32}$$

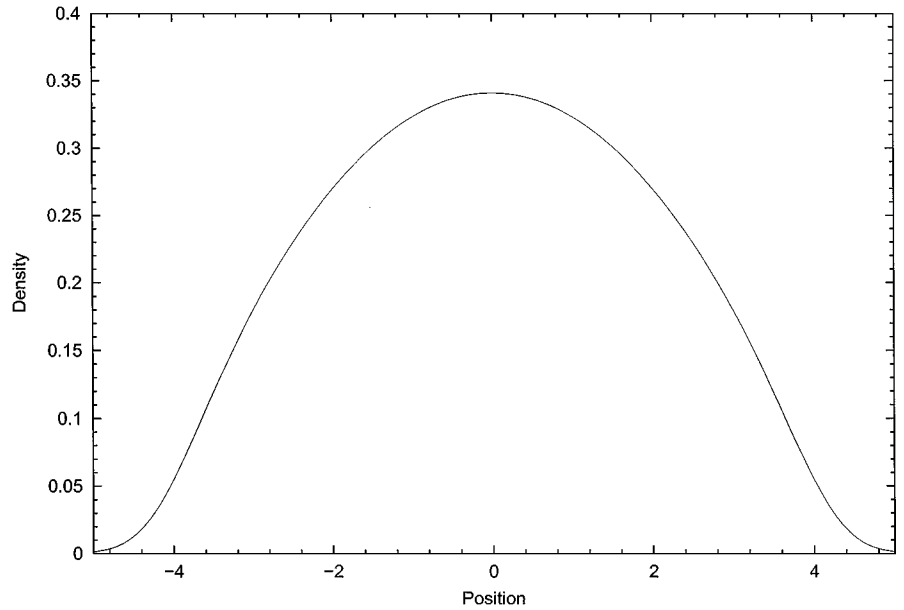

FIG. 1. The density of the atomic Bose condensate in ground state, Example I, obtained by evolution in complex time. The values of the numerical parameters are $a_0 = 5$, $L = 28.5$, $N = 1024$, $\Delta t = 0.01$.

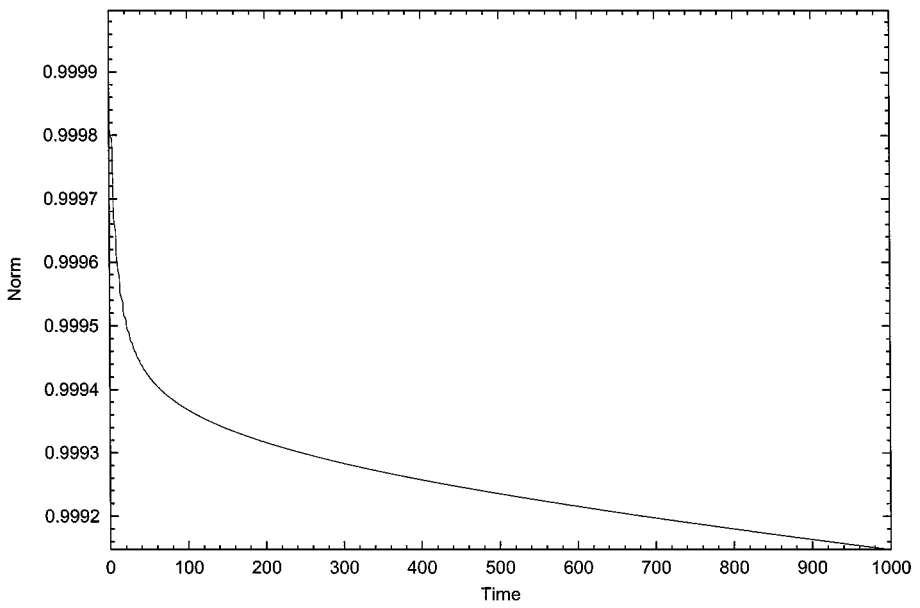

FIG. 2. Behavior of the norm of the wave function of the atomic Bose condensate, Example II—Slightly perturbed ground state used as the initial condition and propagated for 500,000 iterations. The numerical parameters are $a_0 = 5$, $L = 28.5$, $N = 1024$, $\Delta t = 0.002$.

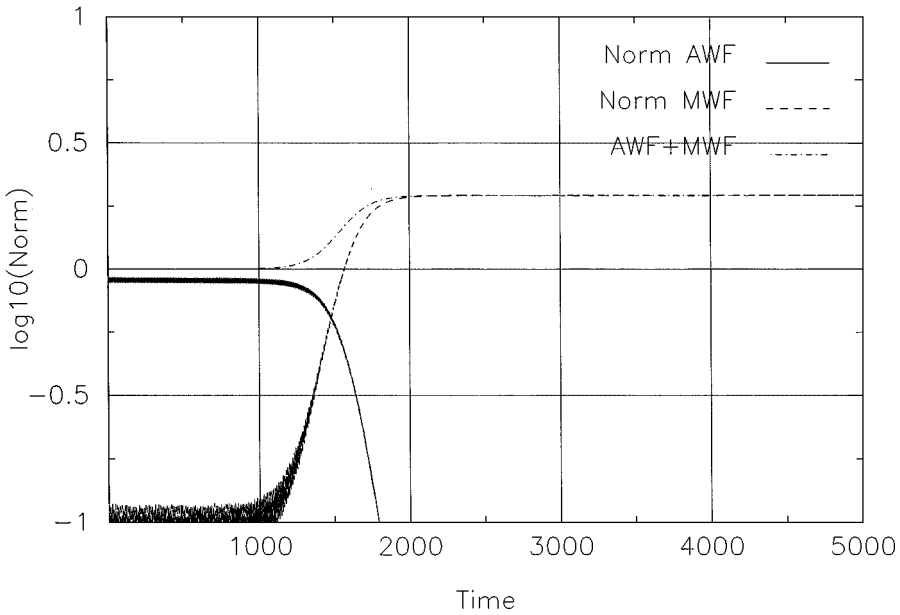

FIG. 3. Squared norm behavior of the distribution functions for fields φ (Norm AWF), ψ (Norm MWF), and their sum (AWF + MWF), as the function of time, as described in Example III. The distribution functions are propagated for 500,000 iterations, using Eqs. (31) and (32). The numerical parameters are $L = 28.5$, $N = 1024$, $\Delta t = 0.01$, $\delta = 2$, $K = 1$.

The initial condition is the ground state obtained by evolving the same system of equations in complex time. Then a random perturbation of 10% of the local amplitude is introduced. The values of all parameters were the same as those for Examples I and II, while the new parameters δ and K have the values 2 and 1, respectively. The behavior of the norm of the wave functions is shown in Fig. 3 calculated for 500,000 iterations. In this case the error in the norm becomes nonnegligible after some $N \sim 150{,}000$ iterations. This growth of norm was actually used as an indicator of chaos in the system. This behavior was expected based on the theoretical analysis of the system over the considered range of parameters.

3. DISCUSSION

In this section we compare the method to one of the standard approaches in dealing with nonlinear Hamiltonians, the so-called split-step group of methods. In the Introduction, we indicated how the method would be implemented for a typical problem. Consider solving the initial value problem, with the splitting along the lines outlined in Eqs. (7) and (8),[3] where the Runge–Kutta fourth-order method is used for time integration of the nonlinear part. Then a propagation of the solution, $\varphi(t_k)$, for the time step Δt would consist of the calculations

[3] Here alternative splittings are possible. One of the faster splittings is that using as H_0 only a kinetic energy operator. Evolution under action of this operator is then performed using a FFT scheme.

$$
\begin{aligned}
y_1' &= -i\,W[t_k, \varphi(t_k)],\\
y_2' &= -i\,W\left[t_k + \frac{\Delta t}{2}, \varphi(t_k) + \frac{\Delta t}{2} y_1'\right],\\
y_3' &= -i\,W\left[t_k + \frac{\Delta t}{2}, \varphi(t_k) + \frac{\Delta t}{2} y_2'\right],\\
y_4' &= -i\,W[t_k + \Delta t, \varphi(t_k) + \Delta t y_3'],
\end{aligned}
\tag{33}
$$

so that

$$
\varphi_2(t_k + \Delta t) = \varphi(t_k) + \frac{\Delta t}{6}(y_1' + 2y_2' + 2y_3' + y_4'). \tag{34}
$$

This is followed by the evolution due to the H_0 for the time step Δt, resulting in

$$
\varphi(t_k + \Delta t) = u_0(\Delta t)\left(\varphi(t_k) + \frac{\Delta t}{6}(y_1' + 2y_2' + 2y_3' + y_4')\right). \tag{35}
$$

Compare the split-step method, Eqs. (33) to the proposed method

$$
\begin{aligned}
Y_1' &= -i\,W[t_k, \varphi(t_k)],\\
Y_2' &= -i\,W\left[t_k + \frac{\Delta t}{2}, u_0\left(\frac{\Delta t}{2}\right)\left(\varphi(t_k) + \frac{\Delta t}{2} Y_1'\right)\right],\\
Y_3' &= -i\,W\left[t_k + \frac{\Delta t}{2}, u_0\left(\frac{\Delta t}{2}\right)\varphi(t_k) + \frac{\Delta t}{2} Y_2'\right],\\
Y_4' &= -i\,W\left[t_k + \Delta t, u_0\left(\frac{\Delta t}{2}\right)\left(u_0\left(\frac{\Delta t}{2}\right)\varphi(t_k) + \Delta t Y_3'\right)\right],
\end{aligned}
\tag{36}
$$

with the final result

$$
\varphi(t_k + \Delta t) = u_0(\Delta t)\left(\varphi(t_k) + \frac{\Delta t}{6} Y_1'\right) + \frac{\Delta t}{3} u_0\left(\frac{\Delta t}{2}\right)(Y_2' + Y_3') + \frac{\Delta t}{6} Y_4'. \tag{37}
$$

One observes that our method has five more operations in which the operators $u_0(\Delta t)$ or $u_0(\Delta t/2)$ act on the wave functions. The time integration, on the other hand, has the same number of operations for both methods.

In our opinion, the advantages of our method outweigh the advantages of the splitstep method for this particular class of the problems. We improved the accuracy by at least one order, through only a slightly larger number of computations. Finally, due to the good numerical properties of the operator $u_0(\Delta t)$, for long time iterations, stability of the iterations can be insured by careful examination of the problem and suitable choice of the time integration scheme.

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