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Electronic transport in topological itinerant helical magnet

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A spin system with helical order can exhibit nontrivial topology of the band structure. An example of such a system is the metallic delafossite $PdCrO_2$. To describe its transport properties, a simple two-dimensional quasi-isotropic model of the Fermi surface has been proposed, which takes into account the emergence of spin texture, i. e., it consists of alternating fragments with opposite spin polarization. It has been shown that this model can explain the emergence of non-reciprocal electronic transport observed in the metallic delafossite $PdCrO_2$, as well as the unusual anomalous Hall effect.

Keywords: Helical ordering, Band structure, Fermi surface, Electronic transport, Metallic delafossites, $PdCrO_2$.

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1. Introduction

According to Bloch's theorem, the dispersion dependences of electrons in crystal structures should be periodic functions in momentum space, and their periodicity is determined by the size of the Brillouin zone [1]. Thus, the boundaries of the zone can be „glued“ so as to explicitly specify the periodicity of the dispersion relations, which in this case will be determined on a cylinder for one-dimensional (1D) systems, on a torus for two-dimensional (2D) and a hypertor for three-dimensional (3D) structures [2]. The topological nontriviality of these objects leads to the fact that the zone structure can belong to various topological classes [3]. Traditionally, it is assumed that a nontrivial band structure arises due to the specific phase distribution of the wave function in the Brillouin zone [4]. The phase variation can be represented as a vector field of the Berry vector potential (or connectivity). It has properties similar to the vector potential of a magnetic field, in particular, the ambiguity associated with gauge invariance. It is convenient to move from it to another vector field, the Berry curvature, which is similar in its properties to the induction of a magnetic field. The distribution of the Berry curvature in the Brillouin zone may have a different topology. This is easy to see, for example, for 2D systems: on the surface of a torus, the Berry curvature as a vector field can belong to various topological classes in cases where the „monopole“ is inside or outside the torus [3].

In recent decades, the main efforts of researchers have been focused on studying topological insulators (TI) and edge states in them, since unusual observed effects occur here [5,6], which are determined by surface states with enormous mobility of charge carriers.

It has recently been shown that a new type of nontrivial topological structures may exist in magnetic helicoidal systems that are not related to the Berry vector potential [7]. They arise for two reasons. First, in a helicoidal magnetic field, the dispersion relations $\varepsilon_{\mathbf{k},\sigma}$ have a specific symmetry [8]:

$$\varepsilon_{\mathbf{k},\langle\sigma\rangle} = \varepsilon_{-\mathbf{k},-\langle\sigma\rangle}, \quad (1)$$

where $\mathbf{k}$ is the wave vector, $\langle\sigma\rangle$ is the average spin value. Secondly, two characteristic periods of the structure, i. e., crystallographic and magnetic, together with Born-Karman periodic boundary conditions in the helicoidal system lead to the fact that within the Brillouin magnetic zone, the dispersion dependence is not periodic and forms a group of branches (a multi-sheet dispersion surface), which, in turn, has a nontrivial the topology [7]. A 2D model of palladium layers in metallic delafossite $PdCrO_2$ was considered as an example of such a band structure. One of the features of the band structure with a nontrivial topology turned out to be the spin texture of the Fermi surface [8,9].

Metallic delafossites ($PdCoO_2$, $PtCoO_2$, $PdCrO_2$) have record-breaking electrical conductivity for metallic oxides comparable to values typical for elementary metals such as copper and silver [10]. These compounds have a layered structure in which the dielectric layers CoO_2 and CrO_2 alternate with conductive layers of platinum or palladium [11]. The relatively low concentration of mobile charge carriers and high electrical conductivity lead to abnormal values of the free path. This suggests an unusual mechanism of electronic transport [12].

Among metallic delafossites, $PdCrO_2$ is the only compound in which a long-range magnetic order occurs at $T_N = 38\,\mathrm{K}$ [13]. The magnetic structure turns out to be extremely complex: chromium ions in the CrO_2 interlayers

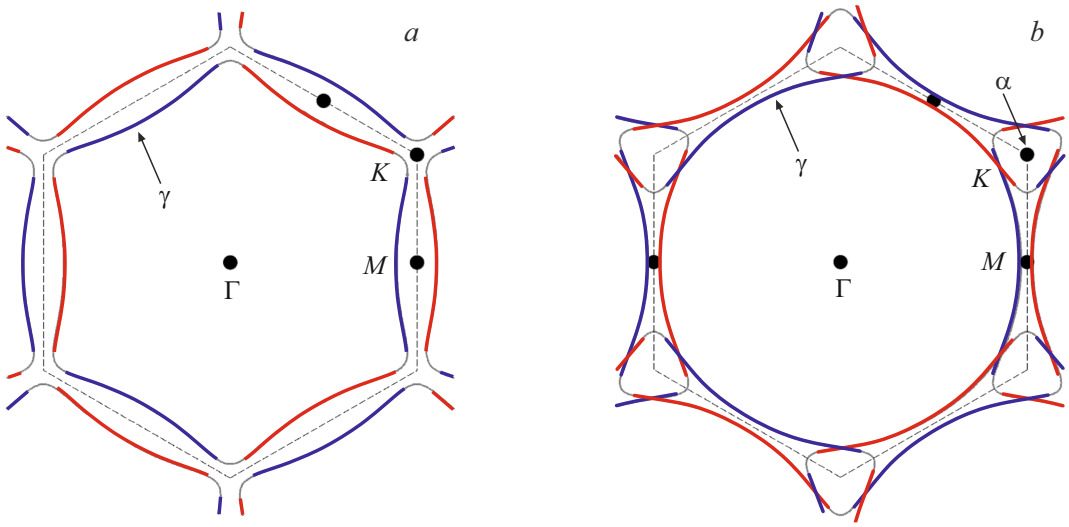

Figure 1. A spin-textured Fermi surface in a 2D model of almost free electrons for a hexagonal palladium layer obtained at different values of the Fermi level (*a* and *b*) [8,9]. Sheets α and γ are designated. Spin polarization is shown in color (blue and red) for spin-up and spin-down polarization.

form the 120°th order with alternating chirality in neighboring interlayers. In total, the magnetic structure consists of 18 sublattices [13]. The transition to a magnetically-ordered state leads to a sharp drop in resistance. In addition to its extremely high conductivity, $PdCrO_2$ has a number of other unexpected transport properties: the non-reciprocity of electronic conductivity [14] and the unusual anomalous Hall effect (UAHE) [15].

It is shown in this paper that all of the above transport properties can be explained within the framework of a 2D model of a Fermi surface with a spin texture.

2. Quasi-isotropic two-dimensional Fermi surface model

The Fermi surface in $PdCrO_2$ is currently well studied, both in the paramagnetic (PM) and magnetically ordered phases [10,16–18]. In the first case, there is a single sheet (α) of a quasi-two-dimensional Fermi surface with an electronic conductivity. The Fermi surface reconstruction takes place in the magnetically ordered phase below T_N, due to the transition to the Brillouin magnetic zone [17,18], as a result of which the main α sheet becomes a hole sheet γ and an electronic sheet α (pocket) near the K-point.

In particular, it was proven in Ref. [7], that a non-trivial band structure appears under the action of a 120° magnetic (molecular) field in a two-dimensional hexagonal layer in electrons, when a separate sheet of the dispersion surface is non-periodic in the Brillouin magnetic zone. In this case, the band structure as a whole turns out to be periodic, as required by Bloch's theorem.

Thus, one of the main results of the studies in Refs. [7–9] concluded that a single-sheet Fermi surface with a spin texture corresponding to the ratio (1) is possible in the topological metal regime. At the same time, it is non-degenerate along the back, possibly with the exception of isolated points. In other words, the spin state of an electron on the Fermi surface depends on the wave vector (spin texture) and is uniquely determined by it (absence of degeneracy). Then we can omit the spin index, which we will do in the future.

The band structure of a hexagonal 2D metallic layer in a helicoidal magnetic field in the approximation of almost free electrons [8,9], proposed as a model of conducting layers in $PdCrO_2$, is shown in Figure 1. Under the influence of the effective field of magnetically ordered chromium ion layers, the main γ sheet, the Fermi surface, and pockets (α sheet) appear, which are in good agreement with experimental data. The spin texture of the Fermi surface also appears, corresponding to the topological metal regime, which consists of six alternating arches with opposite spin polarization. In some cases, a similar structure occurs in the edge states of TI.

The transport properties of the zone structure are largely determined by the main γ sheet. At the same time, it can be approximately considered isotropic. Then, if we ignore pockets near K points, it is possible to proceed to the following 2D model representation: the Fermi surface in the absence of a magnetic field is isotropic in shape and has a spin structure. In the case of a nonzero magnetic field, which is assumed to be perpendicular to the spin plane, the arches of the Fermi surface corresponding to different directions of spin polarization are shifted in opposite directions due to the Zeeman effect. Therefore, we will call the model quasi-isotropic. This model allows performing analytical calculations for transport properties taking into account the spin texture. We will also assume a parabolic law of dispersion. Figure 2 shows a model Fermi

surface with a spin texture for cases without a magnetic field and a magnetic field oriented perpendicular to the spin plane.

As was shown earlier in Ref. [19], the spin texture partially suppresses the processes of electron-phonon scattering with overshooting and therefore leads to abnormal conductivity at low temperatures. The following section shows that it also leads to non-reciprocity of electronic transport.

3. Non-reciprocity of electronic transport in $PdCrO_2$ in a magnetic field

It was shown in Ref. [20] that the following condition follows from the Onsager relation in the case of chiral systems in a magnetic field: the electrical conductivity must be invariant with respect to the simultaneous change of the sign of the current and the magnetic field. This means that the reciprocity condition of electronic transport can be violated in a magnetic field. After that, an active search for chiral structures with non-reciprocal electronic transport began. In particular, it was detected in the magnetically ordered phase $PdCrO_2$ for the orientation of current and magnetic field along the crystallographic axis **a** [14], which corresponds to the direction Γ-M in the Brillouin magnetic zone.

When the external homogeneous electric field is oriented along the direction of the magnetic field ($\mathbf{E} \parallel \mathbf{B}$), the kinetic equation takes on a simple form [21]

$$\frac{e}{\hbar}\mathbf{E}\nabla_{\mathbf{k}} f = -\frac{\delta f}{\tau}, \tag{2}$$

where f and δf is the distribution function and its deviation from the equilibrium state, $\mathbf{k}$ is the electron wave vector, τ is the relaxation time, which is considered isotropic, e is the electron charge. The magnetic field is not explicitly included in expression (2), but it changes the equilibrium distribution function (see Figure 2). Here and below we assume that the spin plane is oriented perpendicular to the magnetic field. This condition is always approximately fulfilled in strong magnetic fields, i.e. above the spin-flop transition field B_{sf}. For $PdCrO_2$, the value of B_{sf} is of the order of 7 T [18].

As usual, the deviation of the distribution function from the equilibrium f_0 state in the metal is considered small. Then the deviation from the equilibrium state linear in the electric field can be written as

$$f_1 = e\tau E_x v_x \frac{\mathrm{d}f_0}{\mathrm{d}\varepsilon}, \tag{3}$$

where E_x and v_x are the components of the electric field and velocity along the axis **x** (along the crystallographic direction **a**). The particle energy is assumed in the standard form $\varepsilon = \hbar^2 k^2/(2m)$, and the particle velocity $\mathbf{v} = \hbar^{-1}\nabla_{\mathbf{k}}\varepsilon$.

The current density in the 2D model is determined by the following expression:

$$j_x = \frac{e}{4\pi^2}\int v_x f \,\mathrm{d}\mathbf{k}. \tag{4}$$

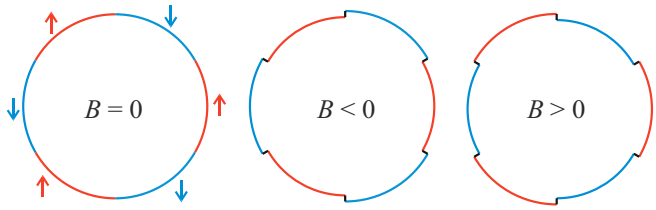

Figure 2. Quasi-isotropic 2D model of a textured Fermi surface (polarization is shown in color) at various magnetic field values (B).

The first-order correction f_1 gives a linear response of the system to an electric field, i.e., ordinary conductivity with minor corrections due to the deviation of the Fermi surface from the isotropic shape in the presence of an external magnetic field.

In normal metals, the equilibrium distribution function is centrally -symmetric, i.e. $f_0(\mathbf{k}) = f_0(-\mathbf{k})$. Then the first-order -correction must be antisymmetric.: $f_1(\mathbf{k}) = f_1(-\mathbf{k})$, and -the second-order correction must be again centrally symmetric $f_2(-\mathbf{k}) = f_2(-\mathbf{k})$. Then the second-order correction by E in the -current density disappears, since the integral expression in the -formula (4) turns out to be an odd function ($\mathbf{k}$, and thus the -transport turns out to be reciprocal. However, this conclusion is unfair -for a spin-textured Fermi surface in the presence of a magnetic field, -since in this case, under the influence of the Zeeman effect $f_0(-\mathbf{k}) \neq f_0(-\mathbf{k})$, as can be seen in Figure 2.

The correction to the second-order distribution function can be obtained by substituting $f_1 \to f$ into the left-hand side of equation (1). Then we get

$$f_2 = (e\tau E_x)^2 \left[\frac{d^2 f_0}{\mathrm{d}^2\varepsilon} v_x^2 + \frac{1}{m}\frac{\mathrm{d}f_0}{\mathrm{d}\varepsilon}\right]. \tag{5}$$

Substituting (5) into (4) after some transformations leads to the expression of the correction to the current density in the second order according to E in the form:

$$j_2 = \frac{e(e\tau E_x)^2}{\sqrt{2}\pi^2 m^{1/2}\hbar^2}\iint \frac{\mathrm{d}^2 f_0}{\mathrm{d}^2\varepsilon}\varepsilon^{3/2}\mathrm{d}\varepsilon\cos^3(\varphi)\mathrm{d}\varphi, \tag{6}$$

where φ is the angle in polar coordinates. In the low temperature limit $(k_B T)/\varepsilon_F \ll 1$), the integral is calculated analytically, and at $B \neq 0$, the value of the nonlinear part of the current turns out to be nonzero

$$j_2 = -\frac{e(e\tau E_x)^2}{8\pi^2\hbar^2}\Delta v_F, \tag{7}$$

where $\Delta v_F = 2\mu_B B/(m v_{F0})$ is the difference of Fermi velocities for different spin directions for a quasi-isotropic model, v_{F0} is the Fermi velocity in the absence of a magnetic field, μ_B is the Bohr magneton. It is also assumed that $\Delta v_F/v_{F0} \ll 1$.

Since the measurement results of non-reciprocal electronic transport were presented in Ref. [14] in terms of

nonlinear resistivity

$$\rho = \rho_0 + \rho_2 j, \tag{8}$$

it is convenient to convert the expression (7) to this kind. The nonlinear correction is small compared to the linear part of the resistivity. Then it can be shown that

$$\rho_2 \propto B/\tau. \tag{9}$$

It can be seen from the expression (9) that ρ_2 is proportional to the magnetic field, which is consistent with experimental data in strong fields [14]. In addition, there is a strong and non-monotonic dependence of ρ_2 on temperature over the relaxation time, which should be proportional to $\rho_0(T)$ to T_N, and then, during the transition to the paramagnetic phase, when the spin texture disappears, the nonlinear part of the resistivity It should go to zero. This behavior is also qualitatively observed experimentally [14].

The effect of non-reciprocity during the flow of current in periodic magnetic structures was studied in Ref. [22], and from fairly general considerations it was shown that a non-planar magnetic structure is necessary for its occurrence. At first glance, this contradicts the results obtained in this section. However, it should be noted that the absence of an external magnetic field was allowed in Ref. [22], whereas its presence was a necessary condition in the approach used above for the non-reciprocity of transport properties. From the analysis of the symmetry of the kinetic coefficients, it can be shown [20] that in a chiral system, the resistance of a bipolar can contain a term of the form $a\mathbf{IB}$, where a is the coefficient, $\mathbf{I}$ and $\mathbf{B}$ is the current and induction of the magnetic field, and when the chirality changes (from left to right and vice versa), the coefficient a must change sign. This contribution corresponds to the magnetochiral anisotropy [20], and the above dependence (9) corresponds precisely to it.

4. Unusual anomalous Hall effect

An anomalous Hall effect is observed in the magnetically ordered phase in $PdCrO_2$, and the Hall resistance cannot be represented as the sum of two terms linear in the magnetic field and magnetization [15]. Therefore, it is referred to as UAHE. Figure 3 shows the experimental dependences of the Hall resistance in $PdCrO_2$ in the magnetically ordered $T = 2\,\mathrm{K}$ and paramagnetic phases $T = 40\,\mathrm{K}$. There are complex models of this effect involving concepts of the Berry phase, scattering in non-planar magnetic systems, etc. On the other hand, it is shown below that a fairly simple explanation can be given, bearing in mind several types of mobile charge carriers in the magnetically ordered phase.

It was already noted above that the magnetic order leads to the reconstruction of the Fermi surface and the appearance of hole-like γ and electronic α sheets. Moreover, the mobility of holes can be significantly higher than that of electrons due to the spin texture (abnormal conductivity)

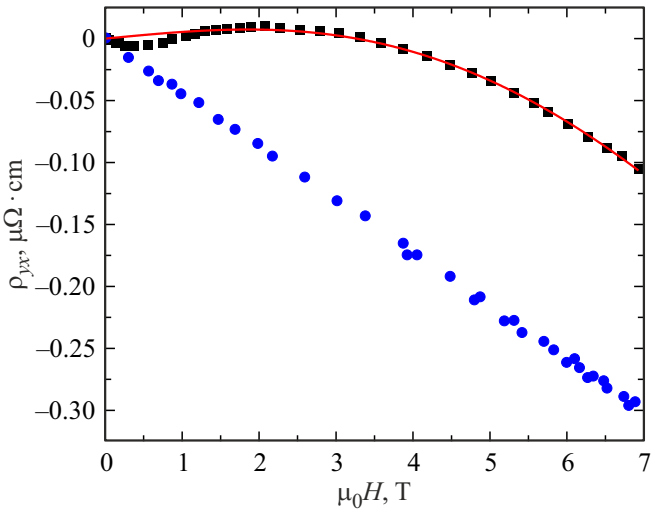

Figure 3. Hall resistance $PdCrO_2$ as a function of the magnetic field at $T = 40\,\mathrm{K}$ (blue circle), $T = 2\,\mathrm{K}$ (black square) from Ref. [15] and the dependence in the two-band model (solid line).

and blocking of scattering processes with flipping [19]. Then, the Hall coefficient in metal has a well-known form in the framework of the two-band model [1]

$$R(H) = \frac{R_e\rho_h^2 + R_h\rho_e^2 + R_eR_h(R_e + R_h)B^2}{(\rho_e + \rho_h)^2 + (R_e + R_h)^2B^2}, \tag{9}$$

where $\rho_{e(h)}$ and $R_{e(h)}$ are the resistivity and Hall constant for the electron (e) and hole (h) zones, respectively. In this case, the Hall constant defined in the expression (9) becomes a function of the magnetic field [1].

Figure 3 shows the dependence of $\rho_{yx} = BR$, where the Hall constant is determined by the formula (9) with the following parameters: $\rho_e = 3.76 \cdot 10^{-8}\,\mathrm{Ohm \cdot m}$, $\rho_h = 1.93 \cdot 10^{-7}\,\mathrm{Ohm \cdot m}$, $R_e = -7.08 \cdot 10^{-10}(\mathrm{C \cdot m^3})^{-1}$, $R_h = 2.09 \cdot 10^{-8}(\mathrm{C \cdot m^3})^{-1}$. It should be noted that the mobilities of electrons and holes ($\mu = |R|/\rho$) are very different in this case: $\mu_e = 0.019\,\mathrm{m^2/V \cdot s}$ and $\mu_h = 0.11\,\mathrm{m^2/V \cdot s}$.

The above example shows that the two-band model, although it is probably too simplified for the electronic structure $PdCrO_2$, nevertheless allows describing UAHE in this compound in a natural way without involving complex theoretical models.

5. Conclusion

In this paper, we propose a simple two-dimensional model of a quasi-isotropic textured Fermi surface corresponding to the nontrivial topology of the band structure of hexagonal conductive layers in a chiral magnetic (molecular) field. It is shown that it makes it possible to explain all the main anomalous transport properties of the magnetic metallic delafossite $PdCrO_2$. In particular, from a microscopic point of view, the non-reciprocity of electron transport is related to the fact that the Fermi surface with a spin

texture becomes asymmetric in a magnetic field (without an inversion center). It was previously shown in Ref. [19] that the texture of the Fermi surface leads to an abnormally high conductivity observed in $PdCrO_2$. It has long been known that the Hall constant becomes dependent on the magnetic field in a two-band metal model [1]. This makes it possible to describe the UAHE in $PdCrO_2$ in the magnetic phase.

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Conflict of interest

The author declares that he has no conflict of interest.

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