ISSN 1062-8738, Bulletin of the Russian Academy of Sciences: Physics, 2018, Vol. 82, No. 5, pp. 550–553. © Allerton Press, Inc., 2018.
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Effect of Total Reflection from a Symmetric Two-Channel Device with Fermion Path Nonanalyticity Points Induced by Rashba Spin-Orbit Coupling

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Abstract—The effect Rashba spin-orbit coupling has on transmission coefficient through a symmetric system with fermion path nonanalyticity points is illustrated using the example of a regular polygon-shaped chain. It is shown that the current passage through a device is blocked at the critical spin-orbit coupling values determined by the system's geometry. At the near-critical spin-orbit coupling values, electron transport is possible only in a narrow range of energies.

DOI: 10.3103/S1062873818050313

The possible existence of points with path nonanalyticity and thus a stepwise change in the direction of the Rashba field is most often ignored in studying the effects Rashba fields have on the properties of low-dimensional systems [1]. The properties of edge states are investigated using models that are infinite in one direction [2, 3]. It is important to clarify if the conclusions of this analysis can be extended to the systems with finite sizes and path nonanalyticity points. Note that, e.g., Lee et al. [4] emphasized the importance of studying a square-shaped system; however, there is still a paucity of detailed studies on the effect angles have on the properties of spin-polarized states. The question of the effect the Rashba spin-orbit coupling constant nonuniformity has on the properties of a system was raised in [5], but the Rashba field was in this case assumed to be constant.

Electrons in a chain with the shape of a regular polygon (Fig. 1) having N sites on each N_s sides and total number of sites $N_s(N-1)$ are described by the Hamiltonian

$$
\begin{aligned}
H_D = &-t_D \sum_{n=1}^{N-1} \sum_{j=1,\sigma}^{N_s} a_{jn+1\sigma}^{+} a_{jn\sigma} - t_D \sum_{j=1,\sigma}^{N_s} a_{j+1,1\sigma}^{+} a_{j,N-1\sigma} \\
&- i\alpha_D \sum_{n=1}^{N-1} \sum_{j=1,\sigma\sigma'}^{N_s} \vec{e}_j \vec{\tau}_{\sigma'\sigma} a_{jn+1\sigma'}^{+} a_{jn\sigma} - i\alpha_D \sum_{j=1,\sigma\sigma'}^{N_s} \vec{e}_j \vec{\tau}_{\sigma'\sigma} a_{j+11\sigma'}^{+} a_{jN-1\sigma} + \text{h.c.}
\end{aligned} \quad (1)
$$

Here, the first two terms correspond to hoppings between nearest neighbors with parameter $t_D > 0$, and the next two correspond to the Rashba spin-orbit coupling associated with an electric potential gradient directed perpendicular to the polygon's plane. The numbering in $j = 1, \ldots, N_s$ corresponds to the polygon side numbers (clockwise); $n = 1, \ldots, N-1$ numbers the sites on each side; α_D is the Rashba spin-orbit coupling constant; $\vec{\tau}$ denotes the Pauli matrices; $\sigma = \pm 1$ corresponds to the electron spin projection onto axis z; and $\vec{e}_j$ is the unit vector along the direction of the Rashba field. The one-electron states in the chain forming a regular polygon are described by the expressions [6]

$$
\begin{aligned}
\Psi_{mls} &= \sum_{jn\sigma} z_{jn\sigma}^{mls} a_{jn\sigma}^{+} |0\rangle, \\
k_{mls} &= \frac{1}{N-1}\left[s \arccos\left(\cos(\varphi/2)\cos\chi\right) + \varphi_l + 2\pi m\right], \\
E_{mls} &= -2\sqrt{t_D^2 + \alpha_D^2}\cos k_{mls}, \ \chi = k_0(N-1), \ \varphi_l = (2l+1)\varphi/2, \\
&l = 1,\ldots,N_s, \ s = \pm 1, \ m = 1,\ldots,(N-1), \ \varphi = 2\pi/N_s,
\end{aligned} \quad (2)
$$

$$z_{1n\sigma}^{mls} = \frac{1}{\sqrt{N_s(N-1)}}\frac{\rho_s^{-\sigma/2}}{\sqrt{\rho_s+\rho_{-s}}}e^{i\sigma k_0(n-n_c)-i\sigma s\pi/4}e^{-ik_{mls}(n-1)},$$
$$\rho_s = \left(\sqrt{\sin^2(\varphi/2)+\cos^2(\varphi/2)\sin^2\chi} - s\cos(\varphi/2)\sin\chi\right)\Big/\sin(\varphi/2),$$
$$z_{1+j,n\sigma}^{mls} = e^{-i\varphi_l j}\left[z_{1n\sigma}^{mls}\cos(\varphi j/2) - \sigma z_{1n\bar{\sigma}}^{mls}\sin(\varphi j/2)\right].$$

Here, the k_0 value is reciprocal to characteristic spin-orbit coupling length L_{SO}; i.e., the distance at which the electron spin rotates around the direction of the Rashba field by angle π, and is determined in the tight binding approximation as

$$k_0 = \arcsin\left(\alpha_D\Big/\sqrt{t_D^2+\alpha_D^2}\right),$$
$$\chi = k_0(N-1) = \frac{\pi}{2}\frac{L}{L_{SO}}, \quad (3)$$

where L is the length of the polygon's side.

We use the Landauer–Büttiker formalism to calculate the transmission coefficient through a device with connected one-dimensional contacts. The transport properties of the system are then determined by the wave function, which is the solution to the Schrödinger equation for Hamiltonian [7]

$$H = H_L + T_L + H_D + T_R + H_R,$$
$$H_L = \sum_{n=-\infty,\sigma}^{-1}\left[t_L\left(c_{n-1\sigma}^{+}c_{n\sigma} + c_{n\sigma}^{+}c_{n-1\sigma}\right) - \varepsilon_d c_{n\sigma}^{+}c_{n\sigma}\right],$$
$$H_R = \sum_{n=1,\sigma}^{\infty} t_R\left(c_{n+1\sigma}^{+}c_{n\sigma} + c_{n\sigma}^{+}c_{n+1\sigma} - \varepsilon_d c_{n\sigma}^{+}c_{n\sigma}\right),$$
$$T_L = \sum_{\sigma} t_{LD}\left(c_{-1\sigma}^{+}a_{L\sigma} + a_{L\sigma}^{+}c_{-1\sigma}\right),$$
$$T_R = \sum_{\sigma} t_{RD}\left(c_{1\sigma}^{+}a_{R\sigma} + a_{R\sigma}^{+}c_{1\sigma}\right),$$
$$H_D = \sum_{mls} E_{mls}b_{mls}^{+}b_{mls}.$$

Here, terms $H_{L,R}$ are the Hamiltonians of contacts; $T_{L,R}$ describes electron tunneling between the contact and device; H_D is diagonalized Hamiltonian (1) of the polygon-shaped chain; $a_{(L,R)\sigma}$ is the operator of annihilation on a device site connected directly to the contacts; b_{mls} is the operator of annihilation of one-electron states (2) in the device; ε_d is the shift of the electron energy in the device, relative to the energy in contacts; and energy E is counted from the seed energy in the device.

The wave function is sought in the form of expansion in the orthogonal basis of the entire system:

$$\Psi = \sum_{n=-\infty}^{-1} u_{n\sigma}c_{n\sigma}^{+}|0\rangle$$
$$+ \sum_{mls} w_{mls}b_{mls}^{+}|0\rangle + \sum_{n=1}^{\infty} v_{n\sigma}c_{n\sigma}^{+}|0\rangle, \quad (4)$$
$$u_{n\sigma} = p_\sigma e^{ik_L n} + r_\sigma e^{-ik_L n},$$
$$v_{n\sigma} = t_\sigma e^{ik_R n},\ |p_\uparrow|^2 + |p_\downarrow|^2 = 1,$$

where the electron wave function in the contacts corresponds to the incoming, reflected, and transmitted waves, respectively, and p_σ determines the incoming electron spin polarization.

Writing the Schrödinger equation and multiplying it by each of the orthogonal basis functions in (4), we obtain the nonuniform system of equations

$$E = 2t_L\cos k_L - \varepsilon_d = 2t_R\cos k_R - \varepsilon_d,$$
$$-t_L r_\sigma + \sum_{mls} t_{LD}w_{mls}z_{L\sigma}^{mls} = t_L p_\sigma,$$
$$-t_R t_\sigma + \sum_{mls} t_{RD}w_{mls}z_{R\sigma}^{mls} = 0, \quad (5)$$
$$(E_{mls}-E)w_{mls} + \sum_{\sigma}\left(t_{LD}r_\sigma e^{ik_L}z_{L\sigma}^{mls*} + t_{RD}t_\sigma e^{ik_R}z_{R\sigma}^{mls*}\right) = -t_{LD}\sum_{\sigma}p_\sigma e^{-ik_L}z_{L\sigma}^{mls*},$$
$$z_{(L,R)\sigma}^{mls} = \langle 0|a_{(L,R)\sigma}b_{mls}^{+}|0\rangle.$$

Reflection and transmission coefficients are in this case determined as

$$R = \sum_{\sigma}|r_\sigma|^2,\ T = \frac{t_R\sin k_R}{t_L\sin k_L}\sum_{\sigma}|t_\sigma|^2. \quad (6)$$

Below, we consider a polygon with an even number of sides and symmetrically connected contacts (Fig. 1). The typical form of the dependence of transmission coefficient through a regular polygon-shaped chain on the incoming electron energy is presented in Fig. 2. The spin-orbit coupling eliminates the fourfold energy degeneracy and results in $(N_s(N-1)/2-1)$ Fano antiresonances between the forming pairs of states caused by the interference of electron wave functions during motion along two channels.

An important effect caused by Rashba spin-orbit coupling is that of total reflection from a two-channel

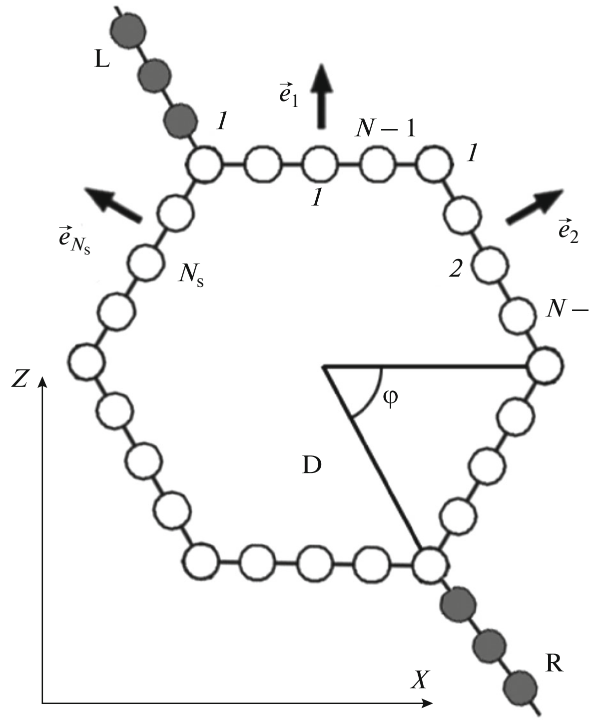

Fig. 1. Geometry and numbering of sites of a regular polygon-shaped chain with symmetrically placed contacts.

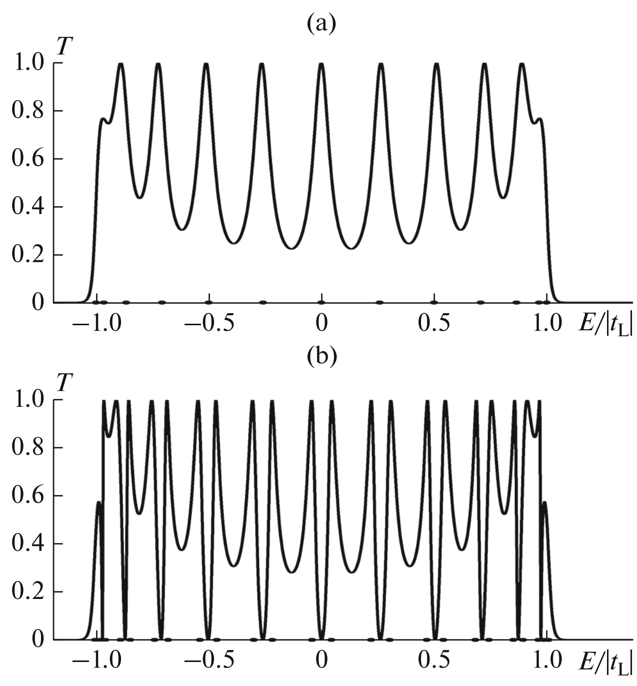

Fig. 2. Transmission coefficient for a regular polygon-shaped chain. $t_L = t_R = -1$; $t_D = 0.5$; $t_{LD} = t_{RD} = -0.5$; $N_s = 6$; and $N = 5$. Top, a chain without spin-orbit coupling; bottom, $\alpha_D = 0.08$. The black dots show the energies of one-electron eigenstates in the chain.

symmetric device at the critical spin-orbit coupling constant values. This effect is illustrated in Fig. 3, which shows the dependence of the transmission coefficient at a specified incoming electron energy on value χ, i.e., the ratio between the polygon side length and characteristic spin-orbit coupling length. The energy parameters of the device change such that the chain conduction band width remains invariable.

A key factor in describing this effect is the expression for the ratio between the expansion coefficients of wave function (2) on the sides connected to the contacts:

$$z_{R\sigma}^{mls} = i(-1)^l \sigma z_{L\bar{\sigma}}^{mls}. \tag{7}$$

It can be seen that this ratio depends only on the evenness of the orbital number and is independent of quantum numbers s and m. If the states with the same quantum number s and different evenness of the orbital number correspond to the same energy E_{mls}, Eqs. (5) can in this case be reduced to the form

$$\begin{gathered}(E_{mls} - E)(w_{mls} - w_{m'l's}) = 2t_{RD}e^{ik_R}\sum_{\sigma} t_\sigma z_{R\sigma}^{mls*}, \\ -t_R t_\sigma + \sum_{mls}{}' t_{RD}(w_{mls} - w_{m'l's}) z_{R\sigma}^{mls} = 0,\end{gathered} \tag{8}$$

where the states with set of quantum numbers (mls) and ($m'l's$) have the same energy E_{mls} and summation with the prime marks is assumed to be done over the pairs of such states. The transmission coefficient in this case is reduced to zero over the range of energies. The value of spin-orbit coupling at which the above condition is met is determined by the equation

$$\cos\chi = \cos(p\varphi)/\cos(\varphi/2), \tag{9}$$

where p is an integer. It can be seen that in the range of $0 \le \chi < 2\pi$, there are ($N_s - 2$) values that correspond to the case when no current is transmitted through the device (Fig. 3).

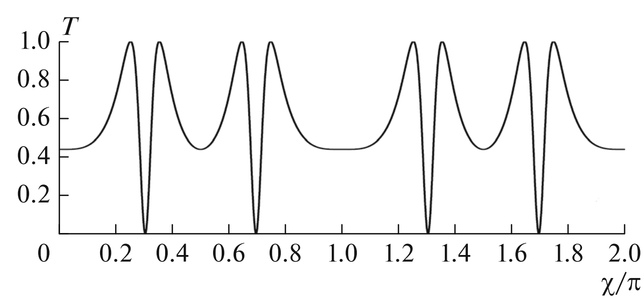

Fig. 3. Dependence of the transmission coefficient for a regular polygon-shaped chain on χ at a fixed chain conduction band width. $t_L = t_R = -1$; $t_{LD} = t_{RD} = -0.5$; $N_s = 6$; $N = 5$; incoming electron energy $E = -0.7$. The zero transmission coefficient in the plot corresponds to the total reflection of electrons from the device.

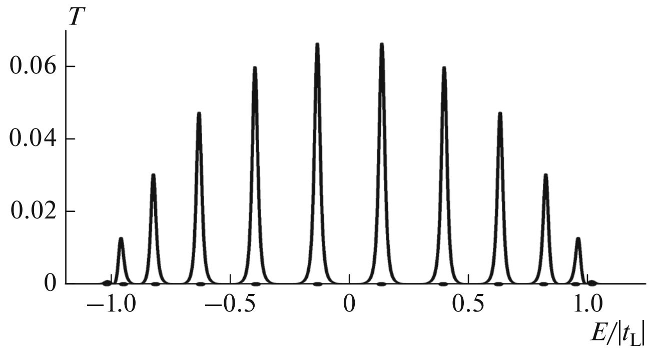

Fig. 4. Transmission coefficient of a regular polygon-shaped chain near the critical spin-orbit coupling constant value. $t_L = t_R = -1$; $t_D = 0.5$; $t_{LD} = t_{RD} = -0.5$; $\alpha_D = 0.12$; $N_s = 6$; and $N = 5$. The black dots show the energies of one-electron states in the chain.

When the spin-orbit coupling constant is close to the critical value, the above considerations remain valid throughout the range of energies, except for the vicinities of the eigenenergies of excitations in a chain. This leads to a situation where only electrons with energies in the narrow ranges near the intrinsic one-electron excitations will be transmitted through the device (Fig. 4). The transmission coefficient in this case changes rapidly upon varying the spin-orbit coupling value, which can be controlled by applying an electric field [8]. This allows the proposed class of systems to be used in microelectronic devices.

CONCLUSIONS

It was shown by the example of a regular polygon-shaped chain that Rashba spin-orbit coupling in combination with fermion path nonanalyticity points leads to size Fano antiresonance in symmetric two-channel systems. At the critical spin-orbit coupling constants determined by the geometry of a device, the interference of electron wave functions upon propagation along two channels results in the total reflection of electrons from it. The slight variation in the spin-orbit coupling constant caused by the change in the electric potential gradient near these critical values results in the narrow-band transmission of electrons by a system. The transmission coefficient in this case changes considerably upon minor variations in the Rashba spin-orbit coupling constant.

ACKNOWLEDGMENTS

The reported study was funded by Russian Foundation for Basic Research (project nos. 16-42-242036, 16-42-243056, and 17-42-240441), Government of Krasnoyarsk Territory, and Krasnoyarsk Region Science and Technology Support Fund to the research (project nos. 22/17, 24/17, and 02/17).

REFERENCES

1. Bychkov, Yu.A. and Rashba, E.I., *JETP Lett.*, 1984, vol. 39, p. 66.
2. Kane, C.L. and Mele, E.J., *Phys. Rev. Lett.*, 2005, vol. 95, p. 226801.
3. Magarill, L.I. and Entin, M.V., *JETP Lett.*, 2014, vol. 100, p. 639.
4. Lee, M., Khim, H., and Choi, M.-S., *Phys. Rev. B*, 2014, vol. 89, p. 035309.
5. Seibold, G., Caprara, S., Grilli, M., and Raimondi, R., *J. Magn. Magn. Mater.*, 2017, vol. 400, p. 63.
6. Val'kov, V.V. and Fedoseev, A.D., *J. Magn. Magn. Mater.*, 2017, vol. 400, p. 185.
7. Val'kov, V.V. and Aksenov, S.V., *J. Exp. Theor. Phys.*, 2011, vol. 113, p. 266.
8. Nitta, J., Akazaki, T., and Takayanagi, H., *Phys. Rev. Lett.*, 1997, vol. 78, p. 1335.

Translated by E. Bondareva