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Original article

On spin flip for electron scattering by several delta-potentials for 1D Hamiltonian with spin-orbit interaction

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ABSTRACT One-dimensional Rashba and Dresselhaus Hamiltonians with spin-orbit interaction are studied. It is assumed that there are point-like potentials on the line. The scattering problem is solved and the possibility of spin-flip is discussed.

KEYWORDS spin-orbit interaction; point-like potential; spin filtering; Schrödinger equation

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1. Introduction

Conventional electronics is based on the charge transport. However, during last decades, a new branch of electronics, spintronics, was developing rapidly. In contrast to electronics which ignores the electron spin, spintronics deals with spinbased electron transport. It is not the electron charge but the electron spin that carries information [1]. The new wave of interest was inspired by the development of quantum computing and quantum computations (see, e.g., [2, 3]). Correspondingly, one needs electronic devices which can distinguish the spin orientation and can control it. The most popular theoretical idea for creating the background for such device is taking into account the spin-orbit interaction. There are two types of spin-orbit coupling: the Rashba Hamiltonian [4] and the Dresselhaus Hamiltonian [5]. The Rashba effect is a direct result of inversion symmetry breaking in the direction perpendicular to the two-dimensional plane. The Dresselhaus Hamiltonian describes the spin-orbit coupling in a two-dimensional semiconductor thin film grown with appropriate geometry. A number of works were devoted to spin-orbit coupling in different dimensions (see, e.g., [6–10]). Point-like potentials are rather useful in this situation [11–14]. As for one-dimensional models, quantum graph is very effective in this situation (see, e.g., [15–17]). Particularly, to ensure the spin filtering, spin flip, control of the spin transport one uses, usually, systems of coupled quantum rings (see, e.g., [14, 18–27]). In the present paper, we show an example of the spin-flip in 1D system without rings for the Hamiltonian with spin-orbit interaction.

2. Model construction

We start with the Schrödinger equation for the Rashba Hamiltonian in one-dimensional case. In the case of spin-orbit interaction, we deal with 2-vector functions $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$.

$$\begin{cases} i\hbar\dfrac{\partial\psi_1}{\partial t} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\psi_1}{\partial x^2} + \alpha_R\dfrac{\partial\psi_2}{\partial x}, \\ i\hbar\dfrac{\partial\psi_2}{\partial t} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\psi_2}{\partial x^2} - \alpha_R\dfrac{\partial\psi_1}{\partial x}, \end{cases} \tag{1}$$

where $\hbar$ is the Plank constant, α_R is the parameter of the Rashba spin-orbit interaction, $|\psi|^2 = |\psi_1|^2 + |\psi_2|^2$. Let us separate variables x, t. It means that $\psi(x,t) = e^{i\omega t}\tilde{\psi}(x)$. Correspondingly, the system (1) transforms to the following form:

$$\begin{cases} -\hbar\omega\tilde{\psi_1} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\tilde{\psi_1}}{\partial x^2} + \alpha_R\dfrac{\partial\tilde{\psi_2}}{\partial x}, \\ -\hbar\omega\tilde{\psi_2} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\tilde{\psi_2}}{\partial x^2} - \alpha_R\dfrac{\partial\psi_1}{\partial x}, \end{cases} \tag{2}$$

In the case of the Dresselhaus spin-orbit interaction, the corresponding system has the following form:

$$\begin{cases} -\hbar\omega\tilde{\psi}_1 = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\tilde{\psi}_1}{\partial x^2} - i\alpha_D\dfrac{\partial\tilde{\psi}_2}{\partial x}, \\ -\hbar\omega\tilde{\psi}_2 = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\tilde{\psi}_2}{\partial x^2} - i\alpha_D\dfrac{\partial\tilde{\psi}_1}{\partial x}, \end{cases} \tag{3}$$

where α_D is the parameter of the Dresselhaus spin-orbit interaction.

As for the point-like potential at point x_0, it is determined by the coupling conditions at this point. There are many variants of such conditions (see, e.g., [14]). We choose the condition which corresponds to 1D delta-potential at the point:

$$\begin{cases} \tilde{\psi}(x_0+0) = \tilde{\psi}(x_0-0), \\ \tilde{\psi}'(x_0+0) - \tilde{\psi}'(x_0-0) = -\beta\tilde{\psi}(x_0+0). \end{cases} \tag{4}$$

Let us choose the atomic system of units with $\hbar = 1, m = 1/2$. Consider the case of finite number of point-like potentials at the line. Then, at each half-axis and at each segment between the potentials, one has the following system of differential equations:

$$\begin{cases} \tilde{\psi}_1'' + k^2\tilde{\psi}_1 + \alpha_R\tilde{\psi}_2' = 0, \\ \tilde{\psi}_2'' + k^2\tilde{\psi}_2 - \alpha_R\tilde{\psi}_1' = 0, \end{cases} \tag{5}$$

where k is the wavenumber. Taking $\tilde{\psi}_j = C_j e^{\lambda x}$, $j = 1, 2$, one obtains the following characteristic equation

$$(\lambda^2 + k^2)^2 + \alpha_R^2\lambda^2 = 0 \tag{6}$$

with the following four roots and the corresponding vectors $\begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$:

$$\lambda = i\tilde{k}_1, \begin{pmatrix} 1 \\ -i \end{pmatrix}; \quad \lambda = -i\tilde{k}, \begin{pmatrix} 1 \\ -i \end{pmatrix}; \quad \lambda = i\tilde{k}, \begin{pmatrix} 1 \\ i \end{pmatrix}; \quad \lambda = -i\tilde{k}_1, \begin{pmatrix} 1 \\ i \end{pmatrix},$$

where

$$\tilde{k} = \frac{1}{2}(\sqrt{\alpha_R^2 + 4k^2} - \alpha_R), \quad \tilde{k}_1 = \frac{1}{2}(\sqrt{\alpha_R^2 + 4k^2} + \alpha_R).$$

Correspondingly, at each segment and half-axis, one has a solution in the form of linear combination of standard solutions. Coupling conditions (4) gives one a system for determination the coefficients of the linear combination.

3. Results and discussion

Consider the scattering problem for the case of one point-like potential at point $x_0 = 0$. System (5) has solution of the form

$$\begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix} = e^{i\tilde{k}x}\begin{pmatrix} 1 \\ i \end{pmatrix} + B_1 e^{-i\tilde{k}x}\begin{pmatrix} 1 \\ -i \end{pmatrix} + D_1 e^{-i\tilde{k}_1 x}\begin{pmatrix} 1 \\ i \end{pmatrix}, \quad x < 0, \tag{7}$$

$$\begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix} = A_2 e^{i\tilde{k}x}\begin{pmatrix} 1 \\ i \end{pmatrix} + C_2 e^{i\tilde{k}_1 x}\begin{pmatrix} 1 \\ -i \end{pmatrix}, \quad x > 0. \tag{8}$$

Coupling conditions (4) at point $x_0 = 0$ gives one the following system for coefficients of (7), (8):

$$\begin{cases} 1 + B_1 + D_1 = A_2 + C_2, \\ 1 - B_1 + D_1 = A_2 - C_2, \\ \tilde{k} - \tilde{k}B_1 - \tilde{k}_1 D_1 = \tilde{k}A_2 + \tilde{k}_1 C_2 - i\beta A_2 - i\beta C_2, \\ -\tilde{k} - \tilde{k}B_1 + \tilde{k}_1 D_1 = -\tilde{k}A_2 + \tilde{k}_1 C_2 + i\beta A_2 - i\beta C_2. \end{cases} \tag{9}$$

We are interested in coefficients of the outgoing solution, which are as follows:

$$A_2 = \frac{\tilde{k} + \tilde{k}_1}{\tilde{k} + \tilde{k}_1 - i\beta}, \quad C_2 = 0,$$

i.e. the outgoing solution has the form:

$$\begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix} = \frac{\tilde{k} + \tilde{k}_1}{\tilde{k} + \tilde{k}_1 - i\beta} e^{i\tilde{k}x}\begin{pmatrix} 1 \\ i \end{pmatrix}. \tag{10}$$

The second scattering problem with the solution of the following form

$$\begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix} = e^{i\tilde{k}_1 x} \begin{pmatrix} 1 \\ -i \end{pmatrix} + B_1' e^{-i\tilde{k}x} \begin{pmatrix} 1 \\ -i \end{pmatrix} + D_1' e^{-i\tilde{k}_1 x} \begin{pmatrix} 1 \\ i \end{pmatrix}, \quad x < 0, \tag{11}$$

$$\begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix} = A_2' e^{i\tilde{k}x} \begin{pmatrix} 1 \\ i \end{pmatrix} + C_2' e^{i\tilde{k}_1 x} \begin{pmatrix} 1 \\ -i \end{pmatrix}, \quad x > 0, \tag{12}$$

is solved analogously and gives one the following outgoing solution:

$$\begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix} = \frac{\tilde{k} + \tilde{k}_1}{\tilde{k} + \tilde{k}_1 - i\beta} e^{i\tilde{k}_1 x} \begin{pmatrix} 1 \\ -i \end{pmatrix}. \tag{13}$$

Using the linearity of the problem, one can incorporate (10), (13) and obtain the solution for the general case:

$$\begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix} = \begin{pmatrix} e^{i\tilde{k}x} + e^{i\tilde{k}_1 x} \\ i(e^{i\tilde{k}x} - e^{i\tilde{k}_1 x}) \end{pmatrix} + (B_1 + B_1') e^{-i\tilde{k}x} \begin{pmatrix} 1 \\ -i \end{pmatrix} + (D_1 + D_1') e^{-i\tilde{k}_1 x} \begin{pmatrix} 1 \\ i \end{pmatrix}, \quad x < 0, \tag{14}$$

$$\begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix} = \frac{\tilde{k} + \tilde{k}_1}{\tilde{k} + \tilde{k}_1 - i\beta} \begin{pmatrix} e^{i\tilde{k}x} + e^{i\tilde{k}_1 x} \\ i(e^{i\tilde{k}x} - e^{i\tilde{k}_1 x}) \end{pmatrix}, \quad x > 0. \tag{15}$$

One can see that

$$\begin{pmatrix} e^{i\tilde{k}x} + e^{i\tilde{k}_1 x} \\ i(e^{i\tilde{k}x} - e^{i\tilde{k}_1 x}) \end{pmatrix} = e^{i\tilde{k}x} \begin{pmatrix} 1 + e^{i\alpha_R x} \\ i(1 - e^{i\alpha_R x}) \end{pmatrix}. \tag{16}$$

Here we took into account that $\tilde{k}_1 - \tilde{k} = \alpha_R$.

To obtain the spin flip, one should choose the proper input and output points. Namely, let the input point x_{in} be such that $e^{i\alpha_R x_{in}} = 1$. Then, keeping in mind (16), one obtains that the input wave function in (14) has the form $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$. One can choose the output point x_{out} in such a way that

$$e^{i\alpha_R x_{out}} = -1. \tag{17}$$

We remember that α_R does not depend on the electron energy (i.e. on k). It means that the relation (17) is valid for all energies. Correspondingly, according to (15), the output state at this point has the form $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Thus, one obtains the spin flip.

One observes the analogous situation for the case of several delta-potentials. It can be solved analytically, but the expressions are too large. It is more convenient to solve the equations numerically. Fig. 1 shows $|\psi_1|$ and $|\psi_2|$ at $x = x_{out}$ as functions of k for fixed $x_{in} = -5$ and $x_{out} = 5$ (dimensionless units) for cases of 1, 3, 5, 9 point-like potentials posed at integer points symmetrically in respect to $x = 0$. One can see that in all cases the ratio $\dfrac{|\psi_2|}{|\psi_1|}$ does not depend on k as has been obtained analytically (see (15) and (16)) for the case of one point-like potential at point $x = 0$. We mention that we deal with the diapason of k outside resonances induced by 1D resonators formed by several delta-potentials (see, e.g., [14]).

The case of the Dresselhaus spin-orbit interaction (3) can be considered analogously. Particularly, one obtains the following characteristic equation which is analogous to (6):

$$(\lambda^2 + k^2)^2 + \alpha_D^2 \lambda^2 = 0 \tag{18}$$

with the following four roots and the corresponding vectors $\begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$:

$$\lambda = i\tilde{k}_1, \begin{pmatrix} 1 \\ 1 \end{pmatrix}; \quad \lambda = -i\tilde{k}, \begin{pmatrix} 1 \\ 1 \end{pmatrix}; \quad \lambda = i\tilde{k}, \begin{pmatrix} 1 \\ -1 \end{pmatrix}; \quad \lambda = -i\tilde{k}_1, \begin{pmatrix} 1 \\ -1 \end{pmatrix},$$

where

$$\tilde{k} = \frac{1}{2}(\sqrt{\alpha_D^2 + 4k^2} - \alpha_D), \quad \tilde{k}_1 = \frac{1}{2}(\sqrt{\alpha_D^2 + 4k^2} + \alpha_D).$$

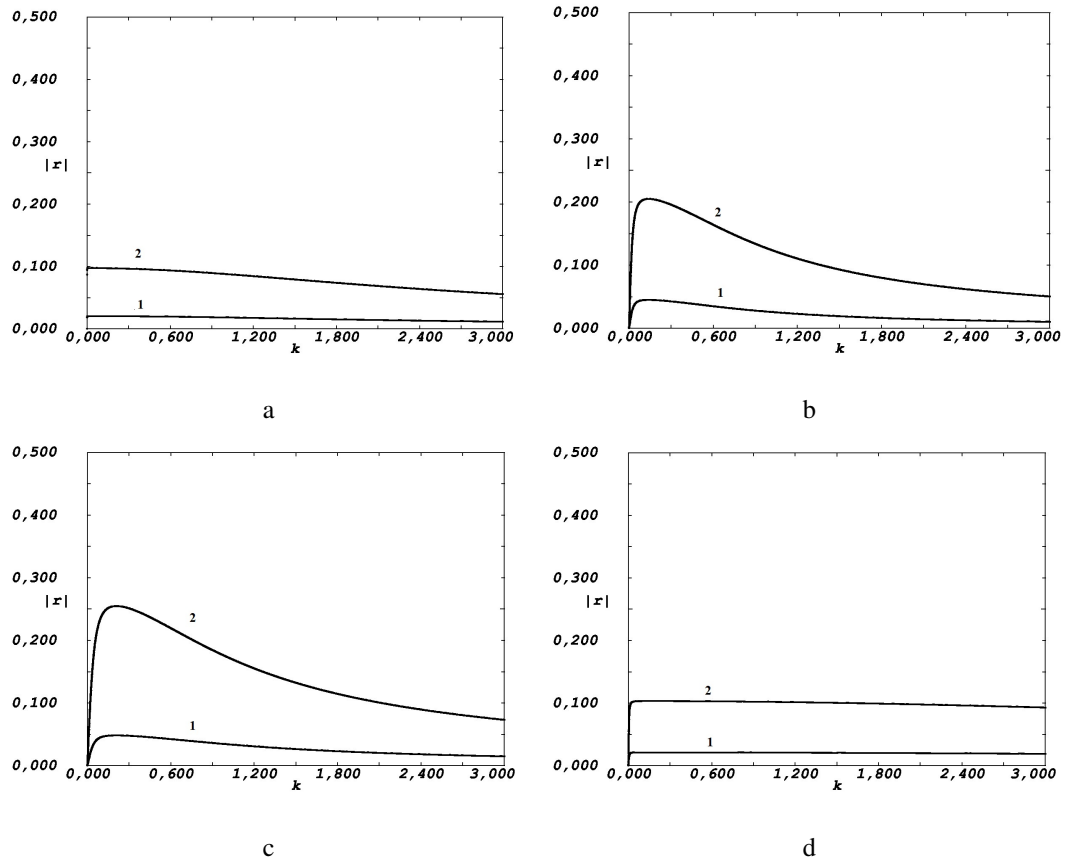

FIG. 1. $r = |\psi_1|$ (curve 1) and $r = |\psi_2|$ (curve 2) as functions of k: a - for one center, b- for 3 centers, c - for 5 centers, d - for 9 centers

Using the same procedure as in the Rashba case, one comes to the solution of the scattering problem for the Dresselhaus Hamiltonian:

$$\begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \end{pmatrix} = \frac{e^{i\tilde{k}x}}{\tilde{k}_1(\tilde{k}+\tilde{k}_1-i\beta)} \times$$

$$\begin{pmatrix} (\tilde{k}+\tilde{k}_1)(\tilde{k}+\tilde{k}_1-i\beta-(\tilde{k}-i\beta)e^{i\alpha_D x})+2\tilde{k}\tilde{k}_1 e^{i\alpha_D x} \\ -(\tilde{k}+\tilde{k}_1)(\tilde{k}+\tilde{k}_1-i\beta+(\tilde{k}-i\beta)e^{i\alpha_D x})+2\tilde{k}\tilde{k}_1 e^{i\alpha_D x} \end{pmatrix}, \quad x>0.$$

One can see that there is no energy independent condition for spin flip as in the case of the Rashba spin-orbit interaction. Moreover, calculations show that the values of transmission coefficients is significantly smaller than in the Rashba case. Correspondingly, the Dresselhaus case is not good for spin-flip applications.

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