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The nonuniform spin polarization in the square-shaped 1D wire induced by spin–orbit coupling

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ABSTRACT

It is shown that the Rashba spin–orbit coupling induces the spatially nonuniform spin state in the square-shaped 1D wire. The electron states of this type are characterized with spin orientation changing according to the harmonic motion along the square side. The period of the oscillation is determined only by the spin–orbital coupling and the hopping parameters ratio. The modulation of spin orientation is caused by step-like changing of Rashba field direction. The obtained results were generalized on the case of polygon-shaped wire.

1. Introduction

The low dimensional systems are of great interest because of their topological insulator properties [1–4]. Amongst other issues, the edge states in such systems are characterized by the strong correlation between the spin direction and the direction of electron propagation. It leads to the possibility of fermion propagation without scattering on nonmagnetic impurities.

The points of fermion path non-analyticity, leading to the step-like changing of the Rashba field orientation, are usually ignored in the investigation of the Rashba spin–orbit coupling [5] influence on the properties of low dimensional systems. The properties of edge states are investigated in the systems infinite in one direction [6,7]. The possibility to extend the conclusions obtained in such analysis on the spatially limited systems, which have the points of fermion path analyticity violation, is a point of discussion. In this connection, it should be noted that the authors of the paper [8] emphasized the importance of the investigation of square-shaped systems, but the detailed research of the influence of corners on the spin-polarized states have not been provided yet.

It was shown earlier in Ref. [9] that the Rashba spin–orbit coupling may lead to the spin symmetry violation in the topological insulators. In this case the quasi-particle state cannot be classified according to spin projection and the effect of symmetry violation manifests as the changing of spin orientation with the propagation. Meanwhile, the authors of Ref. [9] did not take into account the corners and the spin oscillations which are assumed to be dependent on the wave vector.

Neglecting the presence of corners in the system can be a good approximation, if the electron mean free path is much less than the system side length. But in the case of nano-scaled systems this kind of approach may be incorrect. The objective of this article is to investigate the influence of the corners on the properties of spin-polarized states on the example of square-shaped wire.

2. The model Hamiltonian

Let us consider the square-shaped 1D wire (Fig.1) with N sites on each side placed on the substrate. The Hamiltonian of the system is given by

$$\begin{aligned}\widehat{\mathcal{H}} = &-t\sum_{n=1,j\sigma}^{N-1} c^{+}_{jn+1\sigma}c_{jn\sigma} - t\sum_{j\sigma} c^{+}_{j+1,1\sigma}c_{j,N-1\sigma}\\ &- i\alpha\sum_{n=1,j\sigma\sigma'}^{N-1} \vec{e}_j\vec{\tau}_{\sigma'\sigma}c^{+}_{jn+1\sigma'}c_{jn\sigma}\\ &- i\alpha\sum_{j\sigma\sigma'} \vec{e}_j\vec{\tau}_{\sigma'\sigma}c^{+}_{j,1\sigma'}c_{j+1,N-1\sigma} + h.\,c.\end{aligned} \quad (1)$$

Here the first two components describe the nearest neighbor hopping with the parameter $t > 0$, the next two components describe the Rashba spin–orbit coupling caused by the gradient of electric potential oriented perpendicular to the plane of the square. The $j = \text{I, II, III, IV}$ numerates the side of the square (in clockwise direction), $n = 1,\ldots,N-1$ numerates the sites along every side, α is a Rashba spin–orbit coupling constant, $\vec{\tau}$ – Pauli matrices, $\sigma = \pm 1$ – the spin projection in the z direction, $\vec{e}_j$ – a unity vector along the Rashba field (Fig. 1). It is important that this direction is different for each side of the square: the Rashba field vector lies in the plane of the square and oriented perpendicular to its sides.

The one-electron eigenstates of (1) are written in the form:

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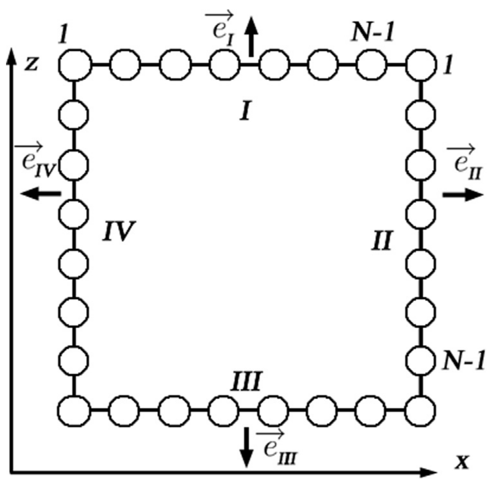

Fig. 1. The geometry and sites numeration in the case of wire, folded in the square form.

$$\psi = \sum_{n=1,\sigma,j}^{N-1} u_{n\sigma}^{j} c_{jn\sigma}^{+}|0\rangle, \tag{2}$$

where $|0\rangle$ is a vacuum state. The studied system has the symmetry axis C_4 that is oriented perpendicular to the square plane and crossing its center, so the wave functions of the one-electron states can be the eigenstates of the $\pi/2$ rotation operator U:

$$U\psi = e^{-i\phi_l}\psi.$$
$$U\psi = \frac{1}{\sqrt{2}} \sum_{jn\sigma} u_{n\sigma}^{j} [c_{(j+1)n\sigma}^{+} - \sigma c_{(j+1)n\bar{\sigma}}^{+}]|0\rangle. \tag{3}$$

Taking into account the spinor property $U^4\psi = -\psi$, the relation between the coefficients (2) can be described in the form:

$$u_{n\sigma}^{j+1} = \frac{e^{-i\phi_l}}{\sqrt{2}} [u_{n\sigma}^{j} - \sigma u_{n\bar{\sigma}}^{j}], \quad \phi_l = \frac{\pi}{2} l + \frac{\pi}{4}, \tag{4}$$

where $l = -2, -1, 0, 1$ is the orbital number.

The coefficients in the expansion (2) are found from the Shrödinger equation. According to the above-mentioned symmetry, it is enough to solve the general equation on the side I and the equations on the right edge of side I and the left edge of side II. The general equation and its solution are

$$\varepsilon u_{n\sigma}^{I} = -(t - i\alpha\sigma)u_{n+1\sigma}^{I} - (t + i\alpha\sigma)u_{n-1\sigma}^{I},$$
$$u_{n\uparrow}^{I} = e^{ik_0(n-1)}[A_1 e^{-ik(n-1)} + A_2 e^{ik(n-1)}],$$
$$u_{n\downarrow}^{I} = e^{-ik_0(n-1)}[A_3 e^{-ik(n-1)} + A_4 e^{ik(n-1)}],$$
$$\varepsilon_k = -2\sqrt{t^2 + \alpha^2}\cos k. \tag{5}$$

where k_0 is the important parameter describing the shift of dispersion curve along the wave vector axis for the different projections of spin

$$k_0 = \arcsin(\alpha/\sqrt{t^2 + \alpha^2}). \tag{6}$$

In general, the wave vector k in the expression (5) may be imaginary and can provide the existence of edge states on the corners of the square.

The unknown parameters in the expression (5) are found from the boundary conditions described by the equations at the edges of the sides:

$$\varepsilon u_{N-1\sigma}^{\mathrm{I}} = -(t - i\alpha\sigma)u_{1\sigma}^{\mathrm{II}} - (t + i\alpha\sigma)u_{N-2\sigma}^{\mathrm{I}},$$
$$\varepsilon u_{1\sigma}^{\mathrm{II}} = -tu_{2\sigma}^{\mathrm{II}} + i\alpha u_{2\bar{\sigma}}^{\mathrm{II}} - (t + i\alpha\sigma)u_{N-1\sigma}^{\mathrm{I}}. \tag{7}$$

Taking into the account that the coefficients are the solutions of general equations (5) the expressions (7) can be rewritten in the simple form:

$$u_{N\sigma}^{\mathrm{I}} = u_{1\sigma}^{\mathrm{II}},$$
$$(t + i\alpha\sigma)u_{N-1\sigma}^{\mathrm{I}} = tu_{0\sigma}^{\mathrm{II}} + i\alpha u_{0\bar{\sigma}}^{\mathrm{II}}. \tag{8}$$

These equations correspond to the continuity condition for the wave function in the continual limit. The coefficients $u_{N\sigma}^{\mathrm{I}}$ and $u_{0\sigma}^{\mathrm{II}}$ are the solutions of general equation (5), which do not enter the expansion (2).

The allowed values of wave vector k are determined by three quantum numbers:

$$k_{lms} = \frac{1}{N-1}\left[s\cdot\arccos\left(\frac{\cos\chi}{\sqrt{2}}\right) + \phi_l + 2\pi m\right],$$
$$l = -2, -1, 0, 1, \quad s = \pm 1, \quad m = 1, \ldots, (N-1),$$
$$\chi = k_0(N-1). \tag{9}$$

One can see that for each allowed k with quantum number $s = +1$ exists the allowed wave vector $-k$ with $s = -1$. All $8(N-1)$ values of k are real, that is why no evanescent states appear in the wire.

The coefficients on the side I of the square take the form:

$$u_{n\uparrow}^{I} = \frac{1}{2\sqrt{N-1}} \frac{1}{\sqrt{1+\rho^2}} e^{ik_0(n-n_c) - is\pi/4} e^{-ikn},$$
$$u_{n\downarrow}^{I} = \frac{1}{2\sqrt{N-1}} \frac{\rho}{\sqrt{1+\rho^2}} e^{-ik_0(n-n_c) + is\pi/4} e^{-ikn}. \tag{10}$$

where ρ is a real positive value

$$\rho = \sqrt{1 + \sin^2\chi} - s\sin\chi. \tag{11}$$

Here the value $n_c = (N+1)/2$ corresponds to the center of the side.

3. The changing of spin orientation along the square side

The mean value of spin vector on the n site of side I for stationary one-electron state is described by the expression

$$\vec{S}_n = \frac{1}{2}\cdot\psi^* \sum_{\sigma\sigma'} \vec{\tau}_{\sigma'\sigma} c_{In\sigma'}^{+} c_{In\sigma}\psi = \frac{1}{2}\cdot A\cdot\vec{s}_n,$$

where $A = 1/4(N-1)$ is the probability of the particle to be found on site n and $\vec{s}_n$ is a unity vector along the spin direction:

$$s_{nx} = s\sin\gamma\sin 2k_0(n - n_c),$$
$$s_{ny} = s\sin\gamma\cos 2k_0(n - n_c),$$
$$s_{nz} = s\cos\gamma. \tag{12}$$

These expressions describe the rotation of quasi-particle spin around the Rashba field direction with the frequency equal to $2k_0$ (6) along the cone (Fig. 2) with the aperture

$$2\gamma = 2\arccos\left(\frac{\sin\chi}{\sqrt{1+\sin^2\chi}}\right). \tag{13}$$

The orientation of spin on each side is not influenced by the quantum numbers, l and m, and depends only on the quantum number s which corresponds to the spin projection on the Rashba field direction. According to (12) the physical meaning of the value χ (9)

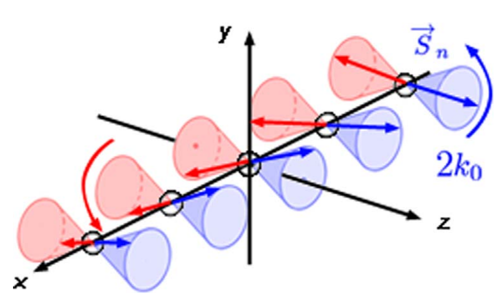

Fig. 2. The quasi-particle spin rotation with the growing of number n of site along the side I.

is a half of the spin rotation angle around the Rashba field direction while the quasi-particle propagates from the first to the last site on one side.

It is useful to compare the obtained states with the ones in the straight wires with various boundary conditions. In the case of N-site wire with periodic boundary conditions (infinite wire with translation symmetry in the case of $N\to\infty$) each energy is twofold degenerated and a pair of states with the same energy has the form:

$$\begin{aligned}&1.\quad u_{n\uparrow}=\frac{1}{\sqrt{N}}e^{-ik_m n},\quad u_{n\downarrow}=0,\quad k_m=2\pi m/N\\&2.\quad u_{n\downarrow}=\frac{1}{\sqrt{N}}e^{ik_m n},\quad u_{n\uparrow}=0,\quad m=1,\ldots,N\\&\varepsilon=-2\sqrt{t^2+\alpha^2}\cos(k_m+k_0).\end{aligned}\tag{14}$$

One-electron states are a pair of plane waves propagating in opposite directions and with oppositely orientated spins.

In the case of square-shaped wire, each of the eigenstates with the same twofold degenerated energy is also a pair of modified plane waves. The spins of quasi-particles are also opposite while the particles propagate along the wire in opposite directions. In this respect they are similar to the eigenstates in the wire with periodic boundary conditions.

The first difference is the essential decrease of the spin projection onto the Rashba field direction, $0\le|s_z|\le 1/\sqrt{2}$, instead of $|s_z|=1$ for the infinite wire. The second feature is the changing of spin direction with the frequency equal to $2k_0$, which does not depend on neither quasi-particle velocity nor on square size but depends only on the ratio between spin–orbital and hopping parameters α/t.

The solutions in the case of the straight unbound wire of length N are:

$$\begin{aligned}&1.\quad u_{n\uparrow}=\sqrt{\frac{2}{N+1}}e^{ik_0 n}\sin k_m n,\ u_{n\downarrow}=0,\\&2.\quad u_{n\downarrow}=\sqrt{\frac{2}{N+1}}e^{-ik_0 n}\sin k_m n,\quad u_{n\uparrow}=0,\\&\varepsilon=-2\sqrt{t^2+\alpha^2}\cos k_m,\quad k_m=\pi m/(N+1)\end{aligned}\tag{15}$$

Each solution is the superposition of two plane waves propagating in opposite directions with codirectional spins due to the internal reflection on the edge sites. The eigenstates in the square are also the superposition of two waves but they propagate in the same direction and have opposite projection of spins.

4. The regular polygon-shaped wire

One can generalize the above investigated model to the case of arbitrary numbers of sides N_s. Such a model has a symmetry axes C_{N_s} and a polygon is invariant to the rotation on angle $\phi=2\pi/N_s$. Using the above described technique we obtained the generalization of the expression for allowed wave vectors (9):

$$\begin{aligned}&k_{lms}=\frac{1}{N-1}[s\arccos(\cos(\phi/2)\cos\chi)\\&\qquad+(2l+1)\phi/2+2\pi m].\\&m=1,\ldots,N-1,\quad l=1,\ldots,N_s,\quad s=\pm1,\\&\phi=2\pi/N_s,\quad \chi=k_0(N-1),\end{aligned}\tag{16}$$

The coefficients in the expansion (2) take the form

$$\begin{aligned}&u_{n\uparrow}=\frac{1}{\sqrt{N_s(N-1)}}\frac{1}{\sqrt{1+\rho^2}}e^{ik_0(n-n_c)-is\pi/4}e^{-ikn},\\&u_{n\downarrow}=\frac{1}{\sqrt{N_s(N-1)}}\frac{\rho}{\sqrt{1+\rho^2}}e^{-ik_0(n-n_c)+is\pi/4}e^{-ikn},\\&\rho=[\sqrt{\sin^2(\phi/2)+\cos^2(\phi/2)\sin^2\chi}-\\&\quad -s\cos(\phi/2)\sin\chi]/\sin(\phi/2).\end{aligned}\tag{17}$$

The changing of quasi-particle spin orientation is described by harmonic motion as in the case of square-shaped wire:

$$\begin{aligned}&s_{nx}=s\frac{\sin(\phi/2)\sin 2k_0(n-n_c)}{\sqrt{\sin^2(\phi/2)+\cos^2(\phi/2)\sin^2\chi}},\\&s_{ny}=s\frac{\sin(\phi/2)\cos 2k_0(n-n_c)}{\sqrt{\sin^2(\phi/2)+\cos^2(\phi/2)\sin^2\chi}},\\&s_{nz}=s\frac{\cos(\phi/2)\sin\chi}{\sqrt{\sin^2(\phi/2)+\cos^2(\phi/2)\sin^2\chi}},\end{aligned}\tag{18}$$

It is useful to investigate the model in the case of $N_s\to\infty$, N=2, corresponding to the ring-shaped wire. The solutions in this case take the form:

$$\begin{aligned}&u_{ns}(l,s)=\frac{1}{\sqrt{N_s}}e^{-isk_l j}\cos\frac{\pi(j-1)}{N_s},\\&u_{n\bar{s}}(l,s)=s\frac{1}{\sqrt{N_s}}e^{-isk_l j}\sin\frac{\pi(j-1)}{N_s},\\&k_l=2\pi l/N_s+\pi/N_s,\ l=1,\ldots,N_s,\\&\varepsilon_k=-2\sqrt{t^2+\alpha^2}\cos(k_0+k_l),\\&s_{nx}=s\sin\frac{2\pi(j-1)}{N_s},\quad s_{ny}=0,\quad s_{nz}=s\cos\frac{2\pi(j-1)}{N_s},\end{aligned}\tag{19}$$

where $j=1,\ldots,N_s$ numerates all sites of the ring. One should use the local axes with the z'-axis orientated in the Rashba field direction to make the expression (19) more clear:

$$\begin{aligned}&u_{ns}(l,s)=\frac{1}{\sqrt{N_s}}e^{-isk_l j},\quad u_{n\bar{s}}(l,s)=0,\\&s_{nz'}=s,\quad s_{nx'}=s_{ny}=0.\end{aligned}\tag{20}$$

It should be expected that the solutions (20) coincide with the ones in the case of straight wire with periodical boundary conditions (14) with the additional term in k_l due to the spinor rotation. This result appears because there is no step-like changing of the Rashba field orientation in this limit.

Another limit is the case N_s=2 corresponding to the flattened ring: two lines with two intersection points. While this limit is unphysical it clarifies that the obtained results are the consequence of the presence of corners in the system but not of the used method. The solutions in this limit have the form:

$$\begin{aligned}&u_{n\uparrow}=\frac{1}{2\sqrt{(N-1)}}e^{ik_0(n-n_c)-is\pi/4}e^{-ik_m n},\\&u_{n\downarrow}=\frac{1}{2\sqrt{(N-1)}}e^{-ik_0(n-n_c)+is\pi/4}e^{-ik_m n},\\&k_m=\frac{\pi m}{N-1},\ m=1,\ldots,2(N-1),\\&\varepsilon_k=-2\sqrt{t^2+\alpha^2}\cos k_m,\\&s_{nx}=s\sin 2k_0(n-n_c),\\&s_{ny}=s\cos 2k_0(n-n_c),\quad s_{nz}=0,\end{aligned}\tag{21}$$

where the quantum number l is included in m.

The solutions for the straight wire with periodical boundary conditions also can be classified as the eigenstate of rotation operator C_2:

$$\begin{aligned}&u_{n\uparrow}=\frac{1}{\sqrt{2N}}e^{-ik_m n-is\pi/4},\quad u_{n\downarrow}=\frac{1}{\sqrt{2N}}e^{ik_m n+is\pi/4},\\&k_m=\frac{2\pi m}{N},\ m=1,\ldots,N,\\&\varepsilon_k=-2\sqrt{t^2+\alpha^2}\cos(k_0+k_m),\\&s_{nx}=s\sin 2k_m n,\quad s_{ny}=s\cos 2k_m n,\quad s_{nz}=0.\end{aligned}\tag{22}$$

While the expressions (21) and (22) are similar they have a significant difference. The oscillation frequency in the case of system without corners depends on the wave vector k_m, and, consequently, on the quasi-particle energy. In contrast to this, the oscillation frequency in the case of system with corners depends only on the ratio between spin–orbital coupling and hopping parameters and is the same for all one-particle solutions.

5. Conclusions

It was shown in the article that in the case of system with non-analyticity points of fermion paths the Rashba spin–orbit coupling induces one-electron states with spatially nonuniform spin orientation. The Shrödinger equation was solved and exact wave functions were obtained in the case of square-shaped wire in the nearest neighbor approximation. It was found that in the wire under investigation the spin oscillations appear with the frequency depending on the ratio between the spin–orbit coupling and hopping parameters and not depending on wire length and particle energy, in contrast to the case of the straight wire with periodical boundary conditions. The presence of the corners in such a system provides the dependence of spin projection on the oscillation frequency and square side length. The extension of the model to the case of regular polygon-shaped wire has been carried out.

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