Numerical implementation of absorbing and injecting boundary conditions for the time-dependent Schrödinger equation

M. Cemal Yalabık and M. İhsan Ecemiş
Department of Physics, Bilkent University, 06533 Ankara, Turkey
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A method is described that enables the absorption and injection of wave functions at the boundaries of a region in a numerical solution to the time-dependent Schrödinger equation. A number of results corresponding to one- and two-dimensional simulations are presented. Such boundary conditions enable the use of time-dependent simulations of geometries connected to contacts that correspond to sources and sinks of particles in thermal equilibrium. The approach presented has a number of attractive features from a numerical-implementation point of view.

Numerical solution of the Schrödinger equation for the analysis of quantum transport properties of small geometries (where the effects of energy dissipation mechanisms may be neglected) is a powerful method that has been utilized extensively. If the analyzed system is "open," i.e., if it has contacts that may inject and absorb particles, then one has a number of approaches available for the solution of the wave equation. One method is to consider the time-independent Schrödinger equation, on which the implementation of the contact boundary conditions is well known (see, for example, Ref. 1). The particle may be assumed to be incident from a contact with a given wave vector, further assumed to be absorbed completely by any contact if incident on it. The transport properties of the geometry may then be determined from a superposition of the associated properties of these single particle solutions, weighed by the appropriate magnitudes of the injected waves dictated by the thermal properties of the contacts.[2] A disadvantage of this method is its inability to describe the time-dependent dynamics of the system.

One may also integrate the time-dependent Schrödinger equation with open boundaries numerically,[3–8] however, implementation of the contact boundary conditions is not straightforward.[9] Main difficulty is due to the influence of the wave function values well outside the boundary (that have left the simulation region at some earlier times) on the wave function within the boundary. This then suggests a non-Markovian process, and a boundary condition based on the values of the wave function at previous times may be constructed.[10,11] Simulations have been performed in which the problem of the boundary conditions may be bypassed completely by injecting wave packets of finite extent into a structure, and their time development have been analyzed until a large portion of the wave function reaches some extremal parts of the geometry.[12] The utility of this approach is limited to systems in which the time associated with this development is not prohibitive.

The Wigner function approach is an elegant method[10,13] in which absorbing and injecting boundary conditions can be applied naturally. However, the algorithm is not straightforward, and the method is feasible at present for application to one-dimensional systems, as it requires a $2d$ dimensional mesh for a d-dimensional system. The availability of absorbing and injecting boundary conditions puts the Schrödinger equation on a par with Wigner function approaches in the numerical study of time-dependent quantum phenomena, and it further has the advantage that it is feasible for application to problems with higher dimensionality.

The method to be described in this work is Markovian (in the sense that the boundary condition does not require any knowledge of the system at previous times), and is applicable to systems in which one can compute the time development of the wave function precisely at some region of space near the contacts. This may be accomplished, for example, by assuming a constant potential at this region. As in other Markovian boundary conditions, the method employs an extrapolation of the wave function outside the simulation region as an estimate of the wave that has already left the boundary at earlier times. An important difference between our method and the previous Markovian approaches is the construction of an estimate based on the values of the wave function in a relatively large region near the boundary. The time development of the wave function, therefore, is based on the progress of the function in this region, and does not require excessively small time steps for stability. The extrapolation further does not require a knowledge of the time derivative of the wave function near the boundary. An appealing point about the approach is the utilization of the efficient fast Fourier transform procedure in conjunction with open boundary conditions, which is normally used for perfectly reflecting or periodic boundaries. We next describe the method, present a number of examples of the application of the approach, and present the conclusions.

The principle idea of the method is to calculate the development of the wave function during a time step twice, once with reflecting or periodic boundary conditions throughout the full simulation space, second near the contact region, using an extrapolation of the wave function outside the contact region consistent with the absorption-injection condition. The full wave function is then updated using a mixture of the two time developments. A number of results corresponding to the application of this method to some simple systems is given.

The time-dependent Schrödinger equation may be dis-

cretized on a set of lattice points a distance Δx apart as

$$\imath(\partial\psi_l/\partial\tau) = [K + v(l,\tau)]\psi_l \ , \tag{1}$$

where ψ_l represents the time-dependent value of the wave function at the lth lattice point, v is the unitless potential function [scaled by the energy $\epsilon_0 = \hbar^2/2m(\Delta x)^2$, with $\hbar$ the Planck constant and m the particle mass], and τ is the unitless time variable (scaled by $\hbar/\epsilon_0$). K is the kinetic energy operator which may be defined through the relation,

$$K\psi_l = 2\psi_l - \psi_{l-1} - \psi_{l+1} \ , \tag{2}$$

for a one dimensional system, generalization for higher dimensions is straightforward.

If Ψ represents the vector of values of $\{\psi\}$, its time development can be formally expressed through the equation

$$\Psi(\tau + \Delta\tau) = \exp\left[-\imath\Delta\tau(K + v)\right]\ \Psi(\tau) \ . \tag{3}$$

The integration procedure used in this work[14] for the time development (i.e., "updating") of the wave function is to break up the exponential in Eq. (3) such that

$$\exp\left[-\imath\Delta\tau(K + v)\right]$$
$$\approx \exp(-\imath v\Delta\tau/2)\exp(-\imath\Delta\tau K)\exp(-\imath v\Delta\tau/2) \ , \tag{4}$$

which is correct to order $(\Delta\tau)^2$, and preserves the normalization and the time reversal symmetry of the wave function. This uncoupling permits the updating of the wave function in the momentum space for the kinetic energy term (where the kinetic energy operator is diagonal), and in the position space for the potential energy term. The availability of fast Fourier transform algorithms make the transformation and inverse transformation of the wave function at each time step feasible. The discrete Fourier transformation implies periodic boundary conditions, however, perfectly reflecting boundary conditions may also be implemented by antisymmetrizing the wave function (through a doubling of the periodicity length).

As mentioned above, in order to implement an absorbing boundary condition, we consider a number (say n) points near the boundary where the potential may be assumed to be constant. We then extrapolate the wave function to another n points *outside* the boundary consistent with absorption. This is in effect, an estimate of the wave function which has left the boundary at earlier times. Admittedly, this estimate cannot be unique. If one assumes that only outgoing waves exist in this boundary region, an estimate consistent with this assumption may be constructed. The wave function in this extended boundary region may be assumed to have only outgoing momentum components. The optimal choice of these momentum values depends upon the form of the wave function leaving the boundary.

In our work, we have chosen these momentum components such that the discrete Fourier transform of the wave function composed of these $2n$ points corresponds to no incoming (therefore only outgoing) momentum components. For example, if the n values of the wave function near the "left" (i.e., $-x$) boundary of the system are given by ϕ_l (with $1 \le l \le n$), the values of ϕ are extrapolated for values of l outside the boundary (with $-n+1 \le l \le 0$) such that for all l,

$$\phi_l = \frac{1}{\sqrt{2n}} \sum_{k=-n+1}^{0} c_k \exp\left(\imath\frac{2\pi}{2n}kl\right) \ . \tag{5}$$

Here, c_k are the $2n$ Fourier coefficients (with $-n+1 \le k \le n$), which are nonzero only for nonpositive values of k. These coefficients may be determined through the solution of the n simultaneous linear equations in Eq. (5) corresponding to the values of the n "known" values of ϕ at the boundary. However, it is also possible to note that Eq. (5) is a polynomial equation

$$\phi_l = \frac{1}{\sqrt{2n}} \sum_{k=0}^{n-1} c_{-k} {z_l}^k \ , \tag{6}$$

where $z_l = \exp(-\imath\pi l/n)$. Hence, the right hand side of Eq. (5) may be interpreted as a polynomial which is specified to take the values ϕ_l at the points z_l with $1 \le l \le n$. Since this polynomial is unique, it may be determined through the Lagrange formula,[15]

$$p[z] = \sum_{l=1}^{n} \phi_l \prod_{k\neq l} \frac{z - z_k}{z_l - z_k} \ . \tag{7}$$

The polynomial $p(z)$ then is the polynomial in Eq. (6) and may be used to obtain all $2n$ values of ϕ_l:

$$\phi_l = p\{\exp[-\imath(2\pi/2n)l]\} \ . \tag{8}$$

The difficulties associated with the numerical stability in the determination of coefficients in polynomials of a high degree are well known.[16] It will only be pointed out here that the evaluation of the extrapolated values through the Lagrange formula is to be preferred over a direct inversion of Eq. (5), and that the method has been applied to polynomials of order up to 16 with no difficulty, using single precision arithmetic.

As discussed earlier, the above choice of the momentum components to be specified is not unique. Our choice was mainly due to its simplicity, and guarantees a "numerically exact" representation of outgoing wave functions nominally of a single wavelength and commensurate with the extended boundary region. Hence, the accuracy of the method would be expected to increase if the size of this boundary region could be increased, as this would allow longer and longer wavelengths to be commensurate with this region. However, as it stands, the method enables the absorption of wavelengths much longer than the boundary region size, although its accuracy decreases for very long wavelengths. In applications where the dynamics of very long wavelengths dominate, one could modify the extrapolation procedure to include these wavelengths at the expense of others. On the other hand, for a numerically efficient implementation, the mesh length Δx should be chosen such that these large wavelengths are not generated, i.e., a smooth wave function should not be represented by a needlessly large number of points.

The boundary wave function composed of the $2n$ values may then be updated for the next time step (at the constant potential of the boundary), using periodic boundary conditions. Although this type of boundary condition would not be appropriate for points near $l \approx n$, it is quite accurate near the boundary ($l \approx 1$). The full wave function is also updated, using perfectly reflecting or periodic boundary conditions. Again, this type of update is obviously not appropriate near the boundary, but is ac-

curate sufficiently away from the boundary. Hence, the two types of updates are complimentary in regions where they are accurate, and for sufficiently small time steps, there is a wide transition region in which both solutions are accurate and coincide. It is then a matter of switching from one type of update to another in the boundary region in order to obtain the solution for an absorbing boundary condition.

The use of an extrapolation based on a relatively large region near the boundary allows the use of time steps which are not excessively small. We have used a time step of $\Delta\tau = 0.1$ in all of the examples that are presented in the next section. Larger values of this unitless increment could introduce intolerable errors in the break up of the exponential term of Eq. (4) anyway. (For an effective mass $m = 0.067m_e$ corresponding to an electron in GaAs, and a mesh spacing of 1 nm, $\Delta\tau = 0.1$ corresponds to a time step of approximately 0.1 fs.)

If the particle is being injected from the same boundary with a particular wave vector q, one then expects the wave function to have the form

$$\phi_l = A\,\exp(\imath q l) + \frac{1}{\sqrt{2n}} \sum_{k=-n+1}^{0} c_k \exp\left(\imath \frac{2\pi}{2n} k l\right) , \qquad (9)$$

where A is the coefficient of the incident wave. In this case, the updating procedure given above for the boundary region is applied to the set of values $\phi_l - A\,\exp(\imath q l)$ instead of ϕ_l, and the injected wave is updated separately [$A \to A\,\exp(-\imath E_q \Delta\tau)$, with E_q the scaled energy of the incident wave]. The sum of the two components then make up the complete update of the wave function in the boundary region. The full wave function is also updated using perfectly reflecting or periodic boundary conditions, and the two updates are combined as before.

In implementing these types of boundary conditions in more than one dimensions with rectangular geometry, one again needs to know the analytic form of the solutions near the boundaries. Depending on the type of problem, a constant potential, or more typically, a "channel" (perpendicular to the boundary) with finite potential walls may be used, for which analytic form of the solutions near the boundary may be constructed. The form of the solution near the absorbing boundary will then be of the

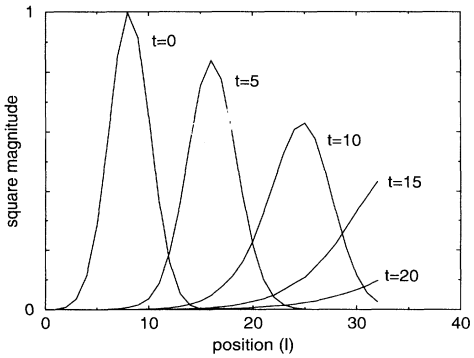

FIG. 1. Motion of a wave packet (corresponding to $\psi_l = \exp[(l-8)^2/16 + \imath 0.982 l]$ initially) under the effect of a perfectly reflecting boundary at the left, and a perfectly absorbing one at the right. The size n of the boundary region is 8. The broken lines connect the discrete values of ψ_l at the indicated values of the unitless time variable.

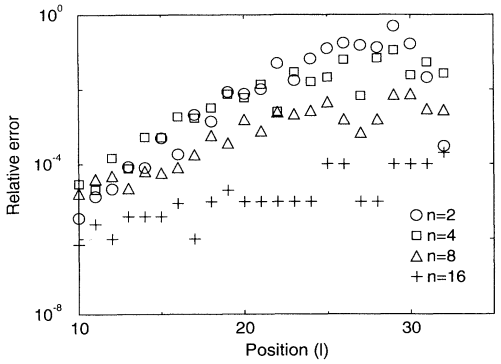

FIG. 2. The relative error in the wave function at $t = 15$ of Fig. 1, displayed for various values of the size n of the boundary region. The relative error is defined as $|\psi_l/\Psi_l - 1|$, where ψ_l and Ψ_l are the values of the wave function on a simulation mesh of sizes 32 and 128, respectively.

form

$$\phi(l_x, l_y, l_z) = A\,u(l_y, l_z)\exp(\imath q l_x) + \frac{1}{\sqrt{2n}} \sum_{k=-n+1}^{0} c_k(l_y, l_z) \exp\left(\imath \frac{2\pi}{2n} k l_x\right) \qquad (10)$$

with a particle injected with wave vector q in the $+x$

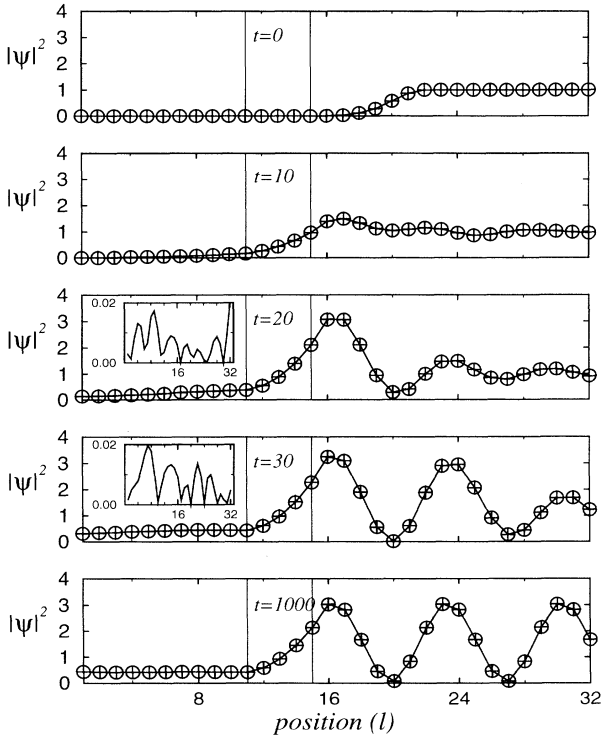

FIG. 3. The progress of a monochromatic wave with a Gaussian wave front injected into initially empty space containing a tunneling barrier, at various values of the unitless time variable. The wave has a scaled unitless energy value of $\epsilon = 0.198$, corresponding to a wavelength of 14 mesh spacings. The potential is zero except between the vertical lines where it has a scaled value of 0.2. The circles (connected by straight lines) correspond to the result of a simulation based on the method described in this work (with a boundary length of $n = 8$), the pluses correspond to the result of a computation on a mesh with 4096 points and with periodic boundary conditions. Two insets display the difference between the two magnitudes at an expanded scale.

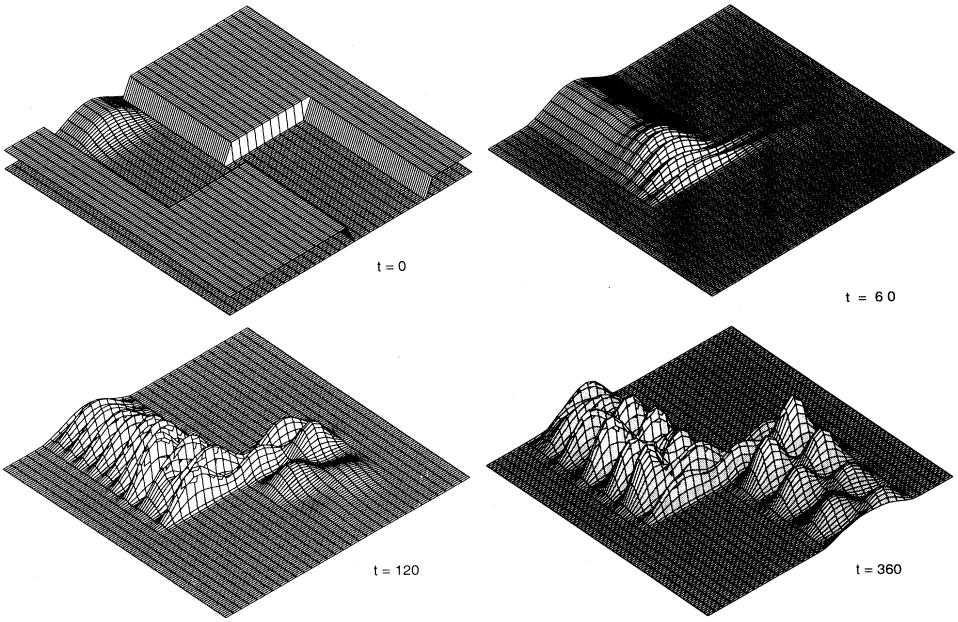

FIG. 4. The development of the wave function in an electron waveguide with a kink. The figure shows the square magnitude of the wave function on a 32×128 simulation mesh. The boundary region has a length of $n = 8$, and the wavelength of the injected wave is approximately 14 mesh units. The scaled value of time is indicated on the figure. The potential profile is superimposed on the wave function for $t = 0$. The oscillations in the outgoing channel are due to the interference between the components of the electron wave function in the first and the second subbands.

direction and in the eigenstate $u(l_y, l_z)$ near the boundary. The integers l_x, l_y, l_z label the position coordinates on the three-dimensional mesh, and the expansion coefficients $c_k(l_y, l_z)$ may be determined as before for fixed l_y and l_z.

Three applications of the boundary conditions are displayed in Figs. 1–4. (All computations have been carried out using single precision arithmetic.) Figure 1 displays the motion of an initially Gaussian wave packet with a momentum in the $+x$ direction, in the presence of a perfectly reflecting boundary at $l_x = 1$, and a perfectly absorbing boundary at $l_x = 33$. The accuracy of the wave packet leaving the boundary at the scaled time value of 15 has been checked against a simulation of the same wave packet on a mesh which extends to 128 points. At this value of the scaled time, one expects no errors on this larger mesh due to the boundary condition, as the wave packet is a safe distance away from the boundary. The "error" in the wave packet on the smaller mesh in comparison to that on the larger mesh is displayed in Fig. 2. As apparent in this figure, there is a dramatic improvement in the approximation as the size n of the boundary region is increased, in fact at the scale of Fig. 1, the wave function generated with $n = 8$ and 16 are indistinguishable from the one generated on the larger mesh. A boundary size corresponding to $n = 8$ seems to be optimal for a large class of problems in terms of accuracy-computational resource tradeoff.

Figure 3 shows the progress of a wave injected into an initially empty space containing a tunneling barrier. A Gaussian wave front has been imposed on the wave. The results of the simulation implementing the method described above have been compared with the results of a simulation carried out on a periodic mesh of size 4096. Again, this large mesh avoids the problems associated with boundary conditions for the values of the time variable indicated in the figure. The difference between the results of the two simulations is not visible in the scale of the figure, two insets are provided to display this difference at an expanded scale.

The method has been tested for a large class of problems corresponding to various potential functions and initial conditions. It was found to be robust in these applications.

The boundary condition described in this work has also been applied to two-dimensional systems in which the wave function is incident (and absorbed) through channel like potentials. By carrying out an ensemble of single particle simulations (each corresponding to a different incident wave) in parallel, it is possible to study quantum transport through two-dimensional structures in the presence of time-dependent boundary conditions. Figure 4 displays the progress of the wave function through a kink (or "double-bend") shaped channel at different times. This structure is expected to have interesting nonlinear transport properties.[17] The results of this study will be reported elsewhere.

An implementation of absorbing and injecting boundary conditions for numerical simulations of the time-dependent Schrödinger equation has been described. The method is Markovian and is stable under a large range of conditions. The basic idea is probably applicable to other types of wave equations (such as the Maxwell Equations) although we have not tested this.

An important practical point is the application of the fast Fourier transform to the solution of the wave equation for systems with open boundaries, which results in improved numerical efficiency. There may be possibilities for improvement in the method, for example through a different choice of momentum components that are specified in the extrapolation procedure, or indeed possibly through the adaptation of a totally different extrapolation procedure. The removal of the sharp cutoffs in space and momentum are areas of possible improvement.

The method described above is presently being used in a more demanding study of a two-dimensional system in the presence of a self consistent potential. This work will be reported separately.

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