Interband Coulomb Interaction and Horizontal Line Nodes in Triplet Superconductor Sr$_2$RuO$_4$

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A possible mechanism for the horizontal line nodes in triplet superconductor, Sr$_2$RuO$_4$, is proposed. We consider the interlayer Coulomb interaction, as well as the on-site Coulomb repulsion, between electrons in different bands. In the second order perturbation in the interband interaction, the effective interaction becomes dependent on $\cos \frac{qF}{2}$, resulting in the horizontal line nodes.

KEYWORDS: triplet superconductivity, line nodes, Hubbard model, Sr$_2$RuO$_4$

Since the discovery of the superconductivity in Sr$_2$RuO$_4$ by Maeno et al.,$^{1}$ its unique properties have been revealed by many experiments. Experiments on Knight shift$^{2}$ and elastic neutron scattering$^{3}$ show that the electrons make the triplet pairs with the $d$-vector parallel to $\hat{z}$ as predicted by Rice and Sigrist$^{4}$ in analogy with superfluid $^3$He. The superconductivity breaks the time-reversal symmetry, as indicated by $\mu$SR experiment.$^{5}$ The energy gap has line nodes as shown by the temperature dependence of specific heat,$^{6}$ and the relaxation in nuclear magnetic resonance (NMR).$^{7}$ The existence of the line nodes is confirmed by other experiments.$^{8-11}$ The absence of the angle dependence of the thermal conductivity in the magnetic field within the $a$-$b$ plane.$^{10,11}$ shows that the line nodes run horizontally on the Fermi surface.

When we assume that the order parameter depends only on $k_x$ and $k_y$, the phenomenological theory based on the group theory in the point group of D$_{4h}$ shows that existence of line nodes and the breakdown of the time-reversal symmetry are in general incompatible with the symmetry and that only accidental vertical line nodes are possible.$^{12}$ Quasi-two-dimensional nature of the Fermi surface, however, should be taken into account.$^{12}$ The Fermi surface in Sr$_2$RuO$_4$ consists of three cylindrical sheets, which are open in the $k_z$ direction. In this case the order parameter should be expanded in the Fourier series rather than Taylor series ($s$-, $p$-, and $d$- partial waves) in $k_z$. In the presence of the interlayer interaction, the horizontal line nodes are possible.$^{12}$

Triplet superconductivity is shown to be caused when spin fluctuation is anisotropic and the Fermi surface is one-dimensional.$^{13,14}$ Takimoto$^{15}$ showed that triplet superconductivity appears in the three-band Hubbard model when the on-site Coulomb interaction between electrons in different bands is large. Nomura and Yamada$^{16}$ studied the three-band Hubbard model in the perturbation theory up to third order. By solving the linearized Eliashberg equation numerically, they obtained that the triplet-superconductivity with the vertical line-node-like structure in the $\beta$ band is stabilized. The vertical line nodes, however, can be wiped out by the mixing of the order parameters compatible with the symmetry at $T < T_c$. Since they consider only two-dimensional model,$^{13-16}$ the possibility of the horizontal line node has not been studied.

The superconductivity with horizontal line nodes are studied by assuming the interlayer attractive interaction.$^{12,18-20}$ Zhitomirsky and Rice$^{17}$ has proposed the pair hopping model between bands, which they call interband proximity effect. In that model the active band has full gap on the Fermi surface, while the passive band has line nodes. They argued that there exists the pair hopping term from the pair at $\mathbf{r}$ and $\mathbf{r} + (a,0,0)$ in the active band to the pair at $\mathbf{r}$ and $\mathbf{r} + (a/2, a/2, c/2)$ in the passive band, where $a$ and $c$ are the lattice constants. The position of line nodes has not been studied experimentally yet. We have proposed that the existence of the horizontal line nodes in the nested part of the Fermi surface can be observed by the inelastic neutron experiment.$^{21}$

Recently, Kondo$^{22}$ studied the two-dimensional Hubbard model at $T = 0$ in the second order perturbation theory. He obtained that singlet superconductivity is stabilized in the wide range of electron filling.

In this paper we propose a mechanism for the horizontal line node in Sr$_2$RuO$_4$ by applying the Kondo’s approach to the multiband extended Hubbard model. We show that the effective interaction resulting in the line nodes can be derived from the lowest order in the interlayer interband Coulomb interaction.

The interband Coulomb interaction is written as

$$\mathcal{H}_{IB} = \sum_{k,k',\sigma'\sigma} \sum_{l\neq l'} V_{IB}(k-k') \times \sum_{\sigma} \sum_{l} \frac{c_{k',l,\sigma}^\dagger c_{k,l,\sigma}}{\epsilon_{k'} - \epsilon_{k}} \sigma' \sigma,$$

(1)

where $l$ is the band index and

$$V_{IB}(k-k') = V \left( 1 + \alpha \cos \frac{a(k_x - k'_x)}{2} \cos \frac{a(k_y - k'_y)}{2} \right) \times \cos \frac{c(k_z - k'_z)}{2}.$$

(2)

In the above $V$ is the on-site interband interaction and $\alpha V$ is the interlayer interband interaction.

The effective interaction in the second order in $V_{IB}$
is shown in Fig. 1. Note that singlet superconductivity and triplet superconductivity have the same form in this model. We get

\[
V_{\text{eff},l}(q) = -\chi^l(q_x, q_y) (V_{IB}(q))^2 + U \\
= V_0(q_x, q_y) + 2V_1(q_x, q_y) \cos \frac{cq_y}{2} \\
+ 2V_2(q_x, q_y) \cos cq_z,
\]

where \( q = k - k' \), \( U \) is the on-site intraband Coulomb interaction,

\[
V_0(q_x, q_y) = -\chi^l(q_x, q_y)(1 + \frac{a^2}{2} \cos^2 \frac{aq_x}{2} \cos^2 \frac{aq_y}{2}) + U,
\]

\[
V_1(q_x, q_y) = -\alpha \chi^l(q_x, q_y) \cos \frac{aq_x}{2} \cos \frac{aq_y}{2},
\]

\[
V_2(q_x, q_y) = -\frac{\alpha^2}{4} \chi^l(q_x, q_y) \cos^2 \frac{aq_x}{2} \cos^2 \frac{aq_y}{2}
\]

and \( \chi^l(q) \) is the susceptibility in the \( l \) band. We have neglected the \( k_z \) dependence in \( \epsilon_{kl'} \), since the Fermi surface has little warping in Sr\(_2\)RuO\(_4\). Then \( \chi^l(q) \) is independent of \( q_z \) and the \( q_z \) dependence of \( V_{\text{eff},l}(q) \) comes from the interlayer interaction. We have also neglected the second order perturbation in \( U \) and the Coulomb interaction between electrons at the nearest sites in the same plane. The interaction within the same plane changes only \( V_0(k_x, k_y) \) and does not affect \( V_1(k_x, k_y) \) and \( V_2(k_x, k_y) \) in Eq. (3). Since we are interested in the mechanism for the horizontal line nodes, we have neglected these terms.

We write the two-dimensional intersection of the Fermi surface as a function of \( \theta \), i.e. \( k \) on the Fermi surface is written as \( (k_F(\theta) \cos \theta, k_F(\theta) \sin \theta, k_z) \). As shown by Kondo,\(^{22}\) the most stable state at \( T = 0 \) is given by the solution

\[
-\int_{0}^{2\pi} d\theta' V_{F_1}(\theta, \theta') \rho(\theta') z(\theta') = \lambda z(\theta) \quad (i = 0, 1, 2)
\]

with the largest eigenvalue \( \lambda \), where

\[
V_{F_1}(\theta, \theta') = V_1(k_F(\theta) \cos \theta - k_F(\theta') \cos \theta', \theta).
\]

\( \rho(\theta') \) is the density of states on the Fermi surface and \( k_F(\theta) \) is the momentum dependence of the order parameter on the Fermi surface (\( \Delta(k) = \Delta_0(\theta), \Delta_0(\theta) \cos \frac{ck}{k_F} \), or \( \Delta_0(\theta) \cos \frac{ck_z}{k_F} \) for the singlet superconductivity and \( d_1(k) = \Delta_0(\theta), \Delta_0(\theta) \cos \frac{ck_z}{k_F} \), or \( \Delta_0(\theta) \cos \frac{ck_z}{k_F} \) for the triplet superconductivity with \( d(k) \parallel \hat{z} \)). By defining

\[
w(\theta) = \sqrt{\rho(\theta) z(\theta)}
\]

Eq. (7) becomes symmetric form as

\[
-\int_{0}^{2\pi} d\theta' \tilde{V}_{F_1}(\theta, \theta') w(\theta') = \lambda w(\theta) \quad (i = 0, 1, 2)
\]

where

\[
\tilde{V}_{F_1}(\theta, \theta') = V_{F_1}(\theta, \theta') \sqrt{\rho(\theta) \rho(\theta')}
\]

The similar equation is obtained by maximizing the average of the effective interaction on the Fermi surface with respect to the order parameter

\[
\int_{-\pi}^{\pi} d\theta V_{F_1}(\theta, \theta') w(\theta') \to \int_{-\pi}^{\pi} d\theta (\tilde{V}_{F_1}(\theta, \theta') w(\theta'))
\]

Comparing Eq. (14) with Eq. (10), we get

\[
\lambda = -\langle \tilde{V}_{F_1}(\theta, \theta') \rangle
\]

Using the Fourier expansion for \( z(\theta) \) we get the eigenvalue of the non-Hermite matrix\(^{22}\) from Eq. (7). We can obtain the eigenvalue problem with Hermite matrix from Eq. (10),

\[
\sum_{l'} M_{ll'}^{(i)} w_{l'} = \lambda w_l,
\]

where

\[
M_{ll'}^{(i)} = -\frac{1}{2\pi} \int_{0}^{2\pi} \int_{0}^{2\pi} d\theta d\theta' \tilde{V}_{F_1}(\theta, \theta') e^{i(\theta' - \theta)},
\]

and

\[
w(\theta) = \sum_{l} w_l e^{i\theta}.
\]

In Sr\(_2\)RuO\(_4\), the \( \beta \) and the \( \gamma \) band have the cylindrical Fermi surfaces with the cross section of 0.457 and 0.667 of the Brillouin zone, respectively.\(^{23}\) As a first step, we use the simple model that there are two bands which have the same energy dispersion. We take the simple model that there are two bands which have the same energy dispersion

\[
\epsilon_l(k) = \epsilon^l(k)
\]
\[ w(\theta) = \eta_2 w(\theta + \pi) = \eta_4 w(\theta + \frac{\pi}{2}) \]
\[ = \eta_U w(-\theta) = \eta_U' w(-\theta + \frac{\pi}{2}) \]

(20)

where \( \eta_2, \eta_4, \eta_U \) and \( \eta_U' \) are the characters of the \( \pi \)-rotation around the \( z \)-axis, the \( \frac{\pi}{2} \)-rotation around the \( z \)-axis, the \( \pi \)-rotation around the \( x \)-axis, and the \( \pi \)-rotation around the \( x = y \) line, respectively for each one-dimensional irreducible representation. The irreducible representations \( a_1, a_2, b_1, \) and \( b_2 \) behave as extended s-wave, g-wave \( (k_xk_y(k_x^2 - k_y^2)), k_x^2 - k_y^2, \) and \( k_xk_y, \) respectively.

We exclude the constant term \( w_{\theta=0} \), which should be included in the \( a_1 \) symmetry, in the \( k_z \)-independent order parameter in order to avoid a large intraband on-site interaction \( U \). Since \( \rho(\theta) \) is not constant, the effect of \( U \) is not completely avoided by removing \( w_0 \). The intraband on-site interaction, however, changes only superconductivity with the \( k_z \)-independent \( a_1 \) symmetry which is not very important in this study as we show below. Thus we use the approximation of removing \( w_0 \).

For the two-dimensional representation, \( w(\theta) \) should satisfy

\[ w(\theta) = -w(\theta + \pi) = \pm w(-\theta). \]

(21)

In the present approximation that only the lowest order in the order parameter is considered, two-dimensional representation corresponds to two degenerate states for \( \pm \) in Eq. (21), which behaves as \( k_x \) and \( k_y \), respectively. For example, the \( e \) symmetry for \( \tilde{V}_{F1}(\theta, \theta') \) has the order parameter represented by

\[ d_z(k) \approx \Delta_0 k_x \cos \frac{ck_x}{2}, \Delta_0 k_y \cos \frac{ck_y}{2} \]

or

\[ \Delta(k) \approx \Delta_0 k_x \sin \frac{ck_x}{2}, \Delta_0 k_y \sin \frac{ck_y}{2} \]

(22)

(23)

In our approximation triplet and singlet superconductivity have the same stability. The actual order parameter in the two-dimensional representation is expected to be

\[ d_z(k) \approx \Delta_0 (k_x + ik_y) \cos \frac{ck_x}{2} \]

or

\[ \Delta(k) \approx \Delta_0 (k_x + ik_y) \sin \frac{ck_x}{2} \]

(24)

(25)

if the higher order terms in the order parameter is taken into account for the superconducting condensation energy.

In Figs. 2-4 we plot the maximum eigenvalues for each irreducible representation as a function of the electron density \( n_e \) for \( \alpha = 0.1 \). It is seen from Figs. 2-4 that the superconductivity with \( e \times \cos \frac{ck_x}{2} \) symmetry (and \( e \times \sin \frac{ck_x}{2} \) symmetry, which degenerates with \( e \times \cos \frac{ck_y}{2} \) in the present model) has the maximum eigenvalue for \( 0.8 \gtrsim n_e \gtrsim 0.5 \).

In Fig. 5 we show the phase diagram in the \( n_e-\alpha \) plane. The triplet superconductivity with horizontal line nodes \( (e \times \cos \frac{ck_x}{2}) \) is stabilized in some region of parameters, which may be realized in \( \text{Sr}_2\text{RuO}_4 \).

We have shown that the effective interaction due to the interband interaction can cause the superconductivity with horizontal line nodes. The mechanism for the superconductivity proposed in the present paper is the extension of the idea by Little,24 who proposed the attractive interaction between electrons via a side-chain Coulomb interaction. In our case the different band plays the role of the side-chain.

The degeneracy between \( e \times \cos \frac{ck_x}{2} \) and \( e \times \sin \frac{ck_x}{2} \) can be lifted by several effects such as warping of the Fermi surface due to interlayer hopping,19 intra-band
interactions, higher order perturbation, anisotropy of the spin susceptibility, etc.

The order parameter with horizontal line-node is stabilized by the relatively small interlayer interaction ($\alpha \approx 0.1$). The anisotropic superconductivity due to the second order perturbation in the on-site interaction is caused by the variation of $\chi(q)$ from its average in order to avoid the large on-site Coulomb repulsion $U$. On the other hand, the product of the on-site interaction and the interlayer interaction can use the full value of the susceptibility to get the superconductivity. This is why the superconductivity with horizontal line nodes is stabilized by a small interlayer interaction.

We have shown that the triplet superconductivity with horizontal line nodes, i.e. $e \times \cos \frac{k_z}{2}$ state, is shown to be stabilized in a reasonable parameter range. We have neglected the fact that $\chi(q)$ is large due to the nesting nature of the $\alpha$ and $\beta$ bands. If we consider the enhancement of $\chi(q)$, the effective interaction in the $\gamma$ band becomes large due to the mechanism discussed in this paper.

The interband proximity effect is compatible with the effective interaction studied in this paper. When both interband interlayer interaction and interband proximity effect are considered, the superconductivity with the horizontal line nodes will be much favored.

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