Transmission coefficient for ballistic transport through quantum resonator

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Abstract

A model for the description of ballistic transport in 1D-2D-1D system based on the theory of self-adjoint extensions of symmetric operators is suggested. Formula for transmission coefficient for the system, particurlarly, in the case of presense of a magnetic field, is obtained.

1 Introduction

While studying transport properties of low-dimensional systems (particurlarly, nanoelectronic devices), one use, usually, the approach based on Landauer-Buttiker theory [1], [2], [3]. Following this approach, one obtains direct relation between conductivity and transmission coefficient for ballistic channels forming the system. Sufficiently general scheme of construction of solvable model for nanoelectronic device with two contacts was suggested in [9]. General expression for the transmission coefficient for the model is determined. The basic idea is using zero-range potentials with internal structure [10], [5], [4]. The approach is a generalization of some examples of the models which are described in [6], [7], [8]. The expression obtained in [9] is rather general and contains some complicated mathematical constructions (Krein functions etc.). That is why it is interesting, especially for physicists, to consider concrete realization of this abstract approach. It is the main goal of the present paper. Let us describe briefly the general scheme.

Consider a nanoelectronic device with two leads, shown on figure 1. The state space $\mathcal{H}$ divides into a direct sum

$$\mathcal{H} = \mathcal{H}_- \oplus \mathcal{H}_d \oplus \mathcal{H}_+,$$

where $\mathcal{H}_\pm = L^2(\mathbf{R}_\pm), \mathcal{H}_d$ is the state space of the device. At first, we need not the concrete form of $\mathcal{H}_d$ (as for as a form of the Hamiltonian H_d which is introduced below). If "the channel is closed", then the system Hamiltonian H^0 can be represented in a form of a direct sum

$$H^0 = H_- \oplus H_d \oplus H_+.$$

Here $H_\pm$ is the operator $-\frac{d^2}{dx^2}$ in $L^2(\mathbf{R}_\pm)$ with the Neumann boundary condition at the point 0 (it corresponds to the absence of current through contacts $\pm$), H_d is the Hamiltonian of a charged particle in the device. Let us denote as $R_-(z), R_d(z), R_+(z), R^0(z)$ the resolvents of the operators H_-, H_d, H_+, H^0 correspondingly. It is evident that $R^0 = R_- \oplus R_d \oplus R_+$. To switch on the interaction we use conventional "restriction- extension" procedure [5]. Namely, we start from a self-adjoint operator, come to a symmetric operator by a restriction. The obtained operator has self-adjoint extensions which gives us the model in question. Note that among these extensions there is initial self-adjoint operator, but it corresponds to the case of absence of interaction.

Let $S_\pm$ be a symmetric operator being a restriction of the operator $H_\pm$ on the domain

$$D(S_\pm) = \{\varphi \in D(H_\pm) : \varphi(0) = 0\}.$$

Consider, simultaneously, a symmetric operator S_d with the deficiency indices (2,2) such that $S_d = H_d \mid_{D(S_d)}$. We shall identify the deficiency elements of the operator with the contacts $\pm$ in the device. A concrete form of the elements depends, naturally, on the physical interpretation of the space $\mathcal{H}_d$ and the Hamiltonian H_d.

In each case it is a subject of a special analysis. An example is given below. It is important to note that the operator S_d may not be densely defined. Particularly, if $\mathcal{H}_d$ is a finite- dimensional space, then $D(S_d)$, evidently, is not dense in $\mathcal{H}_d$ (examples of such operators are in [5]).

We shall use below the Krein formula for resolvents of self-adjoint operators [10]. For this purpose let us introduce standard deficiency subspaces:

$$\mathcal{N}_- = \mathcal{N}_+ = \mathbf{C}, \mathcal{N}_d = \mathbf{C}^2.$$

A contact of the lead with the device "is realized" by means of the basic elements 1 and (1,0) in $\mathcal{N}_-$ and $\mathcal{N}_d$ correspondingly, and a contact of $\mathbf{R}_+$ with the device- by means of the basic elements 1 and (0,1) in $\mathcal{N}_+$ and $\mathcal{N}_d$.Introduce Krein $\Gamma-$ and Q-functions for the operator S_+, S_d, S_-. Denote as $G_\pm(x,y;\zeta)$ the Green function of the operator $H_\pm$. Then the map $\Gamma_\pm(\zeta) : \mathcal{N}_\pm \to L^2(\mathbf{R}_\pm)$ is defined by the formula

$$\mathbf{C} \ni \xi \mapsto G_\pm(x,0;\zeta) \cdot \xi \in L^2(\mathbf{R}_\pm).$$

Let $\Gamma_d(\zeta)$ and $Q_d(\zeta)$ be Krein $\Gamma-$ function and Q- function of the operator S_d:

$$\Gamma_d(\zeta) : \mathbf{C}^2 \to \mathcal{H}_d, Q_d(\zeta) : \mathbf{C}^2 \to \mathbf{C}^2.$$

Γ-function and Q-function for the operator $S, S = S_- \oplus S_d \oplus S_+$, is a direct sum

$$\Gamma(\zeta) = \Gamma_-(\zeta) \oplus \Gamma_d(\zeta) \oplus \Gamma_+(\zeta),$$
$$Q(\zeta) = Q_-(\zeta) \oplus Q_d(\zeta) \oplus Q_+(\zeta).$$

The Hamiltonian H of the system with "open channels" is a self- adjoint extension of the operator S. For the resolvent of the extension we have Krein formula [11]:

$$R(\zeta) = R^0(\zeta) - \Gamma(\zeta)(Q(\zeta) + A)^{-1}\Gamma^*(\overline{\zeta}). \tag{1}$$

The operator matrix $Q(z) + A$ has a structure:

$$\begin{pmatrix} Q_-(\zeta) & \alpha_- & 0 & 0 \\ \alpha_- & Q_d^{11} & Q_d^{12} & 0 \\ 0 & Q_d^{21} & Q_d^{22} & \alpha_+ \\ 0 & 0 & \alpha_+ & Q_+(\zeta) \end{pmatrix} \tag{2}$$

Here $Q_\pm\ (\zeta) = Q_\pm(\zeta) + \mu_\pm$, where α_- and α_+ are values which characterize the "ideal" contacts "-" and "+", value $\mu_-(\mu_+)$ characterizes the degree of difference between the contact "-" ("+") and the "ideal" one (for instance, if $\mu_+ > 0$ then moving particle in the wire $\mathbf{R}_+$ is repulsed by the contact "+", and if $\mu_+ < 0$ then it is attracted). We shall write Q_{ij} instead of Q_{ij}^d for simplicity.

Using this approach, general formula for the transmission coefficient $T(E)$ may be obtained (see [9]):

$$T(E) = \frac{\mid \alpha_-\alpha_+ Q_{12}(E) \mid^2}{E \mid \det(Q(E) + A) \mid^2} \tag{3}$$

In particular case of ideal contacts $\mu_{\pm} = 0$ one has:

$$T(E) = \frac{E\alpha_-^2\alpha_+^2 \mid Q_d^{21}(E) \mid^2}{E(\alpha_-^2 Q_d^{22}(E) + \alpha_+^2 Q_d^{11}(E))^2 + (\det Q_d(E) - E\alpha_-^2\alpha_+^2)^2} \tag{4}$$

2 Model of transport through quantum resonator

Consider a system of two semi-infinite quantum waveguides which are connected through a quantum dot (resonator Ω). We shall deal with so-called one-mode regime. In this situation waveguides may be simulated by semi-axes $\mathbf{R}_-$ and $\mathbf{R}_+$ (fig. 1). Then an element from the domain of the operator S^* has the form:

$$f(x) = \begin{cases} u_-(x), & x \in \mathbf{R}_-; \\ a_1 G(x, x_1; k_0) + a_2 G(x, x_2; k_0) + u(x), & x \in \Omega; \\ u_+(x), & x \in \mathbf{R}_+, \end{cases} \tag{5}$$

where $G(x, y; k)$ is the Green function for the Neumann problem in Ω, k_0^2 is a regular value for the operator. A choice of a self-adjoint extension is related with a choice of "boundary conditions" at the points x_1, x_2. We shall consider one type of the extensions only, namely, those used by Kiselev and Pavlov [12] (in their work the choice of the extension is justified by a comparison of the model solution with a solution of the problem in which there are narrow channels instead of lines in the model). The corresponding conditions are:

$$\begin{array}{c} a_1 = -\alpha u_-'(0), a_2 = \alpha u_+'(0), \\ u_-(0) = \alpha(f - a_1 G(x, x_1; k_0))|_{x=x_1}, \\ u_+(0) = \alpha(f - a_2 G(x, x_2; k_0))|_{x=x_2}, \end{array} \tag{6}$$

where α is a model parameter.

The Green function for the model self-adjoint operator with a source at a point $x_0 \in \Omega$ can be sought in a form:

$$G_\alpha(x, x_0; k) = \begin{cases} a_- i k^{-1} \exp(-ikx), & x \in \mathbf{R}_-; \\ a_1 G(x, x_1; k) + a_2 G(x, x_2; k) + G(x, x_0; k), & x \in \Omega; \\ a_+ i k^{-1} \exp(ikx), & x \in \mathbf{R}_+. \end{cases} \tag{7}$$

Taking into account (6), one obtains

$$\begin{array}{c} a_1 = -\alpha a_-, a_2 = -\alpha a_+, \\ ik^{-1} a_- = \alpha(a_1 g_1(k, k_0) + a_2 G(x_1, x_2; k) + G(x_1, x_0; k)), \\ ik^{-1} a_+ = \alpha(a_2 g_2(k, k_0) + a_1 G(x_1, x_2; k) + G(x_2, x_0; k)), \end{array} \tag{8}$$

where

$$\begin{array}{c} g_i(k, k_0) = (G(x, x_i; k) - G(x, x_i; k_0))|_{x=x_i} = \\ (k^2 - k_0^2) \sum_n |\phi_n(x_i)|^2 (\lambda_n - k^2)^{-1} (\lambda_n - k_0^2)^{-1}, i = 1, 2, \end{array} \tag{9}$$

λ_n is an eigenvalue of the Neumann problem for the Laplace operator in Ω associated with the eigenfunction ϕ_n. System (8) reduces to

$$a_1 = ik\alpha^2(a_1 g_1(k,k_0) + a_2 G(x_1,x_2;k) + G(x_1,x_0;k)),$$

$$a_2 = ik\alpha^2(a_2 g_2(k,k_0) + a_1 G(x_1,x_2;k) + G(x_2,x_0;k)).$$

Hence,

$$a_1 = D_{-1}(-ik\alpha^2 G(x,x_1;k)(ik\alpha^2 g_2(k,k_0) - 1) - k^2\alpha^4 G(x_1,x_2;k)G(x_2,x_0;k),$$

$$a_2 = D_{-1}(-ik\alpha^2 G(x,x_2;k)(ik\alpha^2 g_1(k,k_0) - 1) - k^2\alpha^4 G(x_1,x_2;k)G(x_1,x_0;k),$$

where

$$D = (ik\alpha^2 g_1(k,k_0) - 1)(ik\alpha^2 g_2(k,k_0) - 1) + k^2\alpha^4(G(x_1,x_2;k))^2.$$

Therefore, the corresponding part of the matrix $(Q(\zeta)+A)^{-1}$ in the Krein formula has the form:

$$D^{-1}\begin{pmatrix} -ik\alpha^2(ik\alpha^2 g_1(k,k_0) - 1) & k^2\alpha^4 G(x_1,x_2;k) \\ k^2\alpha^4 G(x_1,x_2;k) & -ik\alpha^2(ik\alpha^2 g_2(k,k_0) - 1) \end{pmatrix}.$$

To obtain other blocks of the matrix it is necessary to consider a situation when the source x_0 is in $\mathbf{R}_\pm$. Let $x_0 \in \mathbf{R}_-$. Then the Green function has the form

$$G_\alpha(x,x_0;k) = \begin{cases} a_- ik^{-1}\exp(-ikx) + G_-(x,x_0;k), & x \in \mathbf{R}_-; \\ a_1 G(x,x_1;k) + a_2 G(x,x_2;k), & x \in \Omega; \\ a_+ ik^{-1}\exp(ikx), & x \in \mathbf{R}_+. \end{cases}$$

Hence, system (8) is replaced by

$$\begin{gathered} a_1 = -\alpha a_-, a_2 = -\alpha a_+, \\ ik^{-1}(a_- + \exp(-ikx_0)) = \alpha(a_1 g_1(k,k_0) + a_2 G(x_1,x_2;k)), \\ ik^{-1}a_+ = \alpha(a_2 g_2(k,k_0) + a_1 G(x_1,x_2;k)). \end{gathered}$$

Consequently,

$$a_- = -\exp(-ikx_0) - ik\alpha(a_1 g_1(k,k_0) + a_2 G(x_1,x_2;k)),$$

$$a_1(ik\alpha^2 g_1(k,k_0) - 1) + ik\alpha^2 a_2 G(x_1,x_2;k) = \alpha\exp(-ikx_0),$$

$$a_2(ik\alpha^2 g_2(k,k_0) - 1) + ik\alpha^2 a_1 G(x_1,x_2;k) = 0.$$

Thus,

$$a_1 = D^{-1}(ik\alpha^2 g_2(k,k_0) - 1)\alpha\exp(-ikx_0),$$

$$a_2 = -D^{-1}ik\alpha^3\exp(-ikx_0)G(x_1,x_2;k),$$

$$a_- = -\exp(-ikx_0)(2 + D^{-1}(ik\alpha^2 g_2(k,k_0) - 1)).$$

As a result, one obtains the following expression for the corresponding (1x1) matrix block:

$$2 + D^{-1}(ik\alpha^2 g_2(k, k_0) - 1)).$$

The block corresponding to $\mathbf{R}_+$ may be obtained in a similar way.

The model for the case of the Dirichlet condition at the boundary of Ω is more complicated. In this situation we have to deal with the operator extension theory in an indefinite metrics space. As for details, see [13], [14]. Nevertheless, the structure of the model is analogous to one described above. We must make the following alterations. Representation (5) should be replaced by

$$f(x) = \begin{cases} u_-(x), & x \in \mathbf{R}_-; \\ a_1 \frac{\partial G_D(x,x_1;k_0)}{\partial n} + a_2 \frac{\partial G_D(x,x_2;k_0)}{\partial n} + u(x), & x \in \Omega; \\ u_+(x), & x \in \mathbf{R}_+, \end{cases} \tag{10}$$

where $G_D(x, y; k)$ is the Green function for the Dirichlet problem in Ω, n is a normal. Further, system (8) slightly changes:

$$\begin{array}{rcl} & a_1 = \alpha a_-, a_2 = \alpha a_+, & \\ ik^{-1}a_- & = & -\alpha(a_1 g_1^D(k, k_0) + a_2 \frac{\partial G_D(x_1,x_2;k)}{\partial n} + \frac{\partial G_D(x_1,x_0;k)}{\partial n}, \\ ik^{-1}a_+ & = & -\alpha(a_2 g_2^D(k, k_0) + a_1 \frac{\partial G_D(x_1,x_2;k)}{\partial n} + \frac{\partial G_D(x_2,x_0;k)}{\partial n}, \end{array} \tag{11}$$

where

$$g_i^D(k, k_0) = (k^2 - k_0^2) \sum_m |\frac{\partial \phi_m^D(x_i)}{\partial n}|^2 (\lambda_m - k^2)^{-1} (\lambda_m - k_0^2)^{-1}, i = 1, 2, \tag{12}$$

λ_m is an eigenvalue of the Dirichlet problem for the Laplace operator in Ω associated with the eigenfunction ϕ_m^D. The following treatment is analogous to the previous one.

3 The system in a magnetic field

The model allows one to consider two-dimensional system in a constant magnetic field $\mathbf{B}$ which is orthogonal to the system plane. Here we must deal with the Green function for the Landau operator

$$H = \frac{1}{2m}(\mathbf{p} - \frac{e}{c}\mathbf{A})^2.$$

Here m, e are mass and charge of an electron correspondingly, c is the speed of light, $\mathbf{p} = -i\hbar\nabla, \mathbf{A} = 2^{-1}\mathbf{B}\mathrm{x}\mathbf{r}$. Let Ω be a disk $\Omega = \{(r, \varphi) : r \leq r_0\}$. Introduce the followimg notation

$$\omega = \frac{|e\mathbf{B}|}{cm}, \lambda = \left(\frac{\hbar c}{|e\mathbf{B}|}\right)^{1/2}, x_0 = \frac{r_0}{2\lambda^2}.$$

The spectrum of the operator H with the Dirichlet boundary conditions consists of the eigenvalues E_{ln},

$$E_{ln} = \hbar\omega(2^{-1}(l + |l| + 1) - \epsilon_{ln}), l = 0, \pm 1, \pm 2, ..., n = 1, 2, ...,$$

ϵ_{ln} is a root of the equation $\Phi(\epsilon, |l| + 1, x_0) = 0$. Here $\Phi(a, c, x) = M(a, c, x)$ is the Kummer function. The corresponding eigenfunction is

$$\Psi_{ln}(r, \varphi) = \left(\frac{m\omega}{2\pi\hbar c_{ln}}\right)^{1/2} \frac{r^{|l|}}{(2\lambda^2)^{|l|/2}} \exp{(il\varphi - \frac{r^2}{4\pi\lambda^2})} \Phi(\epsilon_{ln}, |l| + 1, \frac{r^2}{2\lambda^2}),$$

where c_{ln} is normalization constant,

$$c_{ln} = \int_0^{x_0} \exp{(-x)} x^{|l|} (\Phi(\epsilon_{ln}, |l| + 1, x))^2 dx.$$

The Green function has a form

$$\begin{array}{c} G(r, \varphi, r', \varphi'; \zeta) = \frac{m\omega}{2\pi\hbar} \exp{(-\frac{r^2 + r'^2}{4\lambda^2})} \\ \sum_{l=-\infty}^{\infty} \frac{(rr')^{|l|}}{(2\lambda^2)^{|l|}} \exp{(il(\varphi - \varphi'))} \\ \sum_{n=1}^{\infty} \frac{\Phi(\epsilon_{ln}, |l|+1, \frac{r^2}{2\lambda^2}) \Phi(\epsilon_{ln}, |l|+1, \frac{r'^2}{2\lambda^2})}{c_{ln}(E_{ln} - \zeta)}. \end{array}$$

One sum can be calculated. Let

$$F_l(s, t, \zeta) = \left\{ \begin{array}{l} \Phi(\zeta, |l| + 1, s)(\Psi(\zeta, |l| + 1, t) - \alpha\Phi(\zeta, |l| + 1, t)), s \leq t; \\ \Phi(\zeta, |l| + 1, t)(\Psi(\zeta, |l| + 1, s) - \alpha\Phi(\zeta, |l| + 1, s)), t \leq s. \end{array} \right.$$

Here

$$\alpha = \frac{\Psi(\zeta, |l| + 1, x_0)}{\Phi(\zeta, |l| + 1, x_0)}, \zeta \neq \epsilon_{ln},$$

$\Psi(a, c, x)$ is the Trikomi function. Then the Green function takes the form

$$\begin{array}{c} G(r, \varphi, r', \varphi'; \zeta) = \frac{m\omega}{2\pi\hbar} \exp{(-\frac{r^2 + r'^2}{4\lambda^2})} \\ \sum_{l=-\infty}^{\infty} \frac{(rr')^{|l|}}{(2\lambda^2)^{|l|}} \exp{(il(\varphi - \varphi'))} \\ \Gamma(\frac{1+l+|l|}{2} - \frac{\zeta}{\hbar\omega}) F_l(\frac{r^2}{2\lambda^2}, \frac{r'^2}{2\lambda^2}, \frac{1+l+|l|}{2} - \frac{\zeta}{\hbar\omega}). \end{array}$$

Substitution of this expression into the formula for the transmission coefficient (4), described above gives us the required result.

4 Conclusion

Quantum waveguide-resonator-waveguide system is considered. Solvable model based on the theory of self-adjoint extensions of symmetric operators is suggested. The model is concrete realization of general construction suggested in [9] and its composition with so-called zero-width slit model. For proper choice of the model parameters we use the results of [12]. The advantage is that the approach allows one to reveal some general features of the physical system. We construct model self-adjoint operator which is similar (in some sense) to that for physical system. Green function, transmission coefficient, etc. for the model operator is obtained in an explicit form. As a result, one can get the dispersion equation and investigate effectively spectral properties. The model is constructed both for the case of absence and presence of a magnetic field. The latter is especially interesting for physical applications, namely, for the investigation of transport properties of quantum dots.

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