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Singularity of the Density of States and Transport Anisotropy in a Two-Dimensional Electron Gas with Spin-Orbit Interaction in an In-Plane Magnetic Field

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Abstract—A two-dimensional electron gas with spin-orbit interaction in an in-plane magnetic field is known to form an anisotropic system with a van Hove singularity of the density of states controlled by a magnetic field. Tensors of the conductivity and spin susceptibility that determine the Edelstein effect for this system are studied. It is established that the conductivity and spin susceptibility have sharp singularities that appear in the process of varying the magnetic field or the Fermi level position when the Fermi level passes through the singularity point.

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1. INTRODUCTION

Low-dimensional electron systems with spin-orbit interaction (SOI) cause exceptionally strong interest associated with a multitude of new physical effects [1, 2], many of which also have large practical value [3–5]. Two-dimensional (2D) systems, in which SOI can be controlled by an external field, attract the greatest attention [2]. This study is devoted to effects appearing in a 2D electron gas (EG) with SOI in the presence of an in-plane magnetic field, which apparently leads to anisotropy of the electron spectrum and, correspondingly, to transport anisotropy. The interest in such an anisotropic system is caused by two reasons. First, it models the anisotropy of the electron system with SOI appearing due to strong electron-electron interaction without an external magnetic field [6], but in contrast with it, it admits the relatively simple solution. Second, the transport in an in-plane magnetic field has recently become an important tool of the experimental investigation of 2D electron systems with strong SOI.

In addition, a two-dimensional electron gas in strong SOI conditions is still investigated insufficiently, and new peculiarities have been recently revealed. For example, recent theoretical investigations of the conductivity of 2D EG with SOI showed that the conductivity (G) has an unusual dependence on electron density n, when it is low, so that only the

bottom spin subband is filled, while at a higher density, it acquires the usual Drude form [7]:

$$G = \frac{e^2 n \tau_0}{2m} \begin{cases} \frac{n^3}{3} + \frac{n}{n_0}, & n \le n_0, \\ 2, & n \ge n_0, \end{cases}$$
(1)

where τ_0 is the characteristic scattering time in the absence of SOI; *m* is the effective mass; $n_0 = E_{so}/(\pi\hbar^2)$ is the concentration at the Fermi level, when it coincides with the Dirac point, below which there is only one spin subband; $E_{so} = \alpha^2 m/(2\hbar^2)$ is the characteristic SOI energy; and α is the Rashba constant.

Calculations of the spin polarization appearing in the presence of an electric field along the 2D layer (the Edelstein effect [8]) show that the spin polarization rises proportionally to the Fermi energy below the Dirac point and reaches saturation above it [9].

The conductivity and spin polarization of 2D EG with SOI in the presence of an in-plane magnetic field was barely studied (especially in the region of low concentrations $n < n_0$), although we can expect the appearance of nontrivial features associated with the van Hove singularity of the density of states. We recently established [10] that the latter is present at an energy below the Dirac point. The singularity has a logarithmic character. It is formed due to the presence of a magnetic field from the root singularity of the density of states occurring in the energy minimum of 2D EG with SOI for zero magnetic field, $N(E) \propto (E + E_{so})^{-1/2}$. The singularity point corresponding to the

saddle point in k space shifts from the band bottom to the Dirac point when the magnetic field in increased, and finally disappears. This interesting feature opens up new possibilities for experimental investigation into the spectrum of systems with strong SOI by scanning the magnetic field and measuring the transport characteristics.

In this article, we present the results of studying the conductivity and spin polarization in the Edelstein effect for 2D EG with the Rashba SOI in an in-plane magnetic field.

2. PROBLEM STATEMENT AND METHODS

The Hamiltonian of 2D EG with the Rashba SOI in a magnetic field **B** directed along axis x has the form

$$H = \frac{p^2}{2m}\sigma_0 + \frac{\alpha}{\hbar}(p_x\sigma_y - p_y\sigma_x) - b_l\sigma_x, \qquad (2)$$

where $\mathbf{p} = (p_x, p_y)$ is the electron pulse; σ_x and σ_y are the Pauli matrices; $b_1 = (g^*/2)\mu_B B$, g^* is the effective *g*-factor, which is assumed isotropic and independent of the magnetic field, and μ_B is the Bohr magneton. The vector potential is selected in the calibration $\mathbf{A} = (0, 0, yB)$, at which the pulse coincides with the generalized pulse.

The dispersion law and wave eigenfunctions for this Hamiltonian in dimensionless notations have the form

$$E_{\lambda}(\mathbf{k}) = k^2 + 2\lambda\sqrt{k^2 + 2kb\sin\phi + b^2}, \qquad (3)$$

$$\Psi_{\lambda}(\mathbf{k}) = \frac{1}{\sqrt{2A}} \begin{pmatrix} 1\\ i\lambda e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)}, \qquad (4)$$

where the wave vector $\mathbf{k} = k(\cos\phi, \sin\phi)$ is normalized to $k_{so} = \alpha m/\hbar^2$, the energy is normalized to E_{so} and the dimensionless magnetic field $b = (g^*/2)\mu_B B/\alpha k_{so}$ is introduced, $\lambda = \pm 1$ is the spin index, and A is the sample area. Angle ϕ determines the spin orientation, and it is associated with ϕ by the relationship:

$\tan \varphi = (k \sin \phi + b)/(k \cos \phi).$

To find the conductivity and polarization in the presence of an electron current, it is necessary to calculate the distribution function $f_{\lambda}(\mathbf{k}, \varepsilon)$. For this purpose, let us use the quasi-classical Boltzmann kinetic equation [11]:

$$-e\mathscr{E}\mathbf{v}_{\lambda}(-\partial_{\varepsilon}f_{0}) = \sum_{\lambda'} \frac{d^{2}k'}{(2\pi)^{2}} W_{\lambda\lambda'}(\mathbf{k},\mathbf{k}')$$

$$\times [f_{\lambda}(\mathbf{k},\mathscr{E}) - f_{\lambda'}(\mathbf{k}',\mathscr{E})],$$
(5)

where \mathscr{E} is the strength of the electric field directed at angle θ to axis x, $\mathscr{E} = \mathscr{E}(\cos\theta, \sin\theta)$, the magnitude of

 \mathscr{C} is normalized to $E_{so}k_{so}/e$, $\mathbf{v}_{\lambda}(\mathbf{k})$ is the group velocity, and f_0 is the equilibrium distribution function.

For simplicity's sake, let us consider the case when scattering occurs at impurities with the short-range potential $V(\mathbf{r}) = V_0 \delta(\mathbf{r})$ and is elastic. This assumption is not fundamental for qualitative evaluation of the behavior of the responses that we calculate. The probability of electron transitions in the Born approximation has the form

$$W_{\lambda\lambda'}(\mathbf{k},\mathbf{k}') = R|\langle \mathbf{k}',\lambda'|V/V_0|\mathbf{k},\lambda\rangle|^2 \delta(E_{\mathbf{k},\lambda} - E_{\mathbf{k}',\lambda'}), \quad (6)$$

where $R = n_i V_0^2 k_{so}^2 / (2\pi E_{so}^2)$ and n_i is the concentration of scattering impurities.

When integrating over **k** in Eq. (5), we should keep in mind that there are two Fermi contours in **k**-space at any energy both above the Dirac point and below the singularity point. In the first case, the two contours refer to states with different spin indices, while two closed contours for states with $\lambda = -1$ occur in the second case. There is one singly connected contour in the energy range above the singularity point and below the Dirac point, but in this case there are also two values of **k** in a definite range of *E*. We note that it follows from (3) that the Dirac point has coordinates (0, *b*) in **k**-space and corresponds to energy b^2 . The variations in the Fermi contour in the magnetic field are presented in more detail in [10].

An important feature of the problem under consideration is the fact that the collision integral cannot be simplified under anisotropy conditions by introducing an effective scattering time [12]. Even the use of the so-called two-time approximation [13, 14] leads to erroneous results. Following [12], we solve the kinetic equation (5) precisely without using approximation of the relaxation time.

Taking into account scattering elasticity, let us represent the solution of Eq. (5) at the Fermi contours in the form

$$\Delta f_{\lambda} = f_{\lambda}(\phi, \theta) - f_{0}$$

$$e \mathscr{C} \partial_{E} f_{0} v_{\lambda}(\phi) [a_{\lambda}(\phi) \cos \theta + b_{\lambda}(\phi) \sin \theta],$$
(7)

where $v_{\lambda}(\phi)$ is the magnitude of the group velocity at the corresponding contour $v_{\lambda}(\mathbf{k}) = v_{\lambda}(\phi)(\cos\xi_{\lambda}, \sin\xi_{\lambda})$, while $\xi_{\lambda}(\phi)$ is the angle determining its direction.

The presence of the δ function in Eq. (6) allows us to perform the integration over k in Eq. (5) so that integrals only over angle ϕ for the corresponding Fermi contours remain in it. This results in two independent sets of equations for quantities a_{λ} and b_{λ} :

$$\begin{cases} \cos \xi_{\pm} = \bar{W}_{\pm} a_{\pm}(\phi) - \int d\phi' \left[\frac{v_{\pm}(\phi')}{v_{\pm}(\phi)} W_{\pm\pm}(\phi, \phi') a_{\pm}(\phi') + \frac{v_{\pm}(\phi')}{v_{\pm}(\phi)} W_{\pm\mp}(\phi, \phi') a_{\mp}(\phi') \right], \\ \sin \xi_{\pm} = \bar{W}_{\pm} b_{\pm}(\phi) - \int d\phi' \left[\frac{v_{\pm}(\phi')}{v_{\pm}(\phi)} W_{\pm\pm}(\phi, \phi') b_{\pm}(\phi') + \frac{v_{\pm}(\phi')}{v_{\pm}(\phi)} W_{\pm\mp}(\phi, \phi') b_{\mp}(\phi') \right]. \end{cases}$$

$$\tag{8}$$

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Here,

$$W_{\lambda,\lambda'}(\phi,\phi') = \int_{0}^{\infty} dk' k' W_{\lambda \mathbf{k},\lambda'\mathbf{k}'}$$
⁽⁹⁾

$$= \frac{R}{2} \left[\frac{k^{2} \{1 + \lambda \lambda' \cos[\varphi_{\lambda}(\phi) - \varphi_{\lambda'}(\phi')]\}}{|\mathbf{k}' \nabla_{\mathbf{k}'} E_{\lambda}(\mathbf{k}')|} \right]_{k' = k_{\lambda'}(\phi)}$$

and

$$\overline{W}_{\lambda} = \sum_{\lambda'} d\phi' W_{\lambda,\lambda'}(\phi,\phi') = \sum_{\lambda'} W_{\lambda'}, \qquad (10)$$

where the spin orientation angle $\phi_{\lambda}(\phi)$ is determined by relationship

$$\tan \varphi_{\lambda}(\phi) = \frac{k_{\lambda}(\phi)\sin\phi + b}{k_{\lambda}(\phi)\cos\phi},$$
(11)

calculated at the Fermi contour.

Equations (8) are solved exactly. In this article, we present the results of numerical solution obtained on the grid by angle ϕ for each contour. A nontrivial aspect is the circumstance that the determinant of the formed set of linear equations equals zero, and the rank of the extended matrix of the set equals the determinant rank, and this rank is smaller than the dimensionality of the angular grid by unity. This fact means that an additional equation should be used to solve the set of equations. It is evident that this equation should be derived from the condition of conservation of the number of particles, which coincides with the electroneutrality condition of the system in this case.

At the first it is useful to consider the case of a zero magnetic field and attain an agreement of results found according to the procedure proposed here with those known from publications. Set of Eqs. (8) is substantially simplified at zero magnetic field because the group velocity v_{\pm} = const because of the axial symmetry of the Fermi contours. Finally, we come to the following expression for the distribution function:

$$\nabla f_{\pm}(\phi, 0) = ev_{\pm} \mathscr{E} \partial_E f_0 \frac{2W_{\pm}}{\left(W_{+} + W_{-}\right)^2} \times \cos(\theta - \phi) \begin{cases} \pm 1 & \text{at } E_{\rm F} < 0, \\ 1 & \text{at } E_{\rm F} > 0. \end{cases}$$
(12)

Here, coefficients W_{\pm} depend only on the Fermi-level position (or the electron concentration):

$$W_{\pm} = \frac{1}{2\tau_0} \begin{cases} \frac{1 \pm \sqrt{E_{\rm F} + 1}}{\sqrt{E_{\rm F} + 1}}, & -1 \le E_{\rm F} \le 0, \\ \frac{\sqrt{E_{\rm F} + 1} \pm 1}{\sqrt{E_{\rm F} + 1}}, & E_{\rm F} > 0, \end{cases}$$
(13)

where $\tau_0 = \hbar/RE_{so}$.

The conductivity calculated using expression (12) for the nonequilibrium distribution function coincides with the result found previously in [7] using the Kubo

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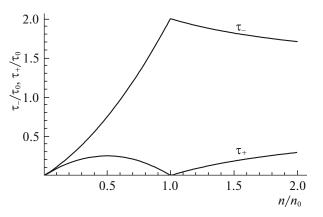


Fig. 1. Scattering times τ_+ and τ_- for two Fermi contours at zero magnetic field depending on the electron concentration *n*. The indices \pm correspond to the spin indices $\lambda = \pm 1$ at $n > n_0$. The indices \pm correspond to two Fermi contours with $\lambda = -1$ for region $n < n_0$.

formula and presented by Eq. (1). The spin polarization also agrees with that found in [8].

The new result, to which our approach leads, is a correct determination of the scattering time using relationships (12) and (13). We found that the set is described by two relaxation times τ_+ and τ_- , which refer to different contours of the Fermi surface: $\tau_{\pm} = 2W_{\pm}/(W_+ + W_-)^2$. They substantially differ by magnitude and, as shown in Fig. 1, have different dependence on the electron concentration.

3. MAIN RESULTS

Components of the conductivity tensor are expressed through functions $a_{\lambda}(\phi)$ and $b_{\lambda}(\phi)$ as follows:

$$G_{xx} = \sum_{\lambda} d\phi F_{\lambda}(\phi) a_{\lambda}(\phi) \cos \xi_{\lambda}(\phi), \qquad (14)$$

$$G_{xy} = \sum_{\lambda} d\phi F_{\lambda}(\phi) b_{\lambda}(\phi) \cos \xi_{\lambda}(\phi), \qquad (15)$$

$$G_{yx} = \sum_{\lambda} d\phi F_{\lambda}(\phi) a_{\lambda}(\phi) \sin \xi_{\lambda}(\phi), \qquad (16)$$

$$G_{yy} = \sum_{\lambda} d\phi F_{\lambda}(\phi) b_{\lambda}(\phi) \sin \xi_{\lambda}(\phi), \qquad (17)$$

where

$$F_{\lambda}(\phi) = \frac{v_{\lambda}^{2}(\phi)k_{\lambda}(\phi)}{\left|\left[\partial_{k}E_{\lambda}(k,\phi)\right]\right|_{k=k_{\lambda}(\phi)}}$$

Here, the conductivity is normalized to the quantity $G_0 = 2e^2/hR$.

It is not difficult to show from symmetry properties of the Fermi contours that nondiagonal elements of the conductivity tensor equal zero ($G_{xy} = G_{yx} = 0$). As for the diagonal components, they have a nontrivial

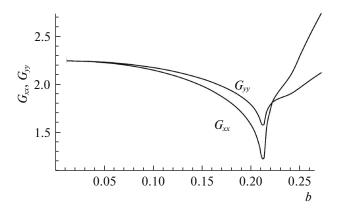


Fig. 2. Dependences of diagonal elements of the conductivity tensor on the magnetic field in the region of the Fermi energy below the Dirac point. Calculations are performed for the Fermi energy $E_{\rm F} = -0.6$.

magnetic-field dependence. It is characterized by the presence of an abrupt minimum in the conductivity at a specific magnetic field. The minimum appears because of the fact that the position of the Fermi level relative to the singularity point of the density of states varies upon varying the magnetic field. The minimum is attained when the Fermi level coincides with the singularity point. Herewith, strongest electron scattering occurs. The position of the conductivity minimum is determined by the condition

$$E_{\rm F} = -1 + 2b. \tag{18}$$

The magnetic-field dependence of diagonal components of the conductivity tensor is shown in Fig. 2 for the case when the Fermi energy is below the Dirac point. If the Fermi energy is above the Dirac point, the conductivity anisotropy is lacking.

Let us now consider the spin density **S** which forms due to an electron current. Density components S_i (i = x, y, z) are determined as follows:

$$S_{i} = \frac{\hbar}{2} \sum_{\lambda} \int \frac{d^{2}k}{4\pi^{2}} \langle \Psi_{\lambda,k}^{+} | \mathbf{\sigma}_{i} | \Psi_{\lambda,k} \rangle \nabla f_{\lambda}(\mathbf{k}).$$
(19)

The corresponding susceptibilities χ_{ij} are determined by the equation

$$S_i = \sum_j \chi_{ij} \mathscr{E}_j.$$
 (20)

Using Eqs. (22) and (12), we derive the following expressions for the spin susceptibility:

$$\chi_{xx} = \sum_{\lambda} \lambda \int d\phi S_{\lambda}(\phi) a_{\lambda}(\phi) \sin \phi_{\lambda}(\phi), \qquad (21)$$

$$\chi_{xy} = \sum_{\lambda} \lambda \int d\phi S_{\lambda}(\phi) b_{\lambda}(\phi) \sin \varphi_{\lambda}(\phi), \qquad (22)$$

$$\chi_{yx} = \sum_{\lambda} \lambda \int d\phi S_{\lambda}(\phi) a_{\lambda}(\phi) \cos \varphi_{\lambda}(\phi), \qquad (23)$$

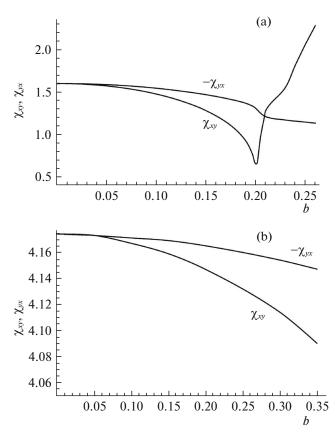


Fig. 3. Magnetic-field dependences of the elements of the tensor of spin susceptibility for the Fermi energy (a) below the Dirac point $E_{\rm F} = -0.6$ and (b) above the Dirac point $E_{\rm F} = 0.8$.

$$\chi_{yy} = \sum_{\lambda} \lambda \int d\phi S_{\lambda}(\phi) b_{\lambda}(\phi) \cos \varphi_{\lambda}(\phi).$$
(24)

Here, all components of the spin polarization are normalized to $e\alpha m\tau_0/h$, and the local density at the Fermi level is determined by the multiplier

$$S_{\lambda}(\phi) = \frac{v_{\lambda}(\phi)k_{\lambda}(\phi)}{[\partial_{k}E_{\lambda}(k,\phi)]_{k=k_{\lambda}(\phi)}}.$$

Symmetry considerations show that the diagonal components of tensor χ_{ij} equal zero and the normal component of the spin polarization is absent, $S_z = 0$. Nondiagonal components χ_{ij} have a magnetic-field dependence with the characteristic feature that appears when condition (18) is fulfilled. Components χ_{yx} has an abrupt minimum, while components χ_{yx} has an inflection point. The behavior of the spin polarization as a function of the magnetic field is shown in Fig. 3 for positions of the Fermi level below and above the Dirac point.

4. CONCLUSIONS

We showed that two characteristic features in the behavior of the conductivity and spin susceptibility of

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2D EG with SOI appear under the action of an inplane magnetic field. First, a rather abrupt singularity (the conductivity minimum and susceptibility χ_{xy}) is formed at the Fermi energy below the Dirac point. It is formed under the condition when the Fermi level coincides with the van Hove singularity point. The experimental observation of such a singularity can be used to determine the SOI constant with the help of Eq. (18). Second, the anisotropy of conductivity and spin susceptibility appears. It can also be a tool for studying electronic systems with SOI. However, we note that the regularities found in this work are obtained for noninteracting electron systems. Neglect by the interaction is justified at a rather large dielectric permeability and for systems with strong SOI such that the SOI energy E_{so} considerably exceeds the energy of the Coulomb interaction between electrons. Such conditions can be fulfilled for widely studied electron systems with giant SOI based on BiTeI [15, 16], LaAlO₃/SrTiO₃ interfaces [17], and surface alloys [18, 19]. In particular, the evaluation for BiTeI, where $E_{so} \approx 0.1$ eV, $m \approx 0.2m_0$, and the dielectric permeability $\varepsilon = 15$ [15] lead to the concentration $n_0 \approx 1.9 \times$ 10¹³ cm⁻² and the Coulomb interaction energy $e^2 \sqrt{n_0} / \epsilon \approx 0.04$ eV. The scale of the magnetic fields, at which the singularities that we predicted can be observed, is evaluated from equality b = 1 and numerically has an order of 10 T.

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