Simulation of coherent quantum transport in a magnetic field: recovery of conductance quantization

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Abstract

We extend the Quantum Transmitting Boundary Method (QTBM), a numerical algorithm for solving the two-dimensional Schrödinger equation for scattering states, to include an applied magnetic field to 2D systems. We apply this technique to simulate the magneto-transport of a periodically corrugated electron channel. The conductance quantization of such structure is recovered when the channel is long. The index of this quantization is a non-monotonic function of energy.

I. Introduction

For structures of ultra-submicron dimension, electron transport is in the quantum regime. The shapes of these devices and the potential landscapes can be flexibly tailored, for example, by electro-static gating on top of the 2DEGs. Understanding the details of transport in these structures inevitably involves numerical solutions of the 2D Schrödinger equation.

Figure 1 schematically shows the type of structures we consider: the region of interest can be partitioned into several input and output lead regions ($\Omega_i, \Omega_j,...$) and a "device region" (Ω_0), where scattering states are to be solved. A perpendicular magnetic field is present. For device modeling, a mode matching approach is widely adopted [1,2]. The problem with this method is that, though useful for the most simple structures, it is difficult to apply for arbitrary potential profiles. A general numerical algorithm, the Quantum Transmitting Bound-

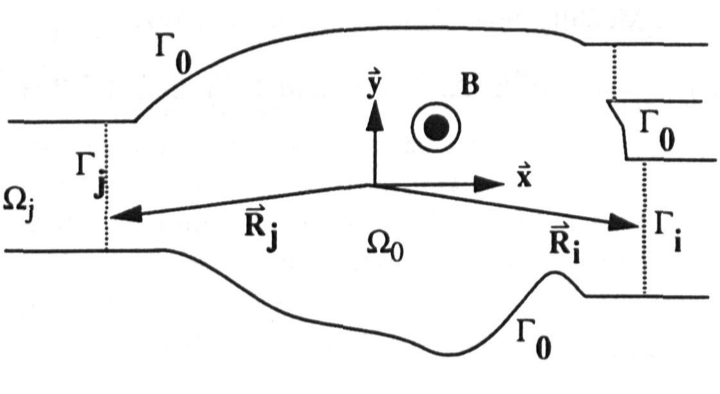

FIGURE 1. The problem geometry. Γ_i is the boundary between the device region Ω_0 and lead i. Γ_0 denotes all the other boundaries, where the wavefunctions vanish. The applied magnetic field B is perpendicular to the 2D system.

ary Method (QTBM) developed by Lent and Kirkner [3], allows more complicated potential profile and can cope with complicated devices. It has proven to be an efficient technique in device modeling in [4].

II. Model And Method

We extend the QTBM to include the effects of applied magnetic fields. With the choice of the vector potential in Landau gauge, $\vec{A} = -By\hat{x}$, the single-band 2D effective-mass Schrödinger equation becomes,

$$\left\{\frac{-\hbar^2}{2m^*}\nabla^2 + \frac{ie\hbar By}{m^*} + \frac{e^2B^2y^2}{2m^*} + V_0(x,y)\right\}\Psi(x,y) = E\Psi(x,y). \tag{1}$$

In the QTBM algorithm, we expand the scattering state in a lead region as a superposition of the local transverse modes, including both traveling and evanescent ones. The modes in the lead regions are obtained by solving (Eq. 1) as a quadratic eigenvalue problem for k at given energy E, using the form $\Psi(x,y) = e^{ikx}\chi(y)$. Part of the difficulty of the problem at non-zero field is that the transverse mode eigenfunction, the $\chi(y)$'s, are not orthogonal, in contrast to the zero field case. Except for the incident modes, the complex amplitude of each mode is an unknown for which we must solve. In the Finite Element Method scheme, we are able to properly implement the boundary conditions and obtain the numerical solutions of full wavefunctions in the whole device by the solution of a single linear problem. We calculate other interested physical quantities of transport, for instance, current density distribution and transmission coefficients directly from the wavefunction. The extended QTBM technique gives us the capability of solving the magneto-transport problem for arbitrarily shaped devices with arbitrary potentials, as that of Figure 1.

III. Application and Results

As an important example, we present the results of this technique applied to a corrugated quantum channel (Figure 2) which illustrates the recovery of conductance quantization for long periodically modulated channels. The conducting width is periodically modulated be-

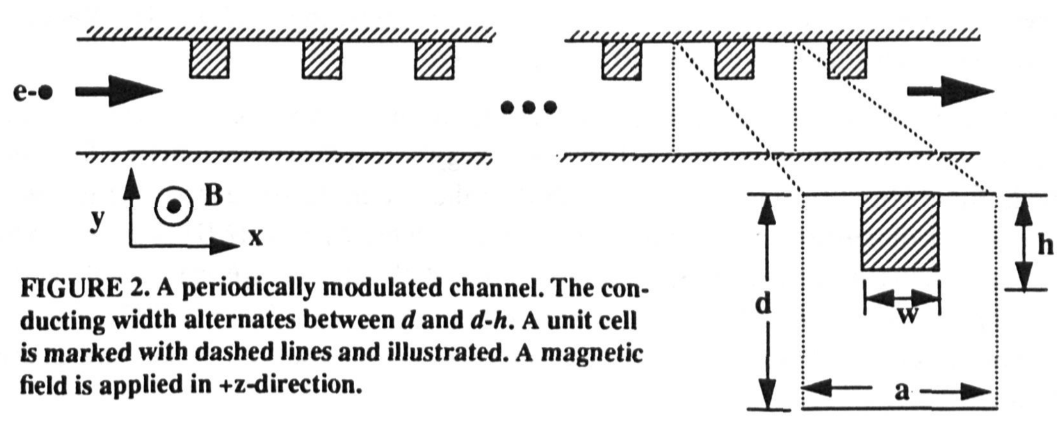

FIGURE 2. A periodically modulated channel. The conducting width alternates between *d* and *d-h*. A unit cell is marked with dashed lines and illustrated. A magnetic field is applied in +z-direction.

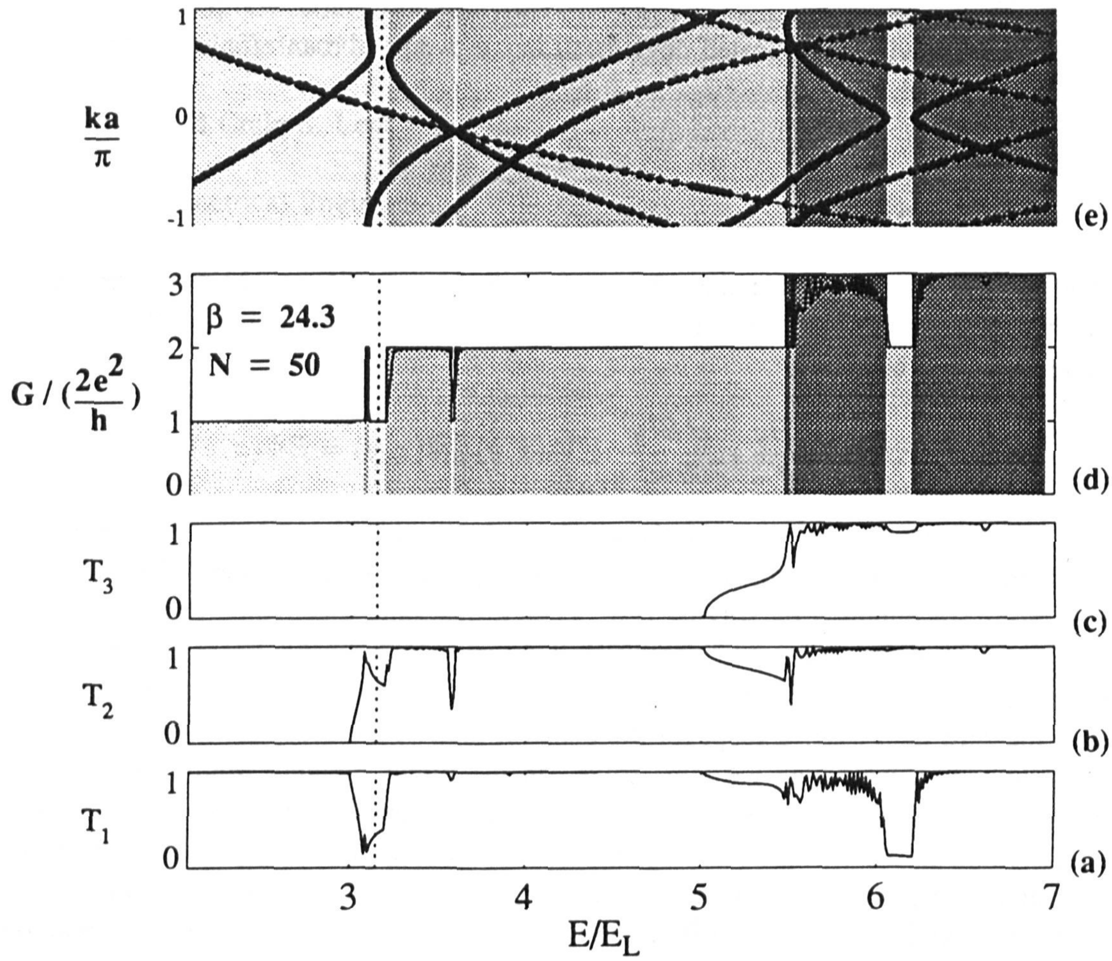

FIGURE 3. Numerical results for the structure in Figure 2 at *d/a=2.0, h/a=0.6, w/a=0.4* and β=*24.3*. (a) Transmission coefficient for a channel of *N=50* unit cells. The incident wave is in the *first* traveling mode; (b) the incident is in the *second* mode; (c) the incident is in the *third* mode. (d) The Landauer Conductance, showing the quantization in a non-monotonic way as the function of energy. (e) The bandstructure of an infinite modulated channel. The *index* of the conductance plateau in (d) has an one-to-one correspondence to the *number* of positive-velocity states at a given energy in the band diagram.

tween d and d-h with a periodicity of a and N periods. The full solution of wavefunctions and scattering matrix is obtained for one unit cell (one corrugation) and the scattering matrix for the structure of N unit cells (periods) is calculated using a cascading method. The Landauer two-terminal conductance is then calculated straightforwardly.

Plotted in Figure 3 are the numerical results of transmission and conductance as a function of energy at a modestly high magnetic field. The energy is expressed in units of first bulk Landau level, $E_L = (\hbar\omega_c)/2$, where $\omega_c = (eB)/m^*$ is the cyclotron frequency; the magnetic field is expressed in dimensionless form by $\beta = (da)/l_H^2$, where $l_H^2 = \hbar/(eB)$ is the magnetic length. For the results presented here, the dimensions of the device are set as $d/a = 2.0$, $h/a = 0.6$, $w/a = 0.4$. The effective mass is chosen to be $m*/m = 0.067$, which is appropriate for GaAs. Hard wall potentials outside the channel and zero inside are chosen for simplicity.

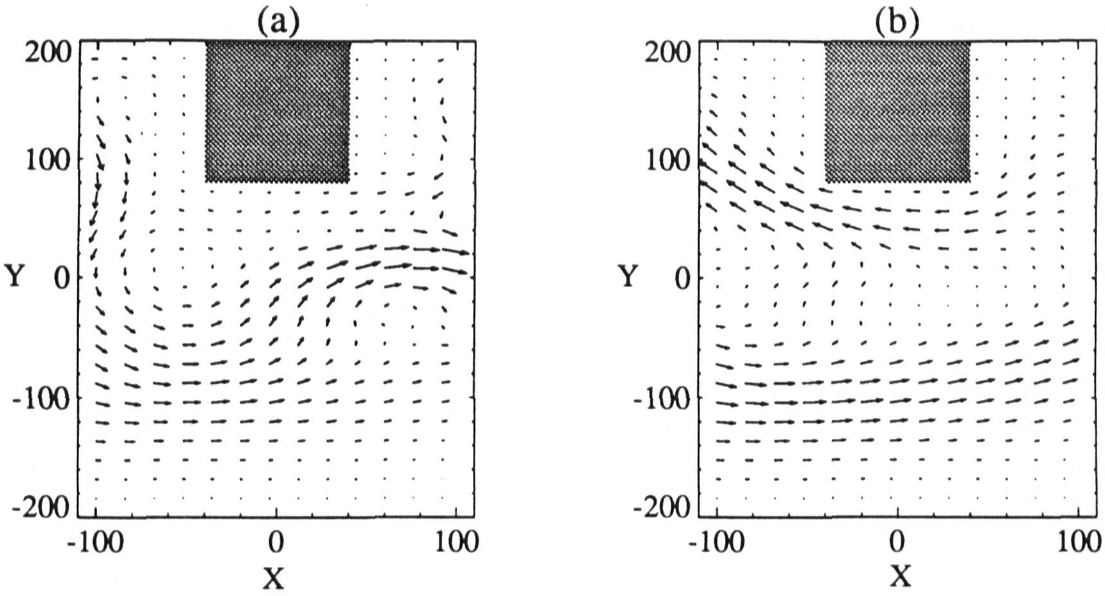

FIGURE 4. Particle current density distribution of the scattering states in the device region of a single unit-cell channel at E/E_L=3.15. Highlighted is the potential barrier "finger" which causes the mixing of edge channels in the device. (a) The input is in the first transverse mode; (b) the input is in the second transverse mode.

Drawn in Figure 3(a), (b) and (c) are the mode transmission coefficients, T_1, T_2, T_3, when the input is in the first, second, and third transverse mode respectively. The channel has *50* periods of modulation. We see a complicated pattern of mode transmission as a function of energy and none of the single mode transmission coefficients is quantized.

In Figure 3(d) we plot the two-terminal Landauer conductance, $G = \frac{2e^2}{h}\sum_i T_i$. It shows that for the long channel of 50 periods, although none of the individual mode transmissions shows the quantization, the total conductance as function of energy is essentially quantized. The height of the plateaus is a non-monotonic function of energy.

In comparison, we also calculated the bandstructure of the infinite periodic system and plot it in the reduced Brillouin zone(Figure 3(e)). We find the index of each conductance plateau has a one-to-one correspondence to the number of positive-velocity (slope) bands in the bandstructure of the infinite problem [5]. The shadings in Figure 3(d) and 3(e) illustrate this correspondence. Full understanding of the variations in conductance from the exact integers is for further study. One reason is that the channel, although long, is still finite.

For an incident energy of E/E_L=3.15, marked with the dashed line in Figure 3(a), there are two allowed traveling modes in the lead region. Figures 4 illustrates the particle current density distributions of a one-cell channel. The modulation causes the mixing of edge states in the device region and makes the single mode transmitting pattern complicated. Shown in Figure 4(a) is the particle current density for electrons incident in the first mode (edge-state). The opposite-going edge states on opposite side walls of the channel are weakly coupled in one unit cell, so the resulting transmission coefficient is T_1=0.96. Figure 4(b) shows the current for electrons incident in the second mode. The transmission coefficient is T_2=0.87

for one unit cell. For the long channel of 50 unit cells, we have T_1 = 0.34 and T_2 = 0.66 which sum to unity for the total transmission and make the plateau index of the quantized conductance 1.

VI. Summary

We have extended the QTBM algorithm to include an applied magnetic field to 2D systems for solving current carrying states governed by effective 2D Schrödinger equation. In this algorithm, we have acquired the capability of modeling of magneto-transport with complicated potential profiles and arbitrarily shaped devices. This technique is applied to studying of a periodically corrugated quantum channel. The results illustrate that the total conductance quantization recovers when the modulated channel is sufficiently long. The plateau index is a non-monotonic function of energy. However, the individual mode transmissions are not quantized.

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