

Absorbing boundary conditions for nonlinear Schrödinger equations

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A local time-splitting method (LTSM) is developed to design absorbing boundary conditions for numerical solutions of time-dependent nonlinear Schrödinger equations associated with open boundaries. These boundary conditions are significant for numerical simulations of propagations of nonlinear waves in physical applications, such as nonlinear fiber optics and Bose-Einstein condensations. Numerical examples are implemented to demonstrate the attractive features of using the LTSM.

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I. INTRODUCTION

Many physical problems require the numerical solution of the nonlinear Schrödinger equation [1] of the form

$$i\hbar[\partial\psi(x,t)]/\partial t = [- (\hbar^2/2m)(\partial^2/\partial x^2) + V(x) + f(|\psi|^2)]\psi, \quad (1)$$

associated with open boundaries, where m is the atomic mass, \hbar is the Planck constant, and $V(x)$ is a potential which is assumed to be constant or almost constant in the far field region. In particular, when the nonlinear term is a cubic one $g|\psi|^2\psi$, Eq. (1) reduces to the one-dimensional Gross-Pitaevskii equation, which describes a Bose-Einstein condensate (BEC) [2] at zero or very low temperature. Here the constant coefficient g is positive for repulsive interactions and negative for attractive interactions. Similar equations also appear in nonlinear optics in fibers [3] where the refractive index due to self-phase modulation leads to the nonlinear effect in optic fibers like the one in Eq. (1). Numerical studies of the Gross-Pitaevskii equation are extremely important as these can provide many interesting phenomena of BECs [4–10]. Consider that the wave function $\psi(x,t)$ of an interacting condensate is expanded in a lattice and propagates indefinitely [11]. In order to simulate the process numerically, one usually uses a periodic boundary condition or a Dirichlet boundary condition $\psi=0$ or a Neumann boundary condition $\frac{\partial\psi}{\partial x}=0$. However, the periodic boundary condition often induces nonphysical wave interactions, and accordingly, it is inappropriate. And the latter two conditions require that the computational domain is very large in order to avoid artificial reflections from the boundary. This would be costly for problems evolving over many time steps or multi-dimensional problems.

An alternative way is to impose an absorbing boundary condition (ABC) [12] such that there is a minor influence to the solution in the interior domain for a finite computational domain. Much attention [13,14] has been paid to develop ABCs for linear Schrödinger equations, which is also available when the nonlinearities of waves are weak [11]. For a general nonlinear case, it is a challenging job to design a suitable ABC of Eq. (1) since many techniques for linear

equations such as the Fourier transformation are invalidated. When the nonlinearity is cubic, the nonlinear Schrödinger equation is integrable, and its exact ABC [15] which is non-local can be obtained through the inverse scattering transform technique. In previous work [16], the perfectly matched layer was introduced for nonlinear waves as an ABC, which was also applied to simulating supersonic BECs [17] and matter waves of the nonpolynomial nonlinear Schrödinger model [18].

In the context of this report we discuss a different method to design ABCs for the nonlinear Schrödinger equation. The so-called local time-splitting method (LTSM) is an extension of our previous work for the advection-diffusion equation [19]. The procedure is simple, effective, and easy to be extended into multidimensional cases. The LTSM can also work well even for a very strong nonlinearity such as the nonlinear Schrödinger equation in the semiclassical regimes. In addition, our method is also available for a general nonlinearity in Eq. (1) such as a quintic nonlinearity [20].

II. ABSORBING BOUNDARY CONDITIONS

The idea of using the LTSM to design ABCs for Eq. (1) is to split the original equation into several subproblems which are easy to be handled, and then solve them alternatively in a small time step Δt . The essential idea of the time-splitting procedure has been widely applied to optical communications [3,21] and modeling of BECs [9]. In these literatures, the time-splitting procedure is global, and is available in both the interior domain and boundaries. However, the global procedure is limited in some situations. For example, the time-splitting Fourier method is a powerful tool in solving the nonlinear Schrödinger equation, but periodic boundary conditions have to be implied if one hopes to use the fast Fourier transform algorithm [3]. Conversely, the LTSM splits the equation only on the neighbor grid points of boundaries. It has great advantage since one possesses many choices for discrete schemes in the interior domain.

Consider a standard splitting for Eq. (1) to form a linear subproblem

$$i\hbar[\partial\psi(x,t)/\partial t] = [- (\hbar^2/2m)(\partial^2/\partial x^2) + V(x)]\psi(x,t) \quad (2)$$

and a nonlinear subproblem

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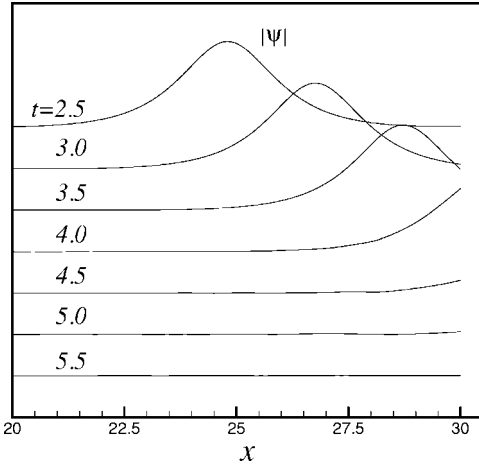


FIG. 1. Propagation of a bright soliton for $|\psi|$. The soliton propagates to the right and is absorbed completely by the boundary at $x=30$. Here $\Delta x=0.1$, $\Delta t=0.05$, $k_0=2$, and $g=-2$ are taken.

$$i\hbar(\partial\psi(x,t)/\partial t) = f(|\psi(x,t)|^2)\psi(x,t). \quad (3)$$

The nonlinear one (3) is an ordinary differential equation, and therefore an extra boundary condition is no more required.

For the linear equation (2) with constant potential function, different methods, by utilizing a rational polynomial to approximate the dispersion relation,

$$\hbar k = \pm \sqrt{2m[\hbar\omega - V]}, \quad (4)$$

have been proposed for obtaining local ABCs. In Eq. (4), the plus sign corresponds to waves moving to the positive x direction, and the minus sign indicates wave motions in opposite direction. The first local ABC was developed in Ref. [13], where the square root is approximated by a linear polynomial after imposing two adjustable parameters which represent the approximate group velocities of the kinetic energy [22]. A second approximation was offered in Ref. [14] by using a rational function to give

$$\hbar k = \pm \hbar k_0(1 + 3z)/(3 + z), \quad (5)$$

with $z=2m(\hbar\omega - V)/\hbar^2 k_0^2$, where $\hbar k_0$ is the expansion point of the rational approximation to Eq. (4). Transforming formula (5) back into a differential equation at the boundaries, one obtains [14]

$$-i\hbar(3\hbar^2 k_0^2/2m - V)(\partial/\partial x)\psi(x,t) + \hbar^2(\partial^2/\partial x^2)\psi(x,t) = \pm \hbar k_0(\hbar^2 k_0^2/2m - 3V)\psi(x,t) \pm 3i\hbar^2 k_0(\partial/\partial t)\psi(x,t). \quad (6)$$

Using the original equation to replace the temporal derivative term yields

$$[\partial^3/\partial x^3 - 3k_0^2(\partial/\partial x) \pm (-3k_0i(\partial^2/\partial x^2) + k_0^3i)]\psi(x,t) = 0. \quad (7)$$

This is an ABC for the $p=3$ case of the form in Ref. [22]. It is important to note that the ABCs (6) and (7) depend on the parameter k_0 , which is related to the group velocity of the waves. Besides these, various ABCs are also available for the linear Schrödinger equation such as discrete ABCs reported

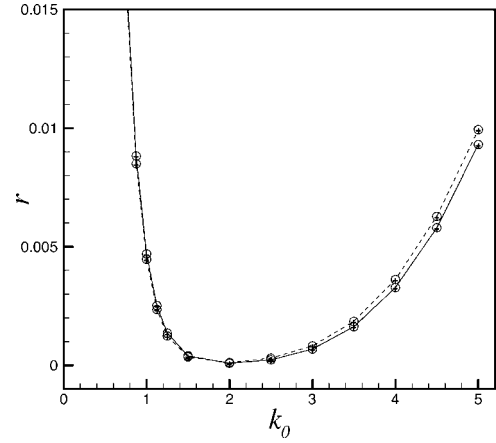


FIG. 2. The reflection coefficient r vs the parameter k_0 with the initial data (12) for different g and grid sizes at time $t=6$. The crosses refer to $g=-2$, and the circles refer to $g=-10$. The curves of two cases almost overlap. The dashed lines show the results for $\Delta x=0.1$ and $\Delta t=0.05$, and the solid lines show the results for $\Delta x=0.05$ and $\Delta t=0.025$.

frequently [23,24] in recent years. In our discussion, the ABC (6) is used as a boundary condition of the linear subproblem.

Now consider the coupling procedure of discretizations for the interior equation and boundary subproblems. Denote Δx and Δt grid sizes in space and time, respectively. To get the numerical solution in the interval $[0, L]$, we use the Crank-Nicholson method [25] to approximate Eq. (1):

$$i\hbar \frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = \left[V_j + f\left(\left|\frac{\psi_j^{n+1} + \psi_j^n}{2}\right|^2\right) \right] \frac{\psi_j^{n+1} + \psi_j^n}{2} - (\hbar^2/2m) \times [(\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1})/2\Delta x^2 + (\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n)/2\Delta x^2] \quad (8)$$

for $j=0, \dots, J$, where ψ_j^n represents the approximation of wave function ψ on the grid point (x_j, t^n) with $t^n = n\Delta t$, $x_j = j\Delta x$, $x_0=0$, and $x_J=L$. Two unknown ghost values ψ_{-1}^{n+1} and ψ_{J+1}^{n+1} cannot be obtained here, and must be provided through boundary conditions. For the purpose, we split Eq. (1) into two subproblems (2) and (3) on the grid points x_α for $\alpha \in \mathcal{S} = \{-1, 0, 1\} \cup \{J-1, J, J+1\}$ in the vicinity of the boundaries, and then solve Eqs. (2) and (3) separately, in which the solution of one subproblem is employed as an initial condition for the next subproblem by imposing intermediate variables ψ_α^* . For Eq. (3), we use the discrete formula

$$\psi_\alpha^{n+1} = e^{-if(|\psi_\alpha^*|^2)\Delta t/\hbar} \psi_\alpha^*, \quad \alpha \in \mathcal{S}, \quad (9)$$

which keeps $|\psi|$ invariant [9]. The first intermediate step is a linear problem, which can generate two extra equalities by discretizing the ABCs (6) with the Crank-Nicholson scheme

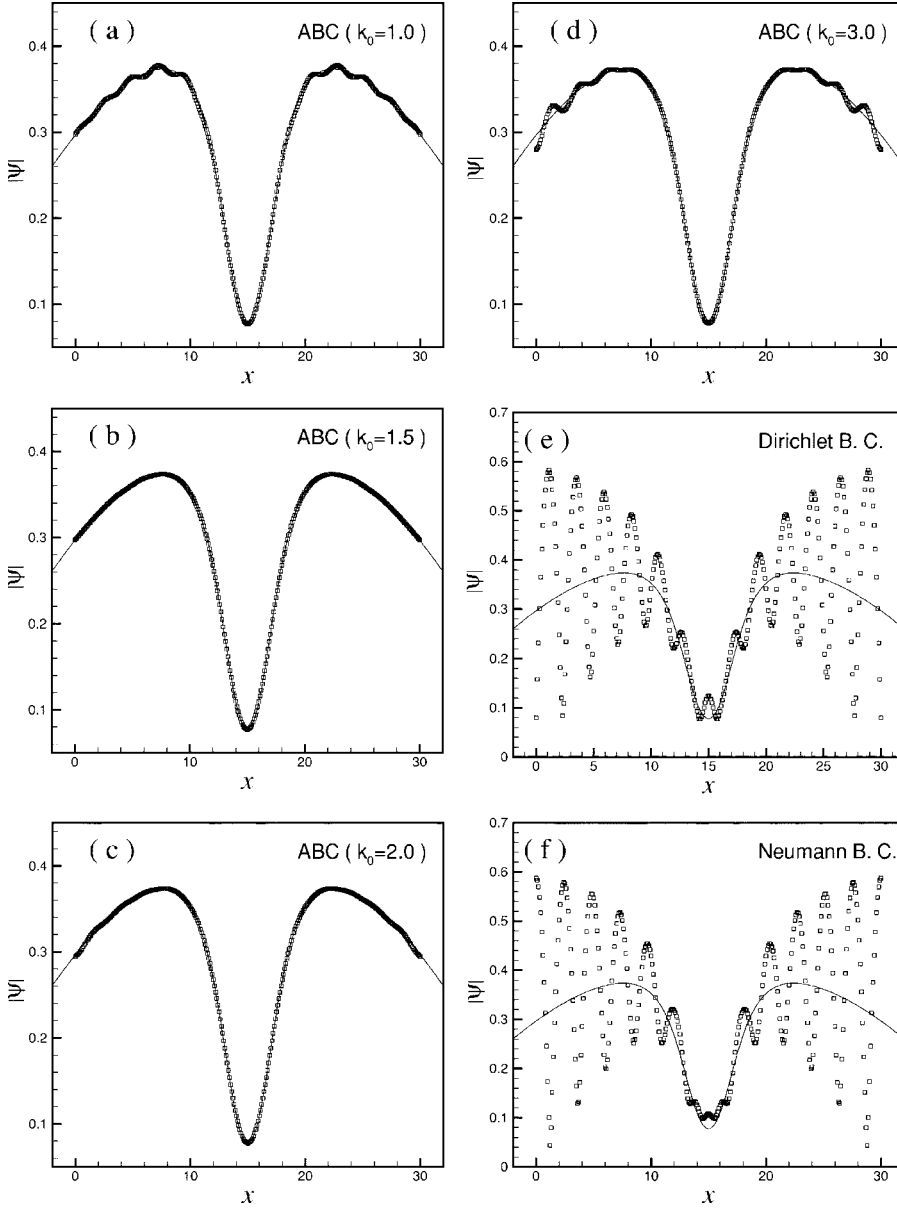


FIG. 3. Expanding of matter waves at $t=6$. The solid line shows the “exact” solution. The squares refer to the numerical solutions in a small domain: (a)–(d) ABCs for $k_0=1, 1.5, 2$, and 3 , respectively; (e) Dirichlet BC; and (f) Neumann BC.

$$\begin{aligned}
 & -i\hbar \left(\frac{3\hbar^2 k_0^2}{2m} - V_s \right) \left(\frac{\psi_{s+1}^* - \psi_{s-1}^*}{4\Delta x} + \frac{\psi_{s+1}^n - \psi_{s-1}^n}{4\Delta x} \right) \\
 & + \hbar^2 [(\psi_{s+1}^* - \psi_{s-1}^*)/2\Delta x \Delta t - (\psi_{s+1}^n - \psi_{s-1}^n)/2\Delta x \Delta t] \\
 & = \pm \hbar k_0 \left(\frac{\hbar^2 k_0^2}{2m} - 3V_s \right) \frac{\psi_s^* + \psi_s^n}{2} \pm 3i\hbar^2 k_0 \frac{\psi_s^* - \psi_s^n}{\Delta t}, \quad (10)
 \end{aligned}$$

where the positive sign in “ \pm ” corresponds to the right boundary $s=J$ and the negative one corresponds to the left boundary $s=0$.

Formulas (8)–(10) represent a nonlinear algebraic system of $J+9$ equations for $J+9$ unknowns $\{\psi_j^{n+1}\}_{j=-1}^{J+1}$ and $\{\psi_\alpha^*, \alpha \in \mathcal{S}\}$. The system can be solved by a nonlinear iterate procedure. To improve the local time-splitting procedure described above, a second-order Strang splitting [26] can be used, where we use two intermediate variables ψ^* and ψ^{**} , which satisfy the approximations

$$\psi_\alpha^* = e^{-if(|\psi_\alpha^n|^2)\Delta t/2\hbar} \psi_\alpha^n \quad \text{and} \quad \psi_\alpha^{n+1} = e^{-if(|\psi_\alpha^*|^2)\Delta t/2\hbar} \psi_\alpha^*. \quad (11)$$

Thus the similar algebraic system can be obtained by using the approximations of the ABCs and Eq. (8).

III. NUMERICAL EXAMPLES

To test the performance of the LTSM, two application examples for the Gross-Pitaevskii equation as $f(|\psi|^2)=g|\psi|^2$ in Eq. (1) are investigated, where dimensionless parameters $\hbar=1$ and $m=\frac{1}{2}$ are taken, and the second-order Strang splitting is used. In calculations, the reduced nonlinear algebraic system is solved by an iterative algorithm as used in Ref. [27], in which the nonlinear parts are linearized at each iterate step.

A. Propagation of a bright soliton

The soliton behavior is of particular interest in optical communications and dynamics of BECs. In the first example,

$V=0$ and $L=30$ are chosen for a propagating bright soliton, which corresponds to attractive interactions. The temporal evolution of an initial bright soliton

$$\psi(x,0) = \sqrt{-2/g} \operatorname{sech}(x-x_0)e^{2i(x-x_0)} \quad (12)$$

with $x_0=15$ is simulated to test the performance of the ABC when the wave propagates to the boundary of computational domain. As is shown for $|\psi|$ in Fig. 1, where k_0 is taken to be equal to the wave number of the wave, the soliton travels until it reaches the boundary and has been absorbed almost completely.

For initial wave functions which are composed of different group velocities, a general method [22] to choose k_0 is the one in which Fourier mode is dominant by a Fourier series expansion. It is important to see the influence of k_0 to the boundary conditions. The reflection ratios at time $t^n=6$ are calculated as [14]

$$r = \frac{\sum_{j=0}^J |\psi_j^n|^2}{\sum_{j=0}^J |\psi_j^0|^2}, \quad (13)$$

which were shown in Fig. 2. The ratio r is handy in the measurement of the quality of the ABC and the dependence of the nonlinear coefficient g and the parameter k_0 . For example, $r=0$ reflects that the soliton has passed through the boundary completely; whereas $r=1$ indicates the wave is completely reflected into the interior domain by the artificial boundaries. In calculations, two grid sizes and two different g are used. In the experimental setting of BECs, g often takes large value so that the nonlinearity is very strong. It can be seen that the ABC works well even for a strong nonlinearity; the reflection ratios for $g=-10$ is almost equal to those for a weaker nonlinearity $g=-2$. The reflection ratio is intensively dependent of the parameter k_0 , which, however, can be chosen in a large interval. When k_0 is chosen in $[0.85, 5]$, r is

less than 1%, but out of this interval, the reflection will increase rapidly.

B. Repulsive interaction

Consider a nonlinear wave with repulsive interaction, such as free expansion of a BEC. The initial wave and potential function are taken to be Gaussian pulses,

$$\psi(x,0) = e^{-0.1(x-x_0)^2} \text{ and } V(x) = e^{-0.5(x-x_0)^2}, \quad (14)$$

with $x_0=15$. In the calculation, $g=2$, $L=30$, $\Delta x=0.1$, and $\Delta t=0.0375$ are chosen. The numerical results with the same mesh sizes by using the proposed ABC in a large domain $[-15, 45]$ are taken to be a reference exact solution, since the analytic solution is unknown. Figures 3(a)–3(d) show the motion of the wave with the ABCs for four different parameters. The reflective wave is very small when the waves hit the boundaries if k_0 is in an appropriate range, such as $[1.5, 2]$. Without the ABC, on the other hand, as is seen in Figs. 3(e) and 3(f), the computational results are very awful.

IV. SUMMARY

Absorbing boundary conditions have been proposed for the nonlinear Schrödinger equation by using a local time-splitting technique, which can be extended into a wide range of applications, such as in the modeling of optical soliton propagations and expanding Bose-Einstein condensates. Numerical examples are performed to show the effectiveness of this approach. Extensions to problems in multidimensions are straightforward, in which we can also split them into several subproblems, and perform similar procedures. These will be reported in detail in further work.

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