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Model of tunnelling through quantum dot and spin–orbit interaction

D A EREMIN[1], E N GRISHANOV[1], I Y POPOV[2],* and A A BOITSEV[2]

[1]Department of Mathematics and Information Technology, Ogarev Mordovia State University, Bolshevistskaya Street 68, Saransk, Russia
[2]Department of Higher Mathematics, ITMO University, Kroverkskiy pr. 49, St. Petersburg, 197101, Russia
*Corresponding author. E-mail: popov1955@gmail.com

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Abstract. Solvable mathematical model is suggested for tunnelling through quantum dot. The model is based on the theory of self-adjoint extensions of symmetric operators. The spin–orbit interaction is taken into account. The transmission coefficient is obtained. The result is compared with the case where spin–orbit interaction is absent.

Keywords. Tunnelling; quantum dot; self-adjoint extension.

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1. Introduction

Many nanoelectronic devices are based on tunnelling through nanostructures. Correspondingly, the dependence of the transmission coefficient on the particle energy and the system parameters plays a crucial role in such engineering applications. Electron tunnelling through quantum dots having connecting leads was studied in [1–6]. To describe the process effectively, one can use a solvable model of quantum dot – point-like potential with internal structure (see e.g. [7–9] and references in [10]). An abstract model for tunnelling was suggested in [5]. As for the mathematical difficulties, they are related to the necessity of connecting manifolds having different dimensions. The general approach to the description of such contacts was developed in [11]. It is based on the theory of self-adjoint extensions of symmetric operators. As for physical aspects, one can mention works dealing with the properties of two-dimensional electron gas on curved surfaces [12,13]. In many cases, the spin–orbit interaction plays an important role (see e.g. [14,15]). The spin–orbit interaction is at the heart of the emerging field of spintronics. New devices are being contemplated based purely on the spin degrees of freedom instead of charge. There are two microscopic origins of spin–orbit interactions. One originates due to structural inversion asymmetry, which is known as Rashba spin–orbit interaction [16], and the other is due to the bulk inversion asymmetry, which is known as Dresselhaus spin–orbit interaction [17]. The Rashba effect makes it possible to control the electron spin by the external electric field (see e.g. [18]). The discovery of the giant Rashba effect [19,20] in bulk crystals such as BiTeI and ferroelectric GeTe and in a number of low-dimensional systems bears a promise of creating devices operating electron spins at nanoscale and possessing short operational times. In this paper we deal with the Rashba Hamiltonian.

All the aforementioned models of tunnelling do not take into account the spin–orbit interaction. In this paper, we construct a model of tunnelling through quantum dots under the assumption that the spin–orbit interaction takes place inside the quantum dot. The model is based on the operator extension theory. One can mention a series of papers related to extension theory models for spin–orbit Hamiltonians [21–23]. We follow the work of Jursenas [24] where the point-like potential in $\mathbb{R}^3$ was constructed for the Rashba Hamiltonian. In our case, the model configuration is as follows. We have two semi-infinite lines with the state space $L_2(\mathbb{R}_+) \otimes \mathbb{C}^2$. These lines are coupled to $\mathbb{R}^3$ at some point. The state space for $\mathbb{R}^3$ is $L_2(\mathbb{R}^3) \otimes \mathbb{C}^2$. Correspondingly, the state space is as follows:

$$L_2(\mathbb{R}_+) \otimes \mathbb{C}^2 \oplus L_2(\mathbb{R}^3) \otimes \mathbb{C}^2 \oplus L_2(\mathbb{R}_+) \otimes \mathbb{C}^2.$$

At each semi-infinite line, we consider two copies of L_2-space corresponding to two values of particle spin. The initial Hamiltonian has the form

$$S = S_1 \oplus S_d \oplus S_2.$$

Here

$$S_1 = S_2 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} \otimes \mathbb{C}^2,$$

$$S_d = -\Delta \otimes I + \imath\alpha(\nabla_1 \otimes \sigma_2 - \nabla_2 \otimes \sigma_1) + \beta I \otimes \sigma_3,$$

$\alpha, \beta \geq 0$, α stands for the spin–orbit coupling strength and β is the strength of the magnetic Zeeman field, Δ denotes the three-dimensional Laplace operator, ∇_j $(j = 1, 2)$ is the gradient in the jth component of a three-dimensional position vector, I is the identity operator and σ_j, $j = 1, 2, 3$, are the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The domain of S is as follows:

$$\mathrm{dom}\, S = \mathrm{dom}\, S_1 \oplus \mathrm{dom}\, S_d \oplus \mathrm{dom}\, S_2,$$

$$\mathrm{dom}\, S_1 = \mathrm{dom}\, S_2 = \{f \in H^2(\mathbb{R}_+),$$

$$f(0) = f'(0) = 0\} \otimes \mathbb{C}^2,$$

$$\mathrm{dom}\, S_d = \{f \in H^2(\mathbb{R}^3),\, f(0) = 0\} \otimes \mathbb{C}^2,$$

where H^2 is the Sobolev space. Operator S is a symmetric operator with the deficiency indices (6, 6). It has self-adjoint extensions. We choose a particular extension (see below) as a model Hamiltonian.

2. Model construction

There are several ways to construct the self-adjoint extension, including Neumann formula approach (see e.g. [7]), Krein formula approach (see e.g. [25]) and boundary triplet approach (see e.g. [26]). We choose the second one. This method uses the fact that it is more convenient to deal with the resolvent instead of the initial operator. It is the resolvent of the extension, which is given by the Krein resolvent formula. The formula contains the Γ-field (the Krein Γ-function) and the Krein Q-function (see e.g. [27]). In our model, the Krein Γ-functions for the half-lines are mappings from the deficiency subspaces to the state space $L_2(\mathbb{R}_+)\otimes\mathbb{C}^2$. It is given by the Green function for the half-line. As for the quantum dot, the situation is analogous, but the state space is $L_2(\mathbb{R}^3) \otimes \mathbb{C}^2$. The Krein Q-function is given by a value of the regular part of the Green function for coinciding arguments. These functions for the full system are constructed from the corresponding functions for the system parts. The expressions are written below.

For the half-line, the Γ-field and the Q-function are as follows [27]:

$$\Gamma_1(z) = \Gamma_2(z) = \mathrm{diag}\left(\frac{\imath}{k}\mathrm{e}^{\imath kx}, \frac{\imath}{k}\mathrm{e}^{\imath kx}\right),$$

$$Q_1(z) = Q_2(z) = \mathrm{diag}\left(\frac{\imath}{k}, \frac{\imath}{k}\right),$$

where $k = \sqrt{z}$ and z is the spectral parameter.

As for the term S_d, we use the expression for the Green function from [24]:

$$\Gamma_s = \mathrm{diag}(G_+(x; z), G_+(x; z)),$$

$$Q_s = \mathrm{diag}(Q_+, Q_-).$$

Here

$$Q_\pm(z) = N_\pm^2\left(\frac{1}{4\sqrt{2}\pi} - \frac{\sqrt{-z}}{4\pi} + G_\pm^{\mathrm{ren}}(0; z) - \mathrm{Re}\, G_\pm^{\mathrm{ren}}(0; \imath)\right),$$

where

$$G_\pm^{\mathrm{ren}}(0; z) = \frac{\sqrt{-z}}{4\pi} - \frac{1}{4\pi}\sqrt{\frac{-z}{2}\left(1 + \sqrt{1 - \left(\frac{\beta}{z}\right)^2}\right)} + \left(\frac{\alpha}{8\pi} \mp \frac{\beta}{4\pi\alpha}\right) \times \mathrm{artanh}\left(\frac{\alpha}{\beta}\sqrt{\frac{-z}{2}\left(1 - \sqrt{1 - \left(\frac{\beta}{z}\right)^2}\right)}\right).$$

The normalisation constant is as follows:

$$N_\pm^{-2} = \frac{1}{8\pi}\left(\sqrt{1 + \sqrt{1 + \beta^2}} + \left(\frac{\alpha}{2} \mp \frac{\beta}{\alpha}\right) \times (\mathrm{Arg}(1 + c(1 + \imath)) - \mathrm{Arg}(1 - c(1 + \imath)))\right),$$

$$c = \frac{\alpha}{2\beta}\sqrt[4]{2 + \beta^2 - 2\sqrt{1 + \beta^2}}.$$

The Γ-field and Q-function for the full operator (i.e. for the orthogonal sum of the operators) are obtained by the following method justified in [28]:

$$\Gamma(z) = \Gamma_1 \oplus \Gamma_s \oplus \Gamma_2,$$

$$Q(z) = Q_1 \oplus Q_s \oplus Q_2.$$

To describe an extension of the initial symmetric operator, it is more convenient to deal with the operator

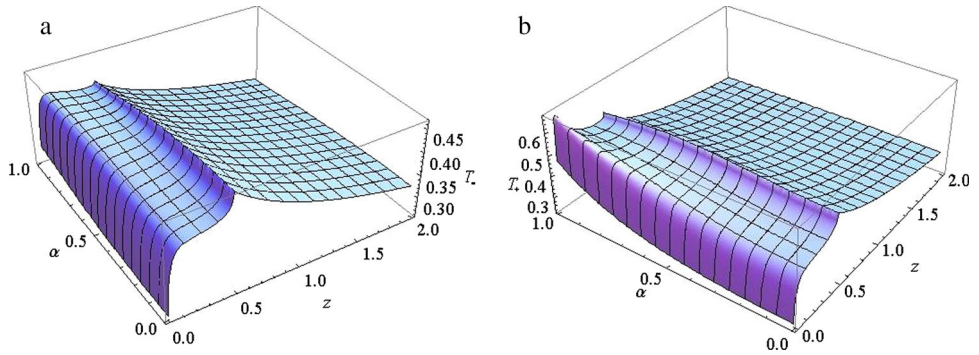

Figure 1. Transmission coefficients $|t_{\pm}|$ via energy z and parameter of spin–orbit interaction α. Values of other parameters are: $\beta = \mu = \gamma = 0.5$ (dimensionless units) (**a**) for T_- and (**b**) for T_+.

resolvent and to use the well-known Krein's resolvent formula:

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

Here a Hermitian matrix A parameterises the extension. We choose this matrix in the following form:

$$A = \begin{pmatrix} \mu & 0 & \gamma & 0 & 0 & 0 \\ 0 & \mu & 0 & \gamma & 0 & 0 \\ \gamma & 0 & 0 & 0 & \gamma & 0 \\ 0 & \gamma & 0 & 0 & 0 & \gamma \\ 0 & 0 & \gamma & 0 & \mu & 0 \\ 0 & 0 & 0 & \gamma & 0 & \mu \end{pmatrix},$$

where parameter μ is related to the properties of the channels. In its turn, non-zero γ corresponds to the existence of interaction between the one-dimensional leads and the quantum dots (i.e. a three-dimensional space in our model). We choose the simplest variant of the matrix ensuring the interaction. The value of γ is related to the probability of transmission from the lead to the dot.

3. Results and discussion

Let us find the transmission coefficient for an electron travelling from the first semi-infinite lead to another one. The incoming wave has the following form:

$$\varphi = \begin{pmatrix} \mathrm{e}^{-\imath kx} \\ \mathrm{e}^{-\imath kx} \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

The solution of the scattering problem is obtained from formula (1):

$$\psi = \varphi - \Gamma(z)(Q(z) + A)^{-1}\Gamma^*(z)(H^0 - z)\varphi. \tag{2}$$

Consequent calculations give us

$$\Gamma^*(z)(H^0 - z)\varphi = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix},$$

$$(Q(z) + A)^{-1}\Gamma^*(z)(H^0 - z)\varphi = \det(Q + A)^{-1} \begin{pmatrix} B_{11} + B_{12} \\ B_{21} + B_{22} \\ B_{31} + B_{32} \\ B_{41} + B_{42} \\ B_{51} + B_{52} \\ B_{61} + B_{62} \end{pmatrix}.$$

Here B_{ij} is the corresponding minor of the matrix $Q+A$. The scattered wave in (2) has the form

$$\Gamma(Q + A)^{-1}\Gamma^*(z)(H^0 - z)\varphi = \det(Q + A)^{-1} \begin{pmatrix} (\imath/k)(B_{11} + B_{12})\mathrm{e}^{\imath kx} \\ (\imath/k)(B_{21} + B_{22})\mathrm{e}^{\imath kx} \\ (B_{31} + B_{32})G_+(x; z) \\ (B_{41} + B_{42})G_-(x; z) \\ (\imath/k)(B_{51} + B_{52})\mathrm{e}^{\imath kx} \\ (\imath/k)(B_{61} + B_{62})\mathrm{e}^{\imath kx} \end{pmatrix}. \tag{3}$$

The transmission coefficients are as follows:

$$t_+ = \frac{\imath(B_{51} + B_{52})}{k \det(Q + A)}, \quad t_- = \frac{\imath(B_{61} + B_{62})}{k \det(Q + A)}.$$

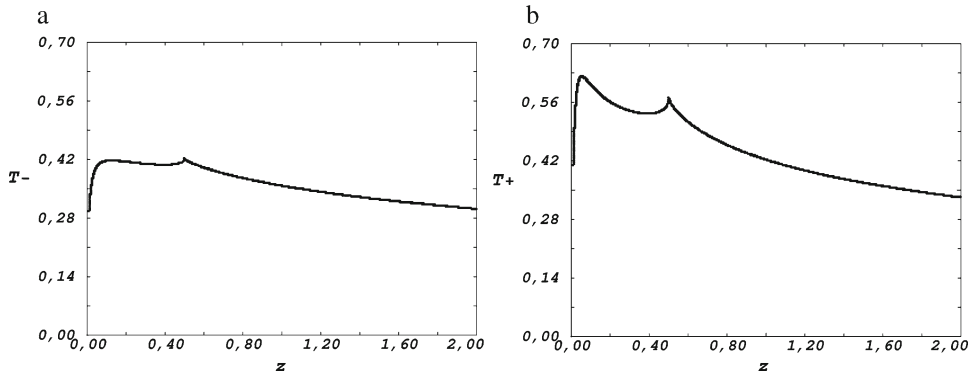

Figure 2. Transmission coefficients $|t_{\pm}|$ via energy z for the spin–orbit interaction $\alpha = 0.9$. Values of other parameters are: $\beta = \mu = \gamma = 0.5$ (dimensionless units) (**a**) for T_{-} and (**b**) for T_{+}.

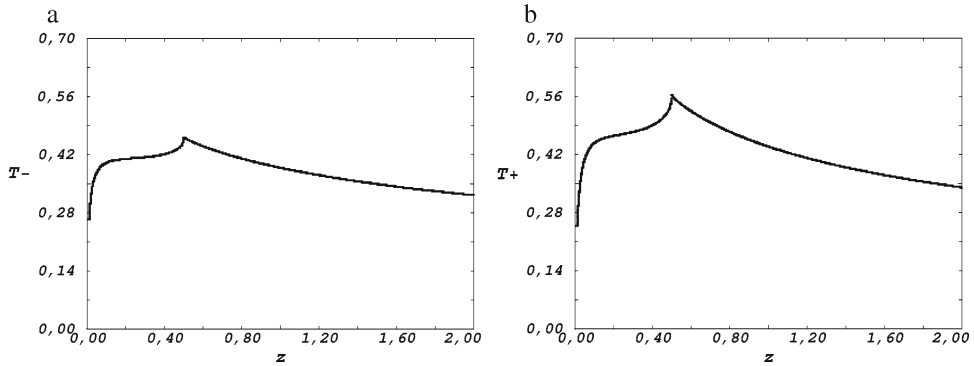

Figure 3. Transmission coefficients $|t_{\pm}|$ via energy z for the spin–orbit interaction $\alpha = 0.3$. Values of other parameters are: $\beta = \mu = \gamma = 0.5$ (dimensionless units) (**a**) for T_{-} and (**b**) for T_{+}.

Here $\pm$ corresponds to the different directions of the spin. The transmission probabilities are given by $P_{\pm} = |t_{\pm}|^2$:

$$P_{+} = \frac{|B_{51} + B_{52}|^2}{z|\det(Q + A)|^2}, \quad P_{-} = \frac{|B_{61} + B_{62}|^2}{z|\det(Q + A)|^2}.$$

Figure 1 shows the dependence of the transmission coefficients $T_{\pm}$ on two variables: energy z and spin–orbit interaction α. We choose dimensionless units. One can see the difference in the behaviour of the coefficients for different directions of the spin. To show this difference in more details and to stress the influence of the spin–orbit interaction, we arrange two cross-sections of figure 1 in figures 2 and 3.

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