Abstract

We consider the two-dimensional, time-dependent Schrödinger equation discretized with the Crank-Nicolson finite difference scheme. For this difference equation we derive discrete transparent boundary conditions (DTBCs) in order to get highly accurate solutions for open boundary problems. We apply inhomogeneous DTBCs to the transient simulation of quantum waveguides with a prescribed electron inflow.

Key words: Quantum waveguide, Schrödinger equation, transparent boundary condition, finite difference scheme

1 Introduction

Quantum waveguides are novel electronic switches of nanoscale dimensions. They are made of several different semiconductor materials such that the electron flow is confined to small channels or waveguides. Due to their sandwiched structure the relevant geometry for the electron current is roughly two dimensional. Using external electrostatic potentials the “allowed region” for the electrons, and hence the geometry can be modified. This allows to control the current flow through such an electronic device. It makes it a switch, which resembles a transistor, but on a nanoscale.
Being quantum particles, the electron transport through a quantum waveguide can be modeled in good approximation by a two dimensional, time dependent Schrödinger equation

\[
\begin{align*}
\frac{i\hbar}{\partial t} \psi(x, t) &= \left( -\frac{\hbar^2}{2m^*} \Delta_x + V(x, t) \right) \psi(x, t), \quad x = (x, y) \in \Omega(t), \ t > 0, \\
\psi(x, 0) &= \psi^I(x), \quad x \in \Omega(0), \\
\psi(x, t) &= 0, \quad x \in \partial\Omega(t)
\end{align*}
\]

on a time-dependent geometry $\Omega(t) \subset \mathbb{R}^2$ with $\psi^I \in L^2(\Omega(0))$ and homogeneous Dirichlet boundary conditions. $h$ and $m^*$ denote the Planck constant and effective mass, respectively. The external potential satisfies $V(., t) \in L^\infty(\Omega(t))$ and $V(x, .)$ is piecewise continuous. The spatial domain consists of (very long) leads and the active switching region, which sometimes has the shape of a stub. Here, we shall only consider domains $\Omega(t)$ that are piecewise constant in $t$ and monotonously growing in time. At the jump discontinuites of the domain we shall extent the solution $\psi$ by zero, as a new initialization.

In typical applications, electrons are continuously fed into the leads. Depending on the size and shape of the stub, the electron current is either reflected (off-state of the device) or it can flow through the device (on-state). Since the applied external potential can modify the stub size, it hence allows to switch the device. Important device data for practitioners are the ratio between the on- and the (residual) off-current as well as the switching time between these two stationary states. These data can be obtained from numerical simulations of the described Schrödinger equation model. The leads are very long compared to the typical size of the active region and they usually only carry (linear combinations of) plane wave solutions. For the efficiency of numerical simulations it is therefore desirable to restrict the simulation model to a small region close to the stub (see Fig. 1). Hence, the leads should to be cut off by using artificial boundary conditions. This is possible without changing the solution of the Schrödinger equation by introducing transparent boundary conditions (TBCs), which are non-local in time (convolution type) and in space.

To illustrate the idea we first consider the one dimensional, time dependent Schrödinger equation (1) with a potential that satisfies $V(x, t) = V_l$ for $x \leq x_l$ and $V(x, t) = V_r$ for $x \geq x_r$ and all $t \geq 0$. The analytic TBC for this equation reads

\[
\psi_x(x_r, t) = -\sqrt{\frac{\hbar}{2\pi m^*}} e^{-i\frac{\hbar}{2m^*} x_r^2} \int_0^t \frac{\psi(x_r, \tau) e^{i\frac{V_r}{\hbar} \tau}}{\sqrt{\tau - t}} d\tau, \quad t > 0,
\]

for the right boundary $x = x_r$ (and analogously for the left boundary) and was first derived in (Pa82), (BaPo91). The numerical discretization of these
artificial boundary conditions is delicate, as it may easily render the initial-boundary value problem unstable. Discrete transparent boundary conditions (DTBCs) for a Crank-Nicolson finite difference discretization of the Schrödinger equation were first given in (Ar98) and (EhAr01) (cf. also (AABES07) for a recent review of the various alternative approaches).

For the 2D-geometry of quantum waveguides, TBCs were rigorously derived in (BeMePi05). A discrete analogue along with a fast evaluation algorithm was given in (ArEhSo03). The topic of this note is to discuss the algorithmic issues of implementing these DTBCs for the 2D-Schrödinger equation (§3.1) and to use them for simulating a quantum waveguide with a resonating stub (§3.2). For a more detailed version including the derivation and analysis of DTBCs for the fourth order “Numerov-scheme” for the 2D-Schrödinger equation we refer to (ScAr07).

2 Finite difference scheme and discrete transparent boundary condition for the 2D-Schrödinger equation

In this section we shall briefly review the derivation of DTBCs for the 2D-Schrödinger equation on a rectangular geometry in conjunction with a finite difference discretization. In this paper we are ultimately interested in solving the Schrödinger equation on a geometry like in Fig. 1 with both leads being rectangular and infinitely long. When discussing TBCs we only need to consider the geometry of the exterior domain, i.e. the domain to be eliminated by the TBC. The interior domain shall be kept in the simulation and can have an irregular geometry (e.g. T-shaped in Fig. 1). For a more realistic model one should actually solve the nonlinear Schrödinger-Poisson equation in the interior domain (cf. (BeMePi05; Sc07)), but this still does not effect the shape of the TBCs.

Here, we choose \( \Omega = \mathbb{R} \times [0, Y] \subset \mathbb{R}^2 \) as the domain of interest. Let \( \psi_{j,k}^n \) be the numerical approximation of the solution \( \psi(x_j, y_k, t_n) \) to the Schrödinger equation (1) on the equidistant grid \( \Omega_{\Delta x, \Delta y} \) with the nodes \( x_j = j \Delta x, \ j \in \mathbb{Z}; \ y_k = k \Delta y, \ 0 \leq k \leq K \) and the time discretization \( t_n = n \Delta t, \ n \in \mathbb{N}_0 \). DTBCs shall be employed at \( x_0 = 0 \) and \( x_J = J \Delta x = X \), hence the computational domain is chosen as the rectangle \([0, X] \times [0, Y]\). At \( y_0 = 0 \) and \( y_K = K \Delta y = Y \) we use zero Dirichlet boundary conditions.

Following (ArEhSo03) we shall now briefly review the derivation of DTBCs for the 2D-Schrödinger equation. Using the 5-point finite difference scheme in space and the Crank-Nicolson scheme in time, the discrete Schrödinger equation on \( \Omega_{\Delta x, \Delta y} \) reads
\[ i\hbar D_t^n \psi_{j,k}^n = -\frac{\hbar^2}{2m^*} \left( D_x^2 \psi_{j,k}^{n+\frac{1}{2}} + D_y^2 \psi_{j,k}^{n+\frac{1}{2}} \right) + V_{j,k}^{n+\frac{1}{2}} \psi_{j,k}^{n+\frac{1}{2}}. \]  

(3)

Here,

\begin{align*}
D_t^n \psi_{j,k}^n &= \frac{\psi_{j,k}^{n+1} - \psi_{j,k}^n}{\Delta t}, \\
D_x^n \psi_{j,k}^n &= \frac{\psi_{j-1,k}^n - 2\psi_{j,k}^n + \psi_{j+1,k}^n}{\Delta x^2}, \\
D_y^n \psi_{j,k}^n &= \frac{\psi_{j,k-1}^n - 2\psi_{j,k}^n + \psi_{j,k+1}^n}{\Delta y^2}
\end{align*}

denote the standard finite difference operators, \( V_{j,k}^{n+\frac{1}{2}} := V\left(x_j, t_{n+\frac{1}{2}}\right) \), and \( \psi_{j,k}^{n+\frac{1}{2}} := \frac{1}{2} \left( \psi_{j,k}^{n+1} + \psi_{j,k}^n \right) \) a time averaging.

**Remark 1** The discretization scheme (3) is of second order both in time and space. Since the discrete \( \ell^2 \)-norm is preserved under the evolution, i.e.

\[ D_t^n ||\psi||_2^2 := \Delta x \Delta y D_t^n \sum_{j \in \mathbb{Z}, 0 \leq k \leq K} |\psi_{j,k}^n|^2 = 0 \text{ for all } n \geq 0 \text{ (cf. (ArEhSo03))}, \]

the scheme is unconditionally stable.

Like in the analytical case we assume that the potential is constant outside of the computational domain: \( V_{j,k}^n = V_0 \) for \( j \leq 1 \) and \( V_{j,k}^n = V_J \) for \( j \geq J - 1 \), and for all \( 0 \leq k \leq K \) and \( n \geq 0 \). This implies that the transversal solution modes (i.e. orthogonal to the channel axis) are decoupled in the exterior domain.

Hence, we shall now Fourier transform equation (3) with respect to the discrete sine-functions

\[ \hat{\psi}_{j,m}^n := \frac{1}{K} \sum_{k=1}^{K-1} \psi_{j,k}^n \sin \left( \frac{\pi km}{K} \right), \quad m = 1, \ldots, K - 1, \]
\[ \hat{\psi}_{j,0}^n = \hat{\psi}_{j,K}^n = 0, \quad 0 \leq j \leq J, \quad n \geq 0. \]

It can be easily shown that

\[ -\frac{1}{2\Delta y^2} \left( \hat{\psi}_{j,k-1}^n - 2\hat{\psi}_{j,k}^n + \hat{\psi}_{j,k+1}^n \right)_m = \frac{1}{\Delta y^2} \left( 1 - \cos \left( \frac{\pi m}{K} \right) \right) \hat{\psi}_{j,m}^n \]

for \( 1 \leq k, m \leq K - 1, \quad j \in \mathbb{Z} \setminus [1, J - 1] \). Since the potential \( V_{j,k}^n \) is constant in the exterior domain, the solution modes \( \hat{\psi}_{j,m}^n \) are independent of each other and we obtain \( K - 1 \) one dimensional discrete Schrödinger equations:

\[ \frac{i\hbar}{\Delta t} (\hat{\psi}_{j,m}^{n+1} - \hat{\psi}_{j,m}^n) = -\frac{\hbar^2}{2m^*\Delta x^2} \left( \hat{\psi}_{j+1,m}^{n+\frac{1}{2}} - 2\hat{\psi}_{j,m}^{n+\frac{1}{2}} + \hat{\psi}_{j-1,m}^{n+\frac{1}{2}} \right) + \tilde{V}_{j,m} \hat{\psi}_{j,m}^{n+\frac{1}{2}}, \]  

(4)
with the modified potential
\[
\tilde{V}_{j,m} := V_j + \frac{\hbar^2}{m^*} \left( 1 - \cos \left( \frac{\pi m}{K} \right) \right), \quad j \in \mathbb{Z} \setminus [1, J - 1], \ m = 1, \ldots, K - 1.
\]

Next we assume that the discrete initial function \( \psi_{j,k}^0 \) is compactly supported in the grid \([1, J - 1] \times [1, K - 1]\). Performing the discrete \( \mathcal{Z} \)-transformation,
\[
\mathcal{Z} \{ \psi^n \} = \Psi(z) := \sum_{n=0}^{\infty} \psi^n z^{-n}, \quad z \in \mathbb{C}, \ |z| > 1,
\]
of (4) on the exterior domain, we derive \( K - 1 \) second order difference equations:
\[
\Psi_{j+1,m}(z) + \left( iR \frac{z - 1}{z + 1} - 2 - w\tilde{V}_{j,m} \right) \Psi_{j,m}(z) + \Psi_{j-1,m}(z) = 0,
\]
j \leq 0 or \ j \geq J,

with \( R = -\frac{4\Delta x^2 m^*}{\hbar} \) and \( w = \frac{2\Delta x^2 m^*}{\hbar} \). For each fixed \( m \), equation (5) has two fundamental solutions of exponential form \( \Psi_{j,m}(z) = \alpha_m(z)^j \). Both for physical reasons and since the discrete solution stays in \( \ell^2(\mathbb{Z} \times [1, K - 1]) \), each mode \( \Psi_{j,m}(z) \) has to decay for \( |j| \to \infty \). This requirement selects a unique root \( \alpha_m(z) \) (with \( |\alpha_m(z)| > 1 \) for \( j \leq 0 \), e.g.) and the \( \mathcal{Z} \)-transformed DTBCs hence read
\[
\Psi_1(z) = \alpha_0(z) \Psi_0(z), \quad \Psi_{J-1}(z) = \alpha_J(z) \Psi_J(z).
\]

**Theorem 2 (DTBCs for the 2D-Schrödinger equation)** Consider the two dimensional, time dependent Schrödinger equation, discretized with the 5-point difference scheme in space and the Crank-Nicolson scheme in time. Then, the sine-transformed DTBCs at \( x_0 = 0 \) and \( x_J = J\Delta x \) read respectively
\[
\hat{\psi}^n_{1,m} - s^{(0)}_{0,m} \hat{\psi}^n_{0,m} = \sum_{\nu=1}^{n-1} s^{(n-\nu)}_{0,m} \hat{\psi}^{n-\nu}_{0,m} - \hat{\psi}^{n-1}_{1,m}, \quad n \geq 1,
\]
\[
\hat{\psi}^n_{J-1,m} - s^{(0)}_{J,m} \hat{\psi}^n_{J,m} = \sum_{\nu=1}^{n-1} s^{(n-\nu)}_{J,m} \hat{\psi}^{n-\nu}_{J,m} - \hat{\psi}^{n-1}_{J-1,m}, \quad n \geq 1,
\]
where the convolution coefficients \( s^{(n)}_{j,m} \) are given by (cf. (ArEhSo03)):
\[
s^{(n)}_{j,m} = \left[ 1 - i\rho \frac{\sigma_j m}{2} \right] \delta_{n,0} + \left[ 1 + i\rho \frac{\sigma_j m}{2} \right] \delta_{n,1}
\]

\[5\]
\begin{align*}
\xi_{j,m} &= \sqrt{(\rho^2 + \sigma_{j,m}^2)(\rho^2 + (\sigma_{j,m} + 4)^2)}, \quad \mu_{j,m} = \frac{\rho^2 + 4\sigma_{j,m} + \sigma_{j,m}^2}{\xi_{j,m}}, \\
\varphi_{j,m} &= \text{arctan} \frac{2\rho(\sigma_{j,m} + 2)}{\rho^3 - 4\sigma_{j,m} - \sigma_{j,m}^2}, \quad \alpha_{j,m} = \frac{i}{2} \sqrt{\xi_{j,m} e^{i\varphi_{j,m}/2}}
\end{align*}

for \( j = 0, J, m = 1, \ldots, K - 1 \). \( P_n \) denotes the Legendre polynomials \( (P_{-1} \equiv P_{-2} \equiv 0) \) and \( \delta_{n,\nu} \) is the Kronecker symbol.

**Remark 3** The decay rate of the convolution coefficients coincides with the decay \( O(t^{-3/2}) \) of the convolution kernel in the analytical TBC (2).

**Remark 4** The discrete Schrödinger equation (3) and the DTBCs (7), (8) are solved iteratively in time. The convolution length in (7), (8) therefore grows with every time step. This makes it impossible to simplify (or accelerate) the numerical evaluation of these time convolution by using a fast Fourier transform (FFT). Hence, the evaluation of the convolution sum up to time level \( n \) requires a memory of the order \( O(Kn) \) and numerical costs of the order \( O(Kn^2) \). The latter can easily surpass the costs of solving the PDE in the interior domain which only grows linearly in \( n \). As a remedy it is possible to approximate the convolution coefficients by a sum of exponentials (say \( L \) terms) and to calculate the convolution sum recursively. This way, the numerical costs may be reduced to \( O(KLn) \) and the memory to \( O(KL) \) with \( L \ll n \), while still keeping high accuracy (cf. (ArEcSo03)).

**Remark 5** In (7), (8) the DTBCs are formulated in sine-transformed space. Hence, these DTBCs are also non-local in space – more precisely in the tangential manifold of the artificial boundary. Due to the sine-modes in \( y \)-direction, this non-locality can easily be dealt with using FFT (cf. §3.1).

If the exterior potential is not constant in the transversal direction (of the channel), the solution can still be expanded in the eigenfunctions of the transversal Schrödinger operator (cf. (BeMePi05)). But then FFTs cannot be used for the evaluation of the DTBCs (cf. §3 of (Sc07)).

**Remark 6** The numerical costs of implementing the DTBCs (7), (8) agree with the costs for “ad-hoc” discretizations of the analytical TBC (2) (or its 2D-analogue) that were proposed in the literature. But (7), (8) have the advantage not to introduce any numerical reflections or to destroy the unconditional stability of the underlying PDE scheme.

**Remark 7** The Crank-Nicolson finite difference scheme (3) is of the order \( O(\Delta x^2 + \Delta y^2 + \Delta t^2) \). With a higher order scheme (compact finite differences) one can again derive modified DTBCs and obtain an order of convergence of \( O(\Delta x^4 + \Delta y^4 + \Delta t^2) \) (cf. (ScAr07)).
3 Numerical results

In this section we discuss the practical implementation of DTBCs and present some numerical results when using them for simulating quantum waveguides.

3.1 Implementation of the DTBC

In (7), (8) the DTBCs are written in sine-transformed space. A direct implementation in position space would necessitate tremendous numerical costs, hence they are implemented in $y$-Fourier space. The discrete convolution

$$C_{J,m}^{(n-1)} := \sum_{\nu=1}^{n-1} s_{J,m}^{(n-\nu)} \hat{\psi}_{J,m}^{\nu}, \quad m = 1, \ldots, K - 1$$

(9)

for the right boundary $x_J = J \Delta x$ is calculated in Fourier space and inverse transformed by

$$C_{J,k}^{(n-1)} = 2 \sum_{m=1}^{K-1} \sin \left( \frac{\pi mk}{K} \right) \left( \sum_{\nu=1}^{n-1} s_{J,m}^{(n-\nu)} \hat{\psi}_{J,m}^{\nu} \right), \quad k = 1, \ldots, K - 1.$$

Since the convolution (9) only involves the solution at the boundary at past time levels (i.e. for $\nu \leq n - 1$), one can directly store the sine-transformed boundary data $\hat{\psi}_{J,m}^{\nu}$. Moreover, this part of the DTBC only enters the inhomogeneity of the linear system to be solved at each time level.

The part $s_{J,m}^{(0)} \hat{\psi}_{J,m}^{n}$ of the left hand side of the DTBC (8) has to be inverse transformed to physical space and we get the couplings

$$\left( s_{J,m}^{(0)} \hat{\psi}_{J,m}^{n} \right)^{\lor}_{J,k,l} = 2 \sum_{m=1}^{K-1} \sin \left( \frac{\pi mk}{K} \right) s_{J,m}^{(0)} \hat{\psi}_{J,m}^{n},$$

$$= \frac{2}{K} \sum_{m=1}^{K-1} \sum_{l=1}^{K-1} s_{J,m}^{(0)} \sin \left( \frac{\pi mk}{K} \right) \sin \left( \frac{\pi kl}{K} \right) \psi_{J,l}^{n}$$

for $k, l = 1, \ldots, K - 1$. Hence, the 5-diagonal system of the discrete 2D-Schrödinger equation (3) obtains additional entries due to the DTBC.

In order to model the electron influx from the left lead, we shall prescribe an incoming plane wave $\varphi(x, y, t)$ at the left boundary. Hence, inhomogeneous DTBCs have to be used at $x_0 = 0$:

$$\hat{\psi}_{1,m}^{n} - \hat{\varphi}_{1,m}^{n} - s_{0,m}^{(0)} \left( \psi_{0,m}^{n} - \varphi_{0,m}^{n} \right)$$
3.2 Simulation of quantum waveguides

Following the simulation of a GaAs-waveguide in (Bu97), we choose the T-shaped geometry shown in Fig. 1 to simulate a quantum waveguide transistor. In x-direction the channel has a length of $X = 60\,\text{nm}$; the channel width $Y$ and the stub width $w$ are $20\,\text{nm}$. In order to control the current through the channel, the stub length can be changed from $L_1 = 32\,\text{nm}$ to $L_2 = 40.5\,\text{nm}$. A homogeneous DTBC is implemented at $x = X$, and an inhomogeneous DTBC at $x = 0$. All other boundaries are considered as hard walls, i.e. we use homogeneous Dirichlet boundary conditions for $\psi$. A (discrete) time harmonic incoming wave function

$$
\varphi_{j,k}^n = \sin \left( \frac{\pi k}{K} \right) e^{ikx_j \Delta x} e^{-it \frac{E_{j,k} \Delta t}{\hbar}}, \quad k = 0, \ldots, K
$$

is modeling the mono-energetic constant incoming current at $x = 0$. Here, $\varphi$ includes only the lowest transversal mode. But any linear combination of higher modes would work equally well, which is a great advantage compared to other artificial boundary conditions (e.g. (Bu97)). In our example the energy $E$ of the incoming wave equals $29.9\,\text{meV}$ and the effective electron mass has
the value $m^* = 0.067m_0$, which corresponds to GaAs. The value of $k_x$ can be derived from the discrete dispersion relation

$$E = \frac{\hbar^2}{m^*} \left( 1 - \cos \left( \frac{\Delta x k_x}{\Delta x^2} \right) \right) + \frac{\hbar^2}{m^*} \left( 1 - \cos \left( \frac{\pi \Delta y}{K} \right) \right)$$

of the Schrödinger equation with $V_0 = 0$ for an incoming wave (11).

For the subsequent simulation we solve the Schrödinger equation (1) by the difference equation (3) without external potential, i.e. $V = 0$. For realistic simulations of MOSFET-channels, (1) should be coupled to the self-consistent Coulomb potential inside the channel. Since we focus on DTBCs, we shall not include this here. But a coupling to the Poisson equation inside the computational domain does not change the derivation or discretization of our open BC. Since we are mostly interested in the switching and the large time behavior of this waveguide, we choose the following (somewhat arbitrary) initial function

$$\psi^I(x, y) = \begin{cases} 
\sin \left( \frac{\pi}{Y} \right) e^{ik_x x} & : 0 \leq x < x_1 \\
\frac{1}{2} \sin \left( \frac{\pi}{Y} \right) e^{ik_x x} \left[ 1 + \cos \left( \frac{\pi}{x_2 - x_1} (x - x_1) \right) \right] & : x_1 \leq x < x_2 \\
0 & : x \geq x_2
\end{cases}$$

with $x_1 = 25\text{nm}$ and $x_2 = 38\text{nm}$, which is consistent with the incoming wave.

Fig. 2 shows the temporal evolution of the solution $|\psi(x, y, t)|$. In this simulation the stub length is first fixed to $L_1 = 32\text{nm}$. After 1.68ps the solution reaches (essentially) a steady state (off-state of the waveguide). Phenomenologically speaking, in this case only $1\frac{1}{2}$ wave packets “fit” into the stub (cf. Fig. 2(c)). Hence, they block the current flow through the waveguide. Then, at $t = 1.68\text{ps}$ the stub is enlarged at once to $L_2 = 40.5\text{nm}$. After some transient phase, the solution converges to a new steady state (on-state of the waveguide, cf. Fig. 2(f)). Here, two wave packets “fit” into the stub, and the current can flow almost unblocked through the device. At $t = 3.60\text{ps}$ the current is already almost constant in $x$ and at its maximum level.
Fig. 2. Absolute value of the solution $\psi(x, y, t)$ to the time-dependent Schrödinger equation on the T-shaped structure of Fig. 1. The discretization parameters are chosen as $\Delta x = \Delta y = 0.5 \text{nm}$, $\Delta t = 0.0002 \text{ps}$, $V = 0 \text{meV}$, $m^* = 0.067m_0$, $E = 29.9 \text{meV}$.

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References


