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Ballistic Transport in Crossed Quantum Wires

An Analytical Approach

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An analytic approach to the ballistic electron transport in crossed 2D wires is presented. It is shown that within and near the first transverse mode the two-mode approximation gives a correct description of the system. Simple formulas for the bound-state energies and the single-mode scattering probabilities are derived.

Eine analytische Näherung an den ballistischen Elektronentransport in gekreuzten 2D-Drähten wird dargestellt. Innerhalb und nahe der ersten transversalen Mode beschreibt die Zweimodennäherung das System korrekt. Einfache Formeln für die Energie des Grundzustandes und die Zweimoden-Streuwahrscheinlichkeit werden abgeleitet.

1. Introduction

Current fine lithographic techniques make it possible to shape electrons at the two-dimensional surfaces into channels the width of which is of the same order as the de Broglie wavelength [1 to 3]. Hence quantum-mechanical effects are strongly manifested in such systems. For example, while from a classical point of view the system of two perpendicular perfect channels of infinite length is characterized by an open potential; the reverse is the case for the quantum channels. Indeed, Peeters [4] and Schult et al. [5] showed that bound states reside at the intersection of the two channels. Beggren and Zhen-Li Ji [6] showed that the bound states give rise to sharp peaks in the conduction. These authors calculated the ballistic transport characteristics (bound-state energies and scattering probabilities) only numerically. It is clear, however, that more realistic theoretical models are numerically more difficult and the various factors which contribute to the process are not always transparent. The purpose of the present work is to present an analytic approach to the ballistic transport in a system of crossed wires in order to bring out the essential approximations and to provide analytic formulas for bound-state energies and scattering amplitudes.

2. Results

To describe the ballistic transport in the X-shaped system of crossed wires we use the Hamiltonian $H = -(\hbar^2/2m^*)\nabla^2$ inside the well (m^* is the effective electron mass) with the boundary condition that the electron wave function goes to zero on the sides of the channels (see insert of Fig. 1). The characteristics of the ballistic transport are determined by

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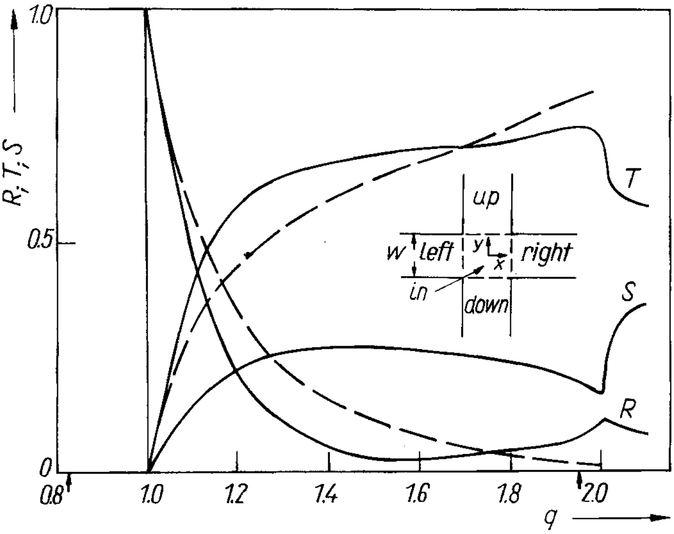

Fig. 1. The reflection (R), forward-transmission (T), and side-transmission (S) probabilities as functions of $q(= w/\pi)\sqrt{2m^*E/\hbar^2}$. $q = 1(2, \ldots)$ corresponds to the opening of the first- (second-, ...) mode propagation. Solid lines two-mode approximation, dashed lines one-mode approximation (see the text). The positions of the two bound states are marked by arrows

scattering-type solutions of the time-independent Schrödinger equation,

$$H\psi = E\psi\,,$$

where the wave function ψ has the form

$$\psi_l = e^{ik(x+d)} \sin \frac{n_0(y + d)\,\pi}{2d} + \sum_{n=1}^{\infty} e^{k_n(x+d)} R_n \sin \frac{n\pi(y + d)}{2d}\,, \tag{1}$$

$$\psi_r = \sum_{n=1}^{\infty} e^{-k_n(x-d)} \sin \frac{n\pi(y + d)}{2d}\, T_n\,, \tag{2}$$

$$\psi_u = \sum_{n=1}^{\infty} e^{-k_n(y-d)} \sin \frac{n\pi(x + d)}{2d}\, U_n\,, \tag{3}$$

$$\psi_d = \sum_{n=1}^{\infty} e^{k_n(y+d)} \sin \frac{n\pi(x + d)}{2d}\, D_n\,, \tag{4}$$

$$\psi_{in} = \sum_{n=1}^{\infty} \left\{(\alpha_n \sinh k_n x + \beta_n \cosh k_n x) \sin \frac{n\pi(y + d)}{2d} + (\delta_n \sinh k_n y + \gamma_n \cosh k_n y) \sin \frac{n\pi(x + d)}{2d}\right\} \tag{5}$$

in each of the five rectangular regions labeled in Fig. 1 with left, right, up, down, and in. The first term in (1) represents an incoming electron wave with the longitudinal wave vector

k and transverse wave number n_0. The electron energy in the channels is

$$E = \frac{\hbar^2}{2m^*}\left(\frac{n^2\pi^2}{4d^2} + k^2\right).$$

The quantities k_n in (1) to (5) are defined by the relations

$$k_n = \left(\frac{n^2 - n_0^2}{4d^2}\pi^2 - k^2\right)^{1/2} \quad \text{for} \quad n^2 \geqq n_0^2 + \frac{4k^2d^2}{\pi^2}$$

and

$$k_n = -i\left(k^2 - \frac{n^2 - n_0^2}{4d^2}\pi^2\right)^{1/2} \quad \text{for} \quad n^2 \leqq n_0^2 + \frac{4k^2d^2}{\pi^2}.$$

The coefficients in (1) to (5) should be chosen so as to match ψ and its derivatives at the boundaries between the five regions. As a result of the matching procedure we get

$$\begin{aligned} &k_nd(1 + \coth 2k_nd + (-1)^n \operatorname{cosech} 2k_nd)\, A_{n,\pm} \\ &\mp \sum_{n'=1}^{\infty} \frac{1 + (-1)^{n+n'}}{2} K_{nn'}A_{n',\pm} = \mp \frac{1 + (-1)^{n+n_0}}{2} K_{nn_0} \\ &+ \delta_{nn_0}k_nd(\coth 2k_nd - 1 + (-1)^n \operatorname{cosech} 2k_nd)\,, \end{aligned} \tag{6}$$

$$\begin{aligned} &k_nd(1 + \coth 2k_nd - (-1)^n \operatorname{cosech} 2k_nd)\, B_{n,\pm} \\ &\mp \sum_{n'=1}^{\infty} \frac{1 - (-1)^{n+n'}}{2} K_{nn'}B_{n',\pm} = \pm \frac{1 - (-1)^{n+n_0}}{2} K_{nn_0} \\ &+ \delta_{nn_0}k_nd(1 - \coth 2k_nd + (-1)^n \operatorname{cosech} 2k_nd)\,, \end{aligned} \tag{7}$$

where

$$A_{n,\pm} = (-1)^n(T_n \pm U_n) - (R_n \pm D_n)\,,$$

$$B_{n,\pm} = (-1)^n(T_n \pm U_n) + (R_n \pm D_n)\,,$$

and

$$K_{nn'} = 2nn'(n^2 + n'^2 - n_0^2 - 4k^2d^2\pi^{-2})^{-1}\,; \qquad n, n' = 1, 2, \dots\,.$$

The set of equations (6) and (7) gives the full description of the scattering process in the system under consideration.

In the following we consider the case $n_0 = 1, 2$ and assume that $E \leqq 4E_t \equiv 4\pi^2\hbar^2/2m^*d^2$. Then the only mode which can propagate through the channels is the $n = 1$ mode, all others are evanescent modes.

From (6) and (7) one obtains

$$U_1 = D_1\,, \tag{8}$$

$$T_1 - R_1 = 1 - 2ikd(B - kd \operatorname{ctg} kd + ikd)^{-1}\,, \tag{9}$$

$$T_1 + R_1 \mp 2U_1 = -1 + 2ikd(\mp A_\pm + kd \operatorname{tg} kd \pm K_{11} + ikd)^{-1}\,. \tag{10}$$

Here we introduce the quantities

$$A_\pm = \sum_{n=1}^{\infty} K_{2n+1,1} a_{n,\pm}\,, \tag{11}$$

$$B = \sum_{n=1}^{\infty} K_{2n,1} b_n\,, \tag{12}$$

where the coefficients $a_{n,\pm}$ and b_n are the solutions of the equations

$$k_{2n}d(1 + \tanh k_{2n}d)\, b_n - \sum_{n'=1}^{\infty} \left(\sum_{n=1}^{\infty} \frac{K_{2n,2m+1}K_{2m+1,2n'}}{k_{2m+1}d(1 + \coth k_{2m+1}d)} \right) b_{n'} = K_{2n,1}\,, \tag{13}$$

$$k_{2n+1}d(1 + \coth k_{2n+1}d)\, a_{n,\pm} \mp \sum_{n'=1}^{\infty} K_{2n+1,2n'+1} a_{n',\pm} = \mp K_{2n+1,1}\,. \tag{14}$$

It is worthwhile to remark that the quantities $A_\pm$ and B describe the contribution to the scattering process only from evanescent modes.

Exact solutions of (13) and (14) can be obtained only numerically. Nevertheless, as is shown below, the equations for the bound-state energies and the scattering probabilities can be expressed in a quite simple analytic form within the accuracy of a few percent.

2.1 Bound-state energies

It is well known that the poles of scattering amplitudes in the upper half of the complex $\boldsymbol{k}$-plane determine the energies of bound states. In our case the energy of the electron bound state is determined by the pole of the function $T_1 - R_1 + 2U_1$,

$$\pi z(1 + e^{-\pi z})^{-1} = 2(1 + z^2)^{-1} - A_+|_{k=i\frac{\pi z}{2d}}\,, \tag{15}$$

where $k = i(z\pi/2d)$ $(z > 0)$. The functions $T_1 - R_1$ and $T_1 - R_1 - 2U_1$ have no poles.

In the one-mode approximation (this means: $A_+ = 0$ in (15)) we obtain that the bound-state energy is given by

$$E_b = (1 - z^2)\, E_t = 0.68 E_t \tag{16}$$

(in [5] $E = 0.66E_t$). Analysis shows that (16) determines the energy of the lowest even-parity bound state. To obtain the energy of the lowest odd-parity bound state we have to consider the case $n_0 = 2$. Using the two-mode approximation to solve (6) and (7) (i.e. the set of equations is truncated on the second mode), we find

$$E'_b = (4 - z_0^2)\, E_t = 3.78 E_t \tag{17}$$

($3.72E_t$ in [5]) where z_0 is the root of the equation

$$\pi z(4 + z^2)(1 - e^{-\pi z})^{-1} = 8\,. \tag{18}$$

It is worthwhile to remark that the bound-state energies obtained in the simplest approximations agree well with the exact values calculated numerically by Schult et al. [5]: the discrepancy does not exceed a few percent. The same statement is valid for some other related systems. For example, the functions (1) to (5) with $T_n = 0$ and $\beta_n = -\alpha_n \tanh k_n d$ describe the ballistic transport in a T-shape system. In this case there is only one bound state and its energy (in the one-mode approximation) is given by

$$E_b = (1 - z_T^2)\, E_t = 0.82 E_t \tag{19}$$

($E_b = 0.81 E_t$ [5]) where z_T is the root of the equation

$$\pi z(1 + z^2)(1 + e^{-\pi z})^{-1/2}(1 - e^{-2\pi z})^{-1/2} = 2^{1/2}\,. \tag{20}$$

The scattering process in an L-shaped system (a right-angle wire bend) is described by the functions (1) to (5) with $T_n = U_n = 0$ and $\beta_n = -\alpha_n \tanh k_n d$, $\gamma_n = -\delta_n \tanh k_n d$. Then, it is easy to show (in the same approximation) that

$$E_b = (1 - z_L^2)\, E_t = 0.95 E_t\,, \tag{21}$$

where z_L is the root of the equation

$$\pi z(1 + z^2)(1 - e^{-2\pi z})^{-1} = 1\,. \tag{22}$$

Comparing (17) and (18) with (21) and (22) we see that the bound-state energy in the L-shaped system, with half the width, coincides with the odd-parity bound-state energy in the X-type system.

It is interesting to remark that the bound states in the L-type system is more loose than in the T- and X-shaped ones. Indeed, from (16), (17), (19), and (21) we see

$$r_X = 1.13d \quad \text{(even parity state)}\,,$$

$$r_X = 1.36d \quad \text{(odd parity state)}\,,$$

$$r_T = 1.50d\,, \qquad r_L = 2.85d\,.$$

This fact may be important when nano-patterns consisting of several "X", "T", and "L" systems are investigated.

2.2 *Scattering probabilities*

We calculate the forward- and side-transmission probabilities, $T = |T_1|^2$ and $S = \frac{1}{2}|U_1|^2$, using the two-mode approximation, i.e. the only evanescent mode which contributes to the scattering process is the $n = 2$ mode. In this case from (13) and (14) we obtain that

$$\begin{aligned} &a_{n,\pm} = 0\,; \qquad n = 1, 2, \dots\,, \\ &b_1 = K_{21}/k_2 d(1 + \tanh k_2 d) \qquad b_n = 0 \quad \text{for} \quad n = 2, 3, \dots\,. \end{aligned} \tag{23}$$

With account of (8) to (12) and (23) the transmission probabilities take the form

$$S = 2F_1 \cos^2 kd(1 + 2F_1 \cos 2kd + F_1^2)^{-1}\,, \tag{24}$$

$$T = \frac{(1 - F_1)^2 \sin^2 kd + (1 - F_2 \cos kd + F_2^2) \cos^2 kd}{(1 - 2F_1 \cos 2kd + F_1^2)(1 - F_2 \cos kd + F_2^2)}\,, \tag{25}$$

$$R = 1 - T - S\,, \tag{26}$$

where

$$F_1 = 4\pi^4 k^{-2} d^{-2} \cos^2 kd (\pi^2 - 4k^2 d^2)^{-2},$$

$$F_2 = \frac{4\pi^2}{\pi^2 - k^2 d^2} \frac{1 + \exp[-(3\pi^2 - 4k^2 d^2)^{1/2}]}{(3\pi^2 - 4k^2 d^2)^{1/2}} \frac{\sin kd}{kd}.$$

Note that putting in (24) to (26) $F_2 = 0$ we obtain the one-mode approximation.

The functions (24) to (26) are plotted in Fig. 1 (solid lines). Despite the roughness of the approximation used, the curves are in excellent agreement with the exact calculations [5]. All important details of the behaviour of the scattering probabilities as functions of the longitudinal wave vector in the range up to the second-mode threshold ($E = 4E_t$) and slightly above are reproduced correctly. Examination of higher approximations shows small quantitative changes not distinguished in the figure scale. At the same time, the one-mode approximation (dashed lines) is valid at small wave vectors only.

3. Conclusions

In conclusion, as demonstrated above, the two-mode approximation gives a reasonable description of the system, revealing the main factors which determine the principle characteristics of the fundamental-mode propagation. An analogous approach seems especially promising for applications to more complex types of wire discontinuity treatments which demand a great amount of computational time.

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