Possible anomalous Doppler shift effect in superconductor Sr$_2$RuO$_4$

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The effect of the Doppler shift is studied in a model for the $\alpha$-$\beta$ bands of Sr$_2$RuO$_4$ consisting of two hybridized 1D bands. Assuming a superconducting gap with nodes in the diagonal directions, we examine the oscillation of the surface density of states and the thermal conductivity under a rotating magnetic field. Upon varying the strength of the hybridization, the oscillation in these quantities is found to exhibit 2D to 1D crossover. In the crossover regime, which corresponds to the actual Sr$_2$RuO$_4$, the thermal conductivity exhibits a two-fold-symmetry oscillation, while the four-fold-symmetry component in the oscillation is barely detectable.

A ruthenate superconductor Sr$_2$RuO$_4$ has attracted much attention as a possible candidate for spin-triplet superconductor. After a theoretical prediction that the pairing should occur in the spin-triplet channel, several experiments have in fact supported this possibility. Early predictions were that the most probable $d$-vector is of the form $\mathbf{d}(\mathbf{k}) = (k_x \pm ik_y)\hat{z}$. In this case, the gap does not have nodes, so the material should be a gapful superconductor. However, recent experiments indicate the existence of nodes (or node-like structures) in the energy gap. Stimulated by these experiments, several theoretical models with gaps having line nodes or node-like structures have been proposed. On the other hand, thermal conductivity measurements under rotating magnetic field have indicated that the gap is almost isotropic within the planes, suggesting indirectly the existence of horizontal nodes in the gap, thereby excluding the possibility of vertical nodes or node-like structures proposed in some theoretical studies. These measurements under magnetic field have motivated our study.

In the presence of a magnetic field, it is known that the energy spectrum of the quasiparticle is influenced by the Doppler shift. The Doppler shifted states around the nodes of the superconducting gap contributes to the density of states at the Fermi energy. If we assume a free-electron-like Fermi surface, the density of states is minimized (maximized) when the magnetic field is applied parallel to the nodal (antinodal) direction, thereby exhibiting a four-fold symmetry oscillation upon rotating the magnetic field. This effect can be used to probe the direction of the nodes by thermal conductivity measurement, but since such experiments can be strongly affected by phonons, we have recently proposed an alternative method: magnetotunneling spectroscopy. Namely, by rotating the magnetic field in the $ab$ plane, the surface density of states (SDOS), and thus the tunneling spectra, oscillates, which enables us to determine the position of the nodes in the gap without using the phase sensitive spectroscopy based on the appearance of the Andreev bound states. As a case study, we have considered the case of the high $T_c$ cuprates and an organic superconductor $\kappa$-(BEDT-TTF)$_2$X, where we found that the SDOS takes its minimum when the applied magnetic field is parallel to the nodal direction, as in systems having free-electron-like Fermi surface. It is not at all clear, however, whether this tendency holds regardless of the shape of the Fermi surface.

This is exactly where the present study sets in. Here we study the effect of the Doppler shift in the $\alpha$-$\beta$ bands, the quasi one-dimensional(1D) bands, of Sr$_2$RuO$_4$. This is motivated by some microscopic theories which propose the presence of superconducting gaps in these bands having nodes or node-like structures in the diagonal direction. Here we concentrate on the $\alpha$-$\beta$ bands, which implicitly assumes that a large nodeless gap opens in the $\gamma$ band and a small one in the $\alpha$-$\beta$ bands, so that the main contribution to the density of states at the Fermi level comes from the latter bands. Considering a 2D model in which two 1D bands are hybridized, and assuming a gap that has nodes in the four diagonal directions (which of course corresponds to vertical nodes in 3D systems), we calculate the SDOS and the thermal conductivity upon rotating the direction of the magnetic field. To our surprise, we find that the four-fold symmetry component in the oscillation of these quantities, which should be clearly visible in 2D systems having free-electron-like Fermi surface, can be barely seen when the hybridization is moderate as in the $\alpha$-$\beta$ bands of Sr$_2$RuO$_4$. What is even more striking in this case is that the thermal conductivity exhibits a strong two-fold-symmetry oscillation reflecting the quasi-one dimensional nature of the Fermi surface.

First let us focus on the tunneling spectrum, namely the SDOS. Assuming that the penetration depth is much longer than the coherence length, the vector potential can be expressed as $\mathbf{A}(\mathbf{r}) = (H \lambda e^{\gamma/\lambda} \sin \theta, -H \lambda e^{\gamma/\lambda} \cos \theta, 0)$,
Then the quasiparticle momenta \( y \) and \( A(r) \) can be approximated as \( A(r) \sim A_0 = (H\lambda \sin \theta, -H\lambda \cos \theta, 0) \). Then the quasiparticle momenta \( k_x \) and \( k_y \) in the \( x \) and \( y \) directions can be given as \( k_x = k_x + (H/\pi H_0) \sin \theta \) and \( k_y = k_y - (H/\pi H_0) \cos \theta \), where \( H_0 = \phi_0/(\pi^2 \lambda) \) with \( \phi_0 = h/(2e) \). Thus, the SDOS at zero energy (the Fermi energy) can be expressed as,

\[
\rho(\theta, H) = \int_{-\infty}^{\infty} d\omega \bar{\rho}_S(\omega) \text{sech}^2 \left( \frac{\omega}{2k_B T} \right), \tag{1}
\]

\[
\bar{\rho}_S(\omega) = \frac{1}{2} \sum_{k,\sigma} \left\{ |u_{k,\sigma}|^2 \left[ \delta(\omega - E_{k,\sigma}) + \delta(\omega - E_{-k,\sigma}) \right] + |v_{k,\sigma}|^2 \left[ \delta(\omega + E_{k,\sigma}) + \delta(\omega + E_{-k,\sigma}) \right] \right\}. \tag{2}
\]

\[
E_{\pm k,\sigma} = \frac{(\xi_{k,\sigma} - \xi_{-k,\sigma}) \pm \sqrt{(\xi_{k,\sigma} + \xi_{-k,\sigma})^2 + 4|\Delta_{k,\sigma}|^2}}{2}, \tag{3}
\]

where \( |u_{k,\sigma}|^2 \) and \( |v_{k,\sigma}|^2 \) are the dispersion of the \( d_{xz} \) and \( d_{yz} \) bands, respectively (see Fig.4) \( t \) and \( \mu \) are fixed at \( t = 0.18t_0 \) and \( \mu = 0.17t_0 \), where \( t_0 \) is the unit of the energy about 1eV, while \( t' \) is varied as a key parameter in the present study which controls the strength of the hybridization between the two bands. Appropriate value of \( t' \) for \( \text{Sr}_2\text{RuO}_4 \) should be \( t' = 0.01 \sim 0.02t_0 \), but \( t' \) is varied in a wider range to see the crossover between 1D and 2D.

As for the gap functions, its absolute value (note that only the absolute value enters in eqns.(3)\&(4)) are chosen as

\[
|\Delta_{k,\alpha}| = |\Delta_{k,\beta}| = \Delta_0 (|\cos(k_x) - \cos(k_y)|), \tag{6}
\]

in order to take into account the node-like structures of the spin-triplet gap functions (having \( p_x + ip_y \) symmetry) found in refs.[14, 15]. Although we assume this phenomenological form for simplicity, our conclusion is not qualitatively affected by the detailed form of the gap, that is, only the direction of the nodes is important. In the following calculation, we fix the parameters \( \Delta_0 = 0.05t_0 \) and \( T = 0.002t_0 \), but our conclusion is not qualitatively affected by the choice of these values.

In Fig.2, we plot the normalized SDOS \( \rho_T = \rho(\theta, H)/\rho(0, H = 0.15H_0) \) as a function of \( \theta \) for several values of \( t' \). In the case of \( t' = 0.11t_0 \), where the hybridization is strong and the Fermi surface is round, \( \rho_T \) is minimized at \( \theta = \pi/4 \), namely the nodal direction, and maximized at \( \theta = 0, \pi/2 \), the antinodal direction, which is consistent with the previous theories for 2D systems. By contrast, when the hybridization is weak and the bands are essentially 1D (\( t' = 0.005t_0 \)), the maximum and the minimum of the oscillation is entirely reversed. Consequently, for a moderate hybridization \( t' = 0.01t_0 \), the SDOS becomes almost constant upon rotating the magnetic field.

\[
\frac{1}{C^+} \approx 0.5 \quad \text{and} \quad \frac{1}{C^-} \approx 1 \quad \text{for} \quad H = 0.15H_0 \text{ with } a: t'/t = 0.1, b: t'/t = 0.01, \text{ and } c: t'/t = 0.005.
\]

This crossover between large and small \( t' \) can be understood as follows. Let us first note that the Doppler

![FIG. 1: Left: magnetic field H in the θ direction. Right: the 2D model considered in the present study.](image-url)
shift is essentially given by $\mathbf{v}_F \cdot \mathbf{A}_0$, where $\mathbf{v}_F$ is the Fermi velocity \([17]\) and the vector potential $\mathbf{A}_0$ is perpendicular to the magnetic field $\mathbf{H}$. When the hybridization is sufficiently strong, the Fermi surface is round as in Figs. (a1) and (a2), so that the situation is the same as in the previous studies for 2D systems. \([18]\) Namely, all the states around the diagonal nodes have non-zero $v_{F,x}$ and $v_{F,y}$, thereby contributing to the density of states when the magnetic field is applied in the antinodal direction (Fig. (a1)). When the field is applied in the nodal direction, on the other hand, the states around the nodes parallel to the field do not contribute to the density of states, while the contribution of the states around the nodes perpendicular to the field is only a factor of $\sqrt{2}$ larger than it is when the field is applied in the antinodal direction (Fig. (a2)). Thus, the SDOS becomes larger when the field is applied in the antinodal direction.

The situation completely changes when we consider the weak hybridization limit, $t' = 0$, where the two one-dimensional bands contribute independently to the density of states. In this case, when the magnetic field is applied along the antinodal direction (Fig. (b1)& (b3)), only the states on the Fermi surface parallel to the field gives contribution. On the other hand, for a field in the nodal direction, states on both Fermi surfaces have contribution that is a factor of $\sqrt{2}$ smaller than it is when the field is in the antinodal direction (Fig. (b2)). Consequently, in the 1D limit, the SDOS becomes larger when the field is applied in the nodal direction.

We now move on to the thermal conductivity. Thermal conductivity $\kappa_{xx}(\theta, H)$ can be expressed as \([24, 28]\)

$$\kappa_{xx}(\theta, H) = -\sum_{k, \sigma} \text{sech}^2 \left( \frac{E_{k,\sigma}}{k_B T} \right) E_{k,\sigma}^2 v_{k,x}^2 \tau_{k,\sigma} \quad (7)$$

with $v_{k,x} = (\partial E_{k,\sigma}/\partial k_x)$, where we assume a constant $\tau_{k,\sigma}$ with $\tau_{k,\sigma} = \tau_0$. As for the energy dispersion $E_k$, we assume the form adopted for the calculation of SDOS for simplicity. Although this may not accurately correspond to the actual experimental situation, we believe that the essential physics can be captured within this formalism.

The thermal conductivity for $H = 0.15H_0$, normalized as $\kappa_T = \kappa_{xx}(\theta, H)/\kappa_{xx}(0, H)$, is shown in Fig. (3a). For $t' = 0.1t_0$, $\kappa_T$ is minimized around $\theta = \pi/4$ and the oscillation essentially has a four-fold symmetry, which is consistent with the previous studies for 2D systems. \([13]\)

By contrast, for $t' = 0.005t_0$ and $t' = 0.01t_0$, $\kappa_T$ exhibits a strong two-fold-symmetry oscillation, taking its maximum at $\theta = \pi/2$ and a minimum at $\theta = 0$. The anomalous two-fold-symmetry oscillation in the case of weak to moderated hybridization can be understood by considering again the $t' = 0$ limit. Namely, when $\theta = 0$, only the states on the $d_{xz}$ branch of the Fermi surface, where $v_{kd} = 0$, gives contribution to the density of states (see Fig. (b1)), so that $\kappa_{xx}(0, H) \sim 0$ according to eq. (7) at zero temperature. When $\theta = \pi/2$, on the other hand, the states on the $d_{xz}$ branch contribute to the density of states (Fig. (b3)), so that $\kappa_{xx}(\theta, H)$ becomes large.

Let us now look into the four-fold-symmetry component of $\kappa_{xx}(\theta, H)$. Since the two-fold-symmetry components in $\kappa_{xx}(\theta, H)$ and $\kappa_{yy}(\theta, H)$ have the same absolute values and the opposite signs to each other, we can focus on the four-fold-symmetry component by looking into $\kappa_{fT}$ defined as $\kappa_{fT} = \kappa_f(\theta, H)/\kappa_f(0, H)$

$$\kappa_f(\theta, H) = \frac{1}{2}[\kappa_{xx}(\theta, H) + \kappa_{yy}(\theta, H)].$$
As seen in Fig. 11(b), the dependence of $\kappa_{xx}$ qualitatively resembles that of the SDOS shown in Fig. 2. Here again, the four-fold-symmetry component in the oscillation of $\kappa_{xx}(\theta, H)$ can be barely seen for moderate (and realistic) values of $t'$. The absence of (or very small) four-fold-symmetry component is consistent with the experimental observations in refs. 8, 9, but the angles where $\kappa_{xx}(\theta, H)$ is maximized and minimized are reversed compared to the two-fold-symmetry oscillation found in ref. 3. However, since we have studied the case of $T \ll \Delta_0$ considering that the effect of phonons can be neglected at low temperatures in the actual experiments, we believe that further experiments at temperatures much lower than the energy scale of the superconducting gap is necessary to verify our prediction for vertical diagonal nodes.

To summarize, we have studied the effect of the Doppler shift on SDOS and the thermal conductivity in a 2D model consisting of hybridized 1D bands, assuming a superconducting gap that has nodes in the diagonal directions. When the hybridization is strong and the Fermi surface is round, both the SDOS and $\kappa_{xx}(\theta, H)$ exhibits a four-fold-symmetry oscillation, taking a maximum (minimum) when the magnetic field is applied parallel to the nodal (anti-nodal) directions. What is more remarkable in the case of weak to moderate hybridization is that the thermal conductivity exhibits a strong two-fold-symmetry oscillation, reflecting the quasi-1D nature of the Fermi surface. Since the actual Sr$_2$RuO$_4$ corresponds to the regime with moderate hybridization, $\kappa_{xx}(\theta, H)$ should exhibit a two-fold-symmetry oscillation, taking its maximum (minimum) when the magnetic field is applied in the $y$ ($x$) direction, while the four-fold-symmetry component in the SDOS and $\kappa_{xx}(\theta, H)$ should be barely detectable.

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