Whether there is the intrinsic Hall effect in a multi-band superconductor?

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The interplay of the microscopic models and the symmetry considerations in application to the superconducting state of putative chiral superconductor $\text{Sr}_2\text{RuO}_4$ are presented. There is demonstrated that chiral two-band superconducting ordering recently proposed as candidate for the superconducting state in this material and having the long-expected property such as the intrinsic Hall effect does not exist as energetically disadvantageous in comparison with the states not supporting the Hall effect. Other chiral multi-band superconducting states with intraband pairing do not support an intrinsic Hall properties as well. The superconducting states with direct interband pairing could serve as the probable candidates for the Hall effect existence.

KEYWORDS: $\text{Sr}_2\text{RuO}_4$, chiral superconductivity

I. INTRODUCTION

During about two decades the layered perovskite material $\text{Sr}_2\text{RuO}_4$ attracts a lot of attention of low temperature community (for the recent review see ). This is mostly due to its putative chiral p-wave superconductivity which is still controversial but supported by several significant experimental observations. The chiral superconductivity breaks the time reversal symmetry. Hence, as a ferromagnet, it has to reveal the anomalous Hall effect. Indeed, there was measured the polar Kerr effect related to the nonzero value of the Hall conductivity at infrared frequencies . On the other hand there was clearly demonstrated that the Hall conductivity in a translationally invariant chiral superconductor is equal to zero . In view of this general statement the proposed explanations of the Hall effect have been purely extrinsic arising from impurity scattering.

Among the attempts to point out the microscopic mechanism of chiral p-wave superconductivity there is recently published model possessing specific properties and based on quasi-one-dimensional character of two conducting bands in this material. (see also ). This model has revealed the important consequence, namely - the intrinsic Hall effect arising from interband transitions involving time-reversal symmetry breaking chiral Cooper pairs as it was analytically demonstrated in the paper. In parallel with the paper there were published the results of numerical calculations of the intrinsic Hall effect in a multi-band superconducting state breaking the time reversal symmetry.

A superconducting state realizing in a compound possesses definite properties dictated by the host crystal symmetry. And a particular microscopic model for superconducting state built theoretically should be constructed in correspondence with the symmetry requirements. Here we discuss the properties of two-band superconducting state introduced in the papers. More generally, we discuss the properties of one component and multi-component superconducting states in a two-band tetragonal superconductor. There is demonstrated that not a single state with intraband pairing obeys the properties necessary to support the intrinsic Hall effect. On the other hand the Hall effect in the superconductors with direct interband pairing still deserves the further studies.

The work presents the explicit analytic expression for the Hall conductivity in terms of exactly formulated microscopic model taking into account not only interband Cooper pairs transitions but formally also the direct inter-band pairing. To formulate the conditions for existence of the intrinsic Hall effect we begin with rewriting several equations from the paper. Then we write the Landau free energy expansions and consider the symmetry properties for the one-component and two-component superconducting states in two band superconductor. The results are formulated in the Conclusion.

II. HALL CONDUCTIVITY

We shall discuss unitary equal spin pairing superconducting states. This case all the calculations for the spin up-up $|\uparrow\uparrow\rangle$ and spin down-down $|\downarrow\downarrow\rangle$ order parameter components are separated and equivalent each other. There are also another type of superconducting states having only one spin component $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ corresponding to the equal spin pairing with spins perpendicular to the spin quantization axis usually chosen parallel to the tetragonal axis $\hat{z}$. This case all the written equation are related to this single component.

The intrinsic Hall conductivity

$$\sigma_H(\omega) = -\frac{1}{2i\omega} \lim_{q \to 0} [\pi_{xy}(q, \omega) - \pi_{yx}(q, \omega)]$$

was found in the paper as analytic continuation of antisymmetric part of the Matsubara current correlator

$$\pi_{xy}(q, \nu_m) = e^2T \sum_{k, \omega_n} Tr[\mathbf{v}_x \mathbf{G}(k, \omega_n)\mathbf{v}_y \mathbf{G}(k + q, \omega_n + i\nu_m)]$$

to the real frequencies $i\nu_m \to \omega + i0^+$. The matrix of electron velocities is determined as derivative of dispersion...
of two-band noninteracting Bloch electrons

\[ \mathbf{v} = \left( \begin{array}{c} v_1(k) \tilde{\tau}_0 \cr v_2(k) \tilde{\tau}_0 \end{array} \right) = \frac{\partial}{\partial k} \left( \begin{array}{cc} \xi_1(k) \tilde{\tau}_0 & \xi_2(k) \tilde{\tau}_0 \\ \xi_2(k) \tilde{\tau}_0 & \xi_1(k) \tilde{\tau}_0 \end{array} \right) . \] (3)

Here,

\[ \xi_1 + \mu = -2t \cos k_x - 2t^z \cos k_y, \]
\[ \xi_2 + \mu = -2t \cos k_y - 2t^z \cos k_x \]  \hspace{1cm}(4)

are the dispersions for the Bloch states in Sr$_2$RuO$_4$ forming bands (numbered by indices 1,2) constructed from the $xz$ and $yz$ ruthenium orbitals correspondingly. To avoid misunderstanding we note, that these bands are often called in the paper by orbitals unlike to real $\alpha$ and $\beta$ bands in this compound those dispersion laws are obtained after usual diagonalization procedure taking into account the interband coupling

\[ \varepsilon_{12} = -2t'' \sin k_x \sin k_y. \] (5)

The 4x4 Green functions for two-band superconductor with equal spin pairing for each spin projection is defined through its inverse matrix

\[ G^{-1}(k, \omega_n) = \left( \begin{array}{cc} i\omega_n \tilde{\tau}_0 - \xi_1 \tilde{\tau}_3 - \Delta_1 & -\xi_2 \tilde{\tau}_3 + \Delta_2 \\ -\xi_1 \tilde{\tau}_3 + \Delta_2 & i\omega_n \tilde{\tau}_0 - \xi_2 \tilde{\tau}_3 - \Delta_2 \end{array} \right). \] (6)

Here, $\tilde{\tau}_0$, $\tilde{\tau}_3$ are the Pauli matrices in the particle-hole space, and the order parameter matrices for intraband and direct interband pairing are correspondingly

\[ \hat{\Delta}_{1,2} = \left( \begin{array}{cc} 0 & \Delta_{1,2}(k) \\ \Delta_{1,2}^*(k) & 0 \end{array} \right) . \] (7)

Following the paper we did not include the interband spin-orbital interaction.

The calculation performed in the paper yields

\[ \pi_{xy}(q = 0, \nu_m) = 4e^2T \nu_m \sum_{k, \omega_n} \frac{(2\omega_n + \nu_m)[(\mathbf{v}_2 - \mathbf{v}_1) \times \mathbf{v}_{12}]}{(\omega_n^2 + E_+^2)(\omega_n^2 + E_-^2)((\omega_n + \nu_m)^2 + E_+^2)} \left[ \varepsilon_{12} \Im(\Delta_1^* \Delta_2) + \xi_1 \Im(\Delta_1^* \Delta_1) - \xi_2 \Im(\Delta_1^* \Delta_2) \right]. \] (8)

Here, $E_{\pm}$ are solutions of the equation $\det G^{-1}(k, \omega_n) = 0$. Unlike to Eqs. (7) and (8) in the paper the above expression is written as it is before the summation over Matsubara frequencies.

Formula (5) contains the terms originating from intraband pairing multiplied by the interband matrix element $\varepsilon_{12}$ and the terms proportional to the direct interband pairing order parameter $\Delta_{12}$. The later are usually ignored in the theory of two band superconductivity due the mismatching of oppositely directed momenta of the Cooper pairs formed by the electrons from different bands. We discuss, first, the terms containing the interband transition matrix element. Then, we have

\[ [(\mathbf{v}_2 - \mathbf{v}_1) \times \mathbf{v}_{12}] \varepsilon_{12} \Im(\Delta_1^* \Delta_2) = -8(t - t^z)(t'')^2(\sin^2 k_x \cos k_y + \sin^2 k_y \cos k_x) \times \sin k_x \sin k_y \Im(\Delta_1^* \Delta_2) \] (9)

The integration in Eq. (5) is produced over the Brillouin cell $\sum_k = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} dk_x dk_y$. The denominator in this formula depending from $E_+$ and $E_-$ is even function both in respect to $k_x$ and $k_y$. Hence, whether there is nonzero value of $\pi_{xy}(q = 0, \nu_m)$, it is determined by the product

\[ \sin k_x \sin k_y \Im(\Delta_1^* \Delta_2) \] (10)

in the last line of Eq. (9). Now, one must fixe the two-band superconducting state for which the integral over Brillouin zone is not zero.

III. SYMMETRY CONSIDERATIONS

A. 1D representations

The authors of paper discuss the superconducting state making use the model of two equivalent bands and corresponding pairing interaction with orthorhombic symmetry ignoring the interband Cooper pairs scattering but taking into account the interband coupling $\varepsilon_{12}$. The orthorhombic point group has onlly one dimensional representations. The superconducting states in two bands are transformed according different 1-D representations of the orthorhombic group, namely, as $\Delta_1 = \eta_1 \sin k_x = |\eta_1| e^{i\varphi_1} \sin k_x$ in the first band and as $\Delta_2 = \eta_2 \sin k_y = |\eta_2| e^{i\varphi_2} \sin k_y$ in the second one. This case, the Landau free energy expansion has the following form

\[ F = \alpha(|\eta_1|^2 + |\eta_2|^2) + \beta(|\eta_1|^4 + |\eta_2|^4) + \beta_{12}|\eta_1|^2|\eta_2|^2 \]
\[ + \beta_{12} \left[ \eta_1^2(\eta_2^*)^2 + (\eta_1^*)^2\eta_2^2 \right]. \] (11)

The coefficients $\alpha = \alpha_0(T - T_0)$ and, hence, the critical temperatures for both bands are equal due the band equivalence. Now, we see, that if the coefficient $\beta_2$ is positive (this is indeed the case in the model), then the phase shift between the superconducting order parameters in bands 1 and 2 is $\varphi_1 - \varphi_2 = \pi/2$. The product (11) proves to be equal to $|\eta_1||\eta_2| \sin^2 k_x \sin^2 k_y$ with obviously nonzero integral over the Brillouin zone.
In fact, it is incorrect to consider the superconducting state in two different bands of tetragonal crystal as relating to the one-dimensional representations of orthorhombic group. Such consideration in terms of a microscopic model means that the Hamiltonian is chosen as not obeying the necessary symmetry conditions. A superconducting state in tetragonal crystal should be transformed according to some representation of tetragonal point group.

The construction, from that follows the coincidence of critical temperatures for the superconducting states transforming according to different representations, is unrealistic. The critical temperatures for the phase transition to the superconducting states relating to different representation are inevitably different. From the point of view of microscopic theory it follows from the difference of bands in the normal state, in given case, the difference between \( \alpha \) and \( \beta \) bands in strontium ruthenate. The model is relevant in the unphysical situation when the superconducting critical temperature is larger than the band hybridization energy \( T_c > > \epsilon_{12} \). Then, at critical temperature, the bands can be treated as equivalent. In reality the opposite inequality takes place. Hence, the \( xz \) and \( yz \) orbitals (bands 1 and 2) should be taken as hybridized and forming different \( \alpha \) and \( \beta \) bands even at temperatures much larger than the temperature of the superconducting transition. We, however, continue our discussion because even at proper treatment of superconducting state realizing in presence of the interband Cooper pairs scattering, \( \sum_{kk'} V_{zz}(k,k')a_{1-k}^\dagger a_{2-k'} \) the Eqs. (8) and (9) are still valid.

According to general rules of nonconventional superconductivity theory the superconducting states arising in a two band metal at the same critical temperature must be related to the same superconducting class. The Landau functional for one-component states has the following form

\[
F = \alpha_1 |\eta_1|^2 + \alpha_2 |\eta_2|^2 + \gamma |\eta_1 \eta_2^* + \eta_2^* \eta_1| \\
+ \beta_1 |\eta_1|^4 + \beta_2 |\eta_2|^4 + \beta_3 |\eta_1\eta_2|^2|\eta_1\eta_2|^2 \\
+ \beta_{12} \left[ |\eta_1^2|^2 + |\eta_2^2|^2 \right].
\]

(12)

The coefficients \( \alpha_1 = \alpha_{10}(T - T_c), \alpha_2 = \alpha_{20}(T - T_c), T_{c1} \) and \( T_{c2} \) are the critical temperatures in the absence of interband pair scattering. The term \( \gamma |\eta_1 \eta_2^* + \eta_2^* \eta_1| \) in Eq. (12) is absent simply due the fact that the superconducting states in different bands belong to different representations. In terms of microscopic theory it means that the interband Cooper pairs transitions are present but only starting from the forth order terms in respect to the order parameter products. These transitions produce in Eqs. (12) the band-mixing terms \( \beta_{12} |\eta_1|^2|\eta_2|^2 \) and \( \beta_{12} |\eta_1^2|^2 + |\eta_2^2|^2 \). The microscopic calculation shows that the fourth and the higher order mixing terms are proportional to the powers of \( \epsilon_{12} \) and completely absent at \( \epsilon_{12} = 0 \). On the contrary, for the superconducting states belonging to the same superconducting class the second order, that is \( |\eta_1 \eta_2^* + \eta_2^* \eta_1| \) term, always exists independently of presence or absence of hybridization \( \epsilon_{12} \).

Note, that in presence \( |\eta_1 \eta_2^* + \eta_2^* \eta_1| \) term, the phase shift between the bands order parameters proves to be 0 for \( \gamma < 0 \) or \( \pm \pi \) for \( \gamma > 0 \).

The symmetry statement that superconducting states in different bands are obligatory related to the same representation has the simple energetic explanation. Indeed, even at \( \alpha_1 = \alpha_2 \) a superconducting state with \( \gamma \) term has higher critical temperature \( T_c = T_{c0} + \frac{|\epsilon_{12}|}{2} \) of the phase transition to the superconducting state than the critical temperature \( T_{c0} \) in the absence \( \gamma \) term. So, the band order parameters belong to the same representation.

The order parameters for the superconducting states in a metal with tetragonal symmetry are listed in Tables 3 and 4 in the book. To take into account the translational symmetry one must simply substitute \( k_x(y) \) by \( \sin k_x(y) \) in these Tables. It is easy to check that for a pair of superconducting states transforming according to the same one-dimensional representation of the tetragonal group the integral over \( k_x, k_y \) from expression (10) vanishes identically yielding \( \eta_{x0}(q = 0, n_m) = 0 \). Hence, all these states do not support the intrinsic Hall effect.

### B. 2D representation

Now one needs to investigate the superconducting state transforming according to two-dimensional representation. The band order parameters for these states have the form

\[
\Delta_1 = \eta_{1x} \psi_{1x} + \eta_{1y} \psi_{1y}, \\
\Delta_2 = \eta_{2x} \psi_{2x} + \eta_{2y} \psi_{2y}
\]

(13)

where the order parameter amplitudes are vectors \( \vec{\eta}_1 = (\eta_{1x}, \eta_{1y}), \vec{\eta}_2 = (\eta_{2x}, \eta_{2y}) \). The functions \( \psi_{1(2)x} \) and \( \psi_{1(2)y} \) of \( E_0 \) irreducible representation are transformed as \( \sin k_x \) and \( \sin k_y \) correspondingly. The Ginzburg-Landau free energy for the two-band superconducting state transforming according to two-dimensional representation has the following form

\[
F = \alpha_1 \vec{\eta}_1 \vec{\eta}_1^* + \beta_1 (|\vec{\eta}_1 \vec{\eta}_1^*|)^2 + \beta_2 |\vec{\eta}_1 \vec{\eta}_1^*| |\vec{\eta}_1 \vec{\eta}_1^*| + \beta_3 (|\vec{\eta}_1 \vec{\eta}_1^*|^4 + |\vec{\eta}_2 \vec{\eta}_2^*|^4) \\
+ \beta_4 (|\vec{\eta}_1 \vec{\eta}_1^*|^2 + |\vec{\eta}_2 \vec{\eta}_2^*|^2) + \beta_5 (|\vec{\eta}_1 \vec{\eta}_1^*|^2 + |\vec{\eta}_2 \vec{\eta}_2^*|^2) \\
+ \beta_6 (|\vec{\eta}_1 \vec{\eta}_1^*|^2 + |\vec{\eta}_2 \vec{\eta}_2^*|^2) + \beta_7 (|\vec{\eta}_1 \vec{\eta}_1^*|^2 + |\vec{\eta}_2 \vec{\eta}_2^*|^2)
\]

(14)

Here, \( \alpha_1 = \alpha_{10}(T - T_{c1}), \alpha_2 = \alpha_{20}(T - T_{c2}), T_{c1} \) and \( T_{c2} \) are the critical temperatures in the absence of interband pair scattering. Again, the fourth order band mixing terms have nonzero values only in presence of the band hybridization term \( \epsilon_{12} \) in Eq. (12). We remind that for each spin component of an equal pairing state the free energy expansion has the same form.

The Landau free energy (14) has completely general character determined only by the crystal symmetry and the dimensionality of representation. The coefficients
$\alpha_1, \ldots, \beta_1, \ldots, \gamma$ can be determined in frame of some microscopic model of pairing. However, even without knowledge of particular values of the coefficients one can make several important conclusions concerning the properties of superconducting states. For example, if we discuss just one-band superconductivity, where the corresponding Landau free energy is given by the first line in Eq. (14), one can conclude that all the superconducting states with $\vec{\eta}_1 \propto (1,0), (1,1), (1,i), \ldots$ have the same critical temperature. The choice between them can be made with aid of the fourth order terms. For example, for coefficients $\beta_1 > 0$ and $\beta'_1 > -2\beta_1$ the most profitable superconducting state proves to be time reversal symmetry breaking state $\vec{\eta}_1 \propto (1,\pm i)$. The beta-coefficients found in frame of weak coupling theory with arbitrary shape of the Fermi surface ($\beta_1 = 2\beta'_1 > 0, \beta'_1 = 0$) support this conclusion (see for instance [10]). On the other hand at $\beta'_1 < 0$ and $\beta'_1 < -2\beta_1$ the state $\vec{\eta}_1 \propto (1,0)$, or $\vec{\eta}_1 \propto (0,1)$ is the most profitable.

In the case of two-band superconductivity, one can also make the model independent conclusion concerning the order parameter form. The superconducting state can consist only of pairs of states belonging to same superconducting class. They are:

(i) $\vec{\eta}_1 \propto (1,0)$ and $\vec{\eta}_2 \propto (1,0)$;
(ii) $\vec{\eta}_1 \propto (1,1)$ and $\vec{\eta}_2 \propto ((1,1)$;
(iii) $\vec{\eta}_1 \propto (1,i)$ and $\vec{\eta}_2 \propto (1,i)$.

It is easy to check that for all these pairs of superconducting states the integral over $k_x, k_y$ from the product $\tilde{\beta}_x, \tilde{\beta}_y$ vanishes identically.

This finding is in an exact correspondence with general statement in [8] that in a translationally invariant chiral superconducting state the Hall conductivity

$$\sigma_H (\mathbf{q} = 0, \omega) \equiv 0.$$ 

C. Direct interband pairing

We have to discuss now the rest of the terms in the equation [8] relating to the direct interband pairing that is proportional to $\Delta_{12}$. The formal consideration of these terms making use the corresponding Landau free energy and symmetry argumentation leads to the same conclusion, namely to the absence of internal Hall effect. This case, however, the similar formal considerations are inapplicable. The point is that the interband pairing (if it exists) due to length mismatching of the oppositely directed momenta in different bands leads inevitably to the space modulated superconducting ordering. The theory actually cannot operate with such a space homogeneous Green functions as given by [8] and space homogeneous Landau expansions. Thus, this problem deserves some special investigation. However, one can suppose that the space inhomogeneous order parameter distribution breaks the system translation invariance. Due to this reason the intrinsic Hall effect in chiral superconductors with interband pairing can in principle exist.

IV. CONCLUSION

We have studied the possibility of intrinsic Hall effect in multiband superconductor with tetragonal symmetry making use the general nonconventional superconductivity theory. There was demonstrated that a superconducting state with intraband pairing including the interband pairs transitions do not support the existence of Hall conductivity. On the other hand this effect in principle can exist in space inhomogeneous superconducting state caused by the direct interband pairing.

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1. Y. Maeno, S. Kittaka, T. Nomura, S. Yonezawa, and K. Ishida, J. Phys. Soc. Jpn. 81, (2012) 011009.
2. C. Kallin, A. J. Berlinsky, J. Phys.: Condens. Matter 21 (2009) 164210.
3. J. Xia, Y. Maeno, P. T. Beyersdorf, M. M. Fejer, and A. Kapitulnik, Phys. Rev. Lett. 97, 167002 (2006).
4. N. Read and D. Green, Phys. Rev. B 61 (2000) 10267.
5. R. M. Lutchin, P. Nagornykh, and V. M. Yakovenko, Phys. Rev. B 80 (2009) 104508.
6. J. Goryo, Phys. Rev. B 78 (2008) 060501(R).
7. S. Raghu, A. Kapitulnik, and S.A. Kivelson, Phys. Rev. Lett. 105 (2010) 136401.
8. T. Takimoto, Phys. Rev. B 62 (2000) R14641.
9. E. Taylor and C. Kallin, Phys. Rev. Lett. 108 (2012) 157001.
10. K. I. Wysokinski, J. A. Annett, B. L. Gyorffy, Phys. Rev. Lett. 108 (2012) 077004.
11. G. E. Volovik, L. P. Gor’kov, Sov. Phys. JETP 61 (1985) 843.
12. V. P. Mineev and K. V. Samokhin, Introduction to unconventional superconductivity (Gordon and Breach, New York, 1999).
13. H. Suhl, B. T. Matthias, and L. R. Walker, Phys. Rev. Lett. 3 (1959) 552.
14. A. P. Mackenzie and Y. Maeno, Rev. Mod. Phys. 75 (2003), 657712.
15. Performing this checking one needs to take into account that considering only the equal state pairing states we
should treat the \{\hat{x}, \hat{y}\} spin components of the order parameters that is \(|\uparrow\uparrow\rangle\) and \(|\downarrow\downarrow\rangle\) pairing states separately from the \(\hat{z}\) component of the order parameter, that is \(|\uparrow\downarrow + \downarrow\uparrow\rangle\) pairing state.

V. Kuznetsova and V. Barzykin, Europhys. Lett. 72 (2005) 437.