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Thermal Hall conductivity of spin-triplet superconductor with time reversal symmetry breaking

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Abstract. The thermal Hall conductivity is investigated for the superconductor Sr\textsubscript{2}RuO\textsubscript{4} assuming a time reversal symmetry breaking order parameter. The \( \gamma \) band of Sr\textsubscript{2}RuO\textsubscript{4} has its Fermi level near the van Hove points, close to the Lifshitz transition. Within a Bogoliubov-de Gennes approach we calculate the thermal Hall conductivity for pairing symmetries including two exemplary cases, the usual chiral \( p \)-wave phase and a \( f_{x^2-y^2} \)-wave phase of the structure \( d = \Delta \hat{z}(k_x^2 - k_y^2)(k_x \pm ik_y) \). In the chiral \( p \)-wave phase the thermal Hall conductivity consists of a universal temperature-linear term and an exponential correction due to quasiparticle activation with a full excitation gap. Due to line-nodes in the gap we find a correction which is quadratic in temperature for \( f_{x^2-y^2} \)-wave state. This difference in the corrections allows to analyze the gap structure of the superconducting phase.

1. Introduction

The transition metal oxide Sr\textsubscript{2}RuO\textsubscript{4} [1, 2] is often viewed as a good candidate for a topological superconductor. Experimental studies indicate that the superconducting state has magnetic properties indicating broken time-reversal symmetry [3, 4]. The symmetry analysis has led to the identification of the pairing channel as chiral \( p \)-wave with a gap function written in \( d \)-vector notation as \( d = \Delta \hat{z}(k_x \pm ik_y) \) with an orbital angular momentum \( L_z = \pm 1 \) along the \( z \) axis [5]. This is the two-dimensional analog of the Anderson-Brinkman-Morel (ABM) state, and has generally a nodeless excitation gap. Recently \( f_{x^2-y^2} \)-wave was proposed an alternative candidate [6], whose gap function has the basic form \( d = \Delta \hat{z}(k_x^2 - k_y^2)(k_x \pm ik_y), \) having vertical line nodes in the excitation gap.

It is well known that the electronic low-energy physics of Sr\textsubscript{2}RuO\textsubscript{4} is governed by the \( \alpha, \beta \) and \( \gamma \) bands composed of the Ru \( 4d \) \( t_{2g} \) orbitals. The topological properties originate from the two-dimensional electron-like \( \gamma \)-band and are characterized by a Chern number [7]. The Fermi energy of the \( \gamma \)-band lies very close to the van Hove point (\( k = (\pi, 0) \)), such that the topology of the Fermi surface may be changed by some form of tuning through a Lifshitz transition, which is then accompanied by the switching of the Chern number [7, 8].

It turns out that the edge currents induced by the time reversal symmetry breaking phase does not change strongly at the Lifshitz transition counter naive expectation [8]. In contrast, the...
thermal Hall effect being directly connected to the Chern number in topological superconductors is certainly more suitable to probe the change of topological features [9]. We have discussed that the temperature dependence of the thermal Hall conductivity in the chiral \( p \)-wave phase is composed of a temperature linear term and an exponential term. The former is proportional to the Chern number and the latter gives the information on the magnitude of the quasiparticle excitation gap and the topological properties [10].

In our present report we propose to examine the thermal Hall conductivity in the superconducting phases with time-reversal symmetry breaking in order to distinguish the pairing symmetry around the Lifshitz transition.

2. Model

To demonstrate the connection between the topological property and the thermal Hall effect, we employ the single band tight-binding model on the two-dimensional square lattice with a structure like the \( \gamma \) band, described by the following Bogoliubov de-Gennes (BdG) Hamiltonian

\[
H_{\text{BdG}} = \sum_k \begin{pmatrix} c_{k\uparrow} & c_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \varepsilon_k & \Delta_k^* \\ \Delta_k & -\varepsilon_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow}^\dagger \\ c_{-k\downarrow}^\dagger \end{pmatrix},
\]

where \( c_{k\sigma} \) (\( c_{k\sigma}^\dagger \)) is the creation (annihilation) operator of an electron with wave vector \( k \) and spin \( \sigma \). \( \varepsilon_k \) and \( \Delta_k \) denote the energy dispersion of the \( \gamma \)-band in the normal phase and the gap function, respectively, given by,

\[
\varepsilon_k = -2t (\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu,
\]

\[
\Delta_k = \begin{cases} \Delta (\sin k_x \pm i \sin k_y), & (\text{chiral } p\text{-wave}) \\ \Delta (\cos^2 k_x - \cos^2 k_y)(\sin k_x \pm i \sin k_y), & (f_{x^2-y^2}\text{-wave}) \end{cases}
\]

where \( t \) (\( t' \)) are the hopping amplitudes between nearest-neighbor (next-nearest-neighbor) sites. \( \mu \) is the chemical potential and \( \Delta \) is the amplitude of the gap function.

Figure 1 displays the Fermi surface for several choices of the chemical potential. The result for \( \mu = 1.3t \) reproduces the electron-like \( \gamma \)-band of bulk \( \text{Sr}_2\text{RuO}_4 \) well. With increasing \( \mu \), the Fermi surface structure switches from the electron-like to hole-like shape when passing through the van Hove points at \( \mu = 1.4t \) (\( \equiv \mu_c \)). Here we implement the change of the Fermi surface topology through the tuning of the chemical potential instead of the direct consideration of physical and/or chemical tunings in \( \text{Sr}_2\text{RuO}_4 \), for simplicity.

The quasiparticle energies of the BdG Hamiltonian are given by \( E_{k\pm} = \pm \sqrt{\varepsilon_k^2 + \Delta_k^2} \).

Thus while the chiral \( p \)-wave phase has fully gapped excitation spectrum, \( E_k \) vanishes at

Figure 1. (Color online) Fermi surface for several choices of \( \mu \) with \( t' = 0.35t \) in the normal phase (\( \Delta = 0 \)). The dashed lines represent line nodes with \( |k_x| = |k_y| \) in the \( f_{x^2-y^2} \)-wave phase.
$k = k_0 \equiv (\pm k_0, \pm k_0)$ and $(\pm k_0, \mp k_0)$ for the $f_{x^2-y^2}$-wave phase due to line nodes, where $k_0$ is given as follows $k_0 = \arccos \left\{ \left(-t + \sqrt{t^2 - t'^2}\mu \right)/(2t') \right\}$. With increasing $\mu$, $k_0$ changes continuously and monotonically even while passing through the Lifshitz transition.

3. Results

In this study we use the following model parameters: the next-nearest-neighbor hopping matrix element and the gap function are $t' = 0.35t$ and $\Delta = 0.1t$, respectively, given in units of $t$. For our further calculation we choose the chiral phases with Chern number +1, noting that the case of $-1$ would yield simply analogous results.

Figure 2 displays the quasiparticle energy dispersions and the density of states (DOS) for the superconducting states. For the chiral $p$-wave ($f_{x^2-y^2}$-wave) phase, DOS reveals a full gap (a pseudogap) in the low-energy sector, whose magnitude is parametrized as $\varepsilon_0$ in both pairing phases. Around the node at $k = k_0$, in the $f_{x^2-y^2}$-wave phase $E_k$ disperse linearly in the momentum approximated by

$$E_k \approx \pm \sqrt{a + b \sin 2\theta} q,$$

with $a = 2\sin^2 k_0 \left\{ 2(t + 2t' \cos k_0)^2 + \Delta^2 \sin^2 k_0 \right\}$ and $b = 2\sin^2 k_0 \left\{ (t + 2t' \cos k_0)^2 - \Delta^2 \sin^2 k_0 \right\}$. The angle $\theta$ denotes the orientation of the momentum relative to $k_0$ and $q = |k - k_0|$. This linear dispersion leads to a DOS linear in energy within the range $|\varepsilon| \leq \varepsilon_0$.

The topological properties are characterized by the Chern number $N_C$, which is defined as

$$N_C = \frac{4\pi}{N} \sum_{n=\pm} \sum_{(E_{kn} < 0)} \text{Im} \left\langle \frac{\partial u_{kn}}{\partial k_x} \frac{\partial u_{kn}}{\partial k_y} \right\rangle,$$

where $N$ stands for the number of sites and $u_{kn}$ is the periodic part of the Bloch wave function of the BdG Hamiltonian.

Let us now discuss the temperature dependence of the thermal Hall conductivity. The formula in the superconducting phase with broken time-reversal symmetry is given by

$$\kappa_{xy} = -\frac{1}{4\pi T} \int d\varepsilon \varepsilon^2 \Lambda(\varepsilon) f'(\varepsilon),$$

$$\Lambda(\varepsilon) = \frac{4\pi}{N} \sum_{kn=\pm} \text{Im} \left\langle \frac{\partial u_{kn}}{\partial k_x} \frac{\partial u_{kn}}{\partial k_y} \right\rangle \theta(\varepsilon - E_{kn}),$$

(a) Band

(b) DOS

![Figure 2](image)

Figure 2. (Color online) (a) Quasiparticle energy dispersion and (b) DOS in the low-energy region. The solid (dashed) lines denote the $\mu = 1.3t$ ($\mu = 1.5t$) result.
where \( f'(\varepsilon) \) and \( \theta(\varepsilon) \) stand for the derivative of the Fermi distribution function and the Heaviside step function, respectively [9]. Note that \( \Lambda(\varepsilon = 0) \) corresponds to the Chern number for both superconducting phases. In the low-temperature limit, the thermal Hall conductivity is linear in temperature to lowest order and proportional to the Chern number [9, 11, 12],

\[
\kappa_{xy} \approx \kappa_{xy}^L = \frac{\pi N_C}{12} T. \tag{8}
\]

We first consider the structure of \( \Lambda(\varepsilon) \), which is important for the correction to the linear temperature dependence of \( \kappa_{xy} \). Figure 3 displays \( \Lambda(\varepsilon) \) for \( \mu = 1.3t \) and \( \mu = 1.5t \). \( \Lambda(\varepsilon) \) has a basically rectangular-like shape and switches from convex downward to convex upward around \( \varepsilon = \varepsilon_0 \). For the larger \( |\varepsilon| \) region, \( \Lambda(\varepsilon) \) decreases towards zero gradually, whose actual structure depends on details of the model, and is not associated with the unique topological aspects and the Lifshitz transition directly.

Since the chiral \( p \)-wave phase has a fully gapped excitation spectrum, \( \Lambda(\varepsilon) \) becomes constant within \( |\varepsilon| \leq \varepsilon_0 \), at value of the Chern number \( N_C \).

On the other hand, in the \( f_{x^2-y^2} \)-wave phase, \( \Lambda(\varepsilon) \) deviates from \( N_C \) except at \( \varepsilon = 0 \) due to gapless excitations around \( k = k_0 \). The derivative of \( \Lambda(\varepsilon) \) in the low-energy region is written as

\[
\Lambda'(\varepsilon) = \frac{\alpha}{\Delta} (2\theta(\varepsilon) - 1), \quad \left( \alpha \equiv \frac{\cos k_0}{2\sqrt{2}\sin^3 k_0} \right). \tag{9}
\]

This formula is analytically obtained by the expansion with respect to wave vector around \( k = k_0 \), and indicates that \( \Lambda(\varepsilon) \) becomes linear in \( |\varepsilon| \) in the low-energy region. Figure 3 shows that the result from Eq. (9) agrees with the \( \Lambda(\varepsilon) \) obtained numerically from Eq. (7). Note that the sign of the coefficient \( \alpha \) becomes negative due to \( \cos k_0 < 0 \) and \( \sin k_0 > 0 \) within the used parameter range and does not change around the Lifshitz transition.

In order to investigate the low-temperature behavior of \( \kappa_{xy} \) analytically, we calculate Eq. (6) by means of \( \tilde{\Lambda}(\varepsilon) \) instead of the exact \( \Lambda(\varepsilon) \), which is given by

\[
\tilde{\Lambda}(\varepsilon) = \left\{ \begin{array}{cc}
N_C + \frac{\alpha}{\Delta} |\varepsilon| & (|\varepsilon| \leq \varepsilon_0) \\
0 & (|\varepsilon| > \varepsilon_0)
\end{array} \right., \tag{10}
\]

\[
\alpha = \left\{ \begin{array}{c}
\frac{\cos k_0}{2\sqrt{2}\sin^3 k_0} \\
\frac{\cos k_0}{2\sqrt{2}\sin^3 k_0}
\end{array} \right. \quad \text{(chiral} \ p \text{-wave)} \\
\frac{\cos k_0}{2\sqrt{2}\sin^3 k_0} \quad \text{(f}_{x^2-y^2} \text{-wave)} \tag{11}
\]

\[\mu = 1.3t \quad \text{chiral} \ p \quad f_{x^2-y^2} \]

\[\mu = 1.5t \quad \text{chiral} \ p \quad f_{x^2-y^2} \]

\[\Lambda(\varepsilon) \text{ for } \mu = 1.3t \text{ and } \mu = 1.5t. \text{ The dotted lines stand for the results from Eq. (9) for the } f_{x^2-y^2} \text{-wave state for } \varepsilon > 0. \]
Then the approximate thermal Hall conductivity $\tilde{\kappa}_{xy}$ is obtained as follows,

$$
\tilde{\kappa}_{xy} \approx \kappa_{xy} = \kappa_{xy}^L + \frac{9\zeta(3)}{4\pi} T^2 - \left\{ \gamma(T) + \gamma'(T) \right\} \epsilon_0 e^{-\frac{\epsilon_0}{T}}, \quad (12)
$$

$$
\gamma(T) = \frac{N_C T}{\pi} \left\{ 2\left( \frac{\epsilon_0}{2T} \right)^2 + 2 \left( \frac{\epsilon_0}{2T} \right) + 1 \right\}, \quad (13)
$$

$$
\gamma'(T) = \frac{2\alpha T^2}{\pi\Delta} \left\{ 2\left( \frac{\epsilon_0}{2T} \right)^3 + 3 \left( \frac{\epsilon_0}{2T} \right)^2 + 3 \left( \frac{\epsilon_0}{2T} \right) + \frac{3}{2} \right\}, \quad (14)
$$

where $\zeta(s)$ is Riemann $\zeta$ function and $\zeta(3) \approx 1.202$. Note that $|\gamma'(T)/\gamma(T)| \sim |\alpha\epsilon_0/(N_C \Delta)| \sim |\alpha/N_C| \approx 0.15 - 0.20$ in the low-temperature region, so that the $\gamma(T)$ term is dominant by the exponential factor in Eq. (12).

This result indicates that the thermal Hall conductivity is expected to sustain the temperature linear behavior at lowest temperature, while having correction terms quadratic in $T$ and exponentially activated. The sign of the exponential term $-\gamma(T)e^{-\frac{\epsilon_0}{T}}$ in Eq. (12) switches from positive for $\mu < \mu_c$ to negative for $\mu > \mu_c$. In contrast the quadratic term remains negative regardless of the chemical potential in our example. Thus while $\tilde{\kappa}_{xy} - \kappa_{xy}^L$ changes the sign around $\mu = \mu_c$ in the chiral $p$-wave phase, $\tilde{\kappa}_{xy} - \kappa_{xy}^L$ has no drastic change due to the contribution of the quadratic term in the $fx_{2-y^2}$-wave phase in the low-temperature region.

The difference $\kappa_{xy} - \kappa_{xy}^L$ as a function of temperature is depicted in Fig. 4 where $\kappa_{xy}$ is obtained numerically from Eq. (6). $\kappa_{xy} - \kappa_{xy}^L$ is well described by the exponential function in the chiral $p$-wave phase [10]. In both amplitudes of the chemical potential ($\mu = 1.3t$ and $\mu = 1.5t$) the low-temperature behavior fits well to the $T$-quadratic term expected for the $fx_{2-y^2}$-wave phase, validating our low-temperature approximation.

For the electron-like Fermi surface with $\mu < \mu_c$, $\kappa_{xy} - \kappa_{xy}^L$ in the chiral $p$-wave phase and the $fx_{2-y^2}$-wave phase have opposite sign. This result indicates that the low-temperature behavior in $\kappa_{xy}$ may give the information concerning the pairing symmetry in bulk Sr$_2$RuO$_4$.

4. Conclusions
Motivated by the transition metal compound Sr$_2$RuO$_4$ we have investigated the thermal Hall conductivity in the spin-triplet superconducting phases with broken time-reversal symmetry. By means of the two-dimensional tight-binding model describing the $\gamma$ band, we obtain the temperature dependence of the thermal Hall conductivity in the chiral $p$-wave phase and the $fx_{2-y^2}$-wave phase. The latter state has gapless quasiparticle excitations due to line nodes yielding a $T^2$ correction to the thermal Hall conductivity on top of the universal $T$-linear term.

![Figure 4](Color online) $\kappa_{xy} - \kappa_{xy}^L$ for $\mu = 1.3t$ and $\mu = 1.5t$. The dotted lines stand for the quadratic term in Eq. (12) in the $fx_{2-y^2}$-wave phase.
We emphasize here that for the electron-like Fermi surface (as realized in Sr$_2$RuO$_4$) the sign of the deviation from universal low-temperature thermal Hall conductivity for the $f_{x^2-y^2}$-wave state is different from that for the chiral $p$-wave state. This qualitative result may, in principle, enable us to experimentally test the pairing state for nodal gaps in Sr$_2$RuO$_4$.

References