Fermi-Surface Topology and Superconductivity Induced by Jahn-Teller Phonons

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Abstract. We discuss emergence of superconductivity in a two-dimensional $e_g$-electron system coupled with Jahn-Teller phonons in the framework of the Migdal-Eliashberg theory. Here we focus on the dependence of superconducting transition temperature $T_c$ on the Fermi-surface structure controlled by the Slater-Koster integrals of $e_g$-electron hopping. When the Fermi-surface structure is abruptly changed, in general, there appears the van Hove singularity in the density of states, leading to the enhancement of $T_c$. In addition to it, for the superconductivity induced by Jahn-Teller phonons, we also observe the increase of $T_c$ apart from the van Hove singularity point, when the $e_g$-electron system exhibits disconnected Fermi surfaces. Even for the pocket-like Fermi-surface structure, we find the relatively high $T_c$ in comparison with the case of single Fermi surface. This is understood by the fact that the pair-hopping attraction between Cooper pairs on different Fermi surfaces is enhanced by Jahn-Teller phonons.

1. Introduction

In the research field of condensed matter physics, it has been an important long-standing issue to develop materials which exhibit high superconducting transition temperature $T_c$. Since the discovery of high-$T_c$ cuprate superconductors [1], it has been widely recognized that there exists a route to obtain anisotropic superconductivity with relatively high $T_c$ originating from strong electron correlation. In particular, concerning the superconductivity characterized by singlet Cooper pair, it has been established that there occurs $d$-wave superconductivity due to spin fluctuations near the antiferromagnetic phase [2, 3, 4].

Recently, another possible route to obtain exotic superconductivity has attracted much attention, even though $T_c$ is not always so high. Namely, multiband effect has been focused in correlated electron materials such as Sr$_2$RuO$_4$ [5], MgB$_2$ [6], Na$_{0.35}$CoO$_2$·1.3H$_2$O [7], and iron pnictides [8, 9]. Several kinds of heavy-electron superconductors also exhibit multi-sheets of Fermi surfaces. Immediately after the Bardeen-Cooper-Schrieffer theory [10], the multiband effect on $T_c$ was discussed in a simple two-band electron model [11]. In recent years, multiband superconductivity has been investigated from various viewpoints [12, 13, 14, 15, 16, 17, 18, 19, 20]. In particular, the discovery of superconductivity in iron pnictides has triggered the revival of the research of multiband superconductivity [21, 22, 23, 24].

In general, in electron systems with degenerate orbitals, Jahn-Teller effect plays an important role, for instance, in manganites [25, 26], since Jahn-Teller distortions are known to lift the degeneracy in electron orbitals. The attractive interaction mediated by Jahn-Teller phonons has been analyzed in a weak-coupling limit by one of the present authors [27]. It has been found
that $T_c$ is significantly enhanced by the interband attraction even within the weak-coupling limit, when Jahn-Teller phonons are active.

In this paper, the effect of the Fermi-surface topology on the emergence of superconductivity is discussed in the two-dimensional $e_g$-electron system coupled with Jahn-Teller phonons on the basis of the strong-coupling theory. It is well known that the van Hove singularity occurs in the density of states due to the abrupt change of the Fermi-surface structure, leading to the enhancement of $T_c$. We find that $T_c$ is increased for the hopping parameters apart from the van Hove singularity point, when the $e_g$-electron system possesses disconnected Fermi surfaces in comparison with the case of single Fermi surface. The increase of $T_c$ is due to the large pair-hopping amplitude between different Fermi surfaces enhanced by the Jahn-Teller phonons.

2. Model and Formulation

We consider the two-dimensional square lattice and the lattice constant is taken as unity. In the unit of $\hbar=k_B=1$, the model Hamiltonian used here is given by

$$
H = \sum_{k,\sigma,\gamma,\gamma'} \varepsilon_{k\gamma\gamma'} d_{k\gamma\sigma}^\dagger d_{k\gamma'\sigma} + \sum_q [g_2(a_{2q} + a_{2q}^\dagger)\tau_{3q} + g_3(a_{3q} + a_{3q}^\dagger)\tau_{2q}]
$$

$$
+ \sum_q [\omega_2(a_{2q}^\dagger a_{2q} + 1/2) + \omega_3(a_{3q}^\dagger a_{3q} + 1/2)],
$$

where $d_{k\gamma\sigma}$ denotes an annihilation operator of an $e_g$ electron with spin $\sigma$ and momentum $k$ in the orbital $\gamma$ (=a and b), $a$ and $b$ indicate $x^2-y^2$ and $3z^2-r^2$ orbitals, respectively, $\varepsilon_{k\gamma\gamma'}$ denotes the electron energy depending on orbitals, $a_{2q}$ and $a_{3q}$ are annihilation operators for $(x^2-y^2)$- and $(3z^2-r^2)$-type Jahn-Teller phonons, respectively, $g_2$ and $g_3$ indicate electron-phonon coupling constants, $\tau_{3q}=\sum_{k,\sigma}(d_{k+q\sigma}^\dagger d_{k\sigma} + d_{k+q\sigma}^\dagger d_{k\sigma})$, $\tau_{2q}=\sum_{k,\sigma}(d_{k+q\sigma}^\dagger d_{k\sigma} - d_{k+q\sigma}^\dagger d_{k\sigma})$, and $\omega_2$ and $\omega_3$ denote Jahn-Teller phonon energies for $(x^2-y^2)$- and $(3z^2-r^2)$-type modes, respectively.

As for the electron kinetic energies $\varepsilon_{k\gamma\gamma'}$, they are expressed as

$$
\varepsilon_{k\alpha\alpha} = (1/2)[(dd\sigma) + (dd\delta)][(cos k_x + cos k_y)],
$$

$$
\varepsilon_{kbb} = (1/2)[(dd\sigma) + 3(dd\delta)][(cos k_x + cos k_y)],
$$

$$
\varepsilon_{kab} = \varepsilon_{k\alpha\beta} = -\sqrt{3}/2)[(dd\sigma) - (dd\delta)][(cos k_x - cos k_y)],
$$

where $(dd\sigma)$ and $(dd\delta)$ denote the Slater-Koster integrals.

In order to evaluate the superconducting transition temperature $T_c$, we solve the gap equation obtained by evaluating both normal and anomalous electron self-energies due to the electron-phonon interaction. Here we consider the spin-singlet $s$-wave Cooper pair with the even function of frequency. In the second-order perturbation theory in terms of $g_2$ and $g_3$, the linearized gap equation at $T=T_c$ is expressed by

$$
\phi_{\mu\nu}(i\omega_n) = T \sum_{n'} \sum_{\mu',\nu'} V_{\mu\mu',\nu\nu'}(i\omega_n - i\omega_{n'}) F_{\mu'\nu'}(i\omega_n),
$$

where $\phi_{\mu\nu}(i\omega_n)$ is anomalous self-energy, $\omega_n$ is fermion Matsubara frequency defined by $\omega_n = (2n+1)\pi T$ with a temperature $T$ and an integer of $n$, $F$ is anomalous Green’s function, and $V_{\mu\mu',\nu\nu'}(i\omega_n)$ is phonon-mediated interaction, given by

$$
V_{aa,aa}(i\nu_n) = V_{bb,bb}(i\nu_n) = -V_{aa,bb}(i\nu_n) = -V_{bb,aa}(i\nu_n) = g_2^2 D_3(i\nu_n),
$$

$$
V_{ab,ab}(i\nu_n) = V_{ab,ba}(i\nu_n) = V_{ba,ab}(i\nu_n) = V_{ba,ba}(i\nu_n) = g_2^2 D_2(i\nu_n),
$$

(4)
and other components are zeros. Here \( \nu_n \) is boson Matsubara frequency defined by \( \nu_n = 2\pi T n \) and \( D_2 \) and \( D_3 \) are phonon Green’s functions, respectively, given by

\[
D_2(i\nu_n) = \frac{2\omega_2}{(i\nu_n)^2 - \omega_2^2}, \quad D_3(i\nu_n) = \frac{2\omega_3}{(i\nu_n)^2 - \omega_3^2}.
\]

In the vicinity of \( T_c \), \( F \) is given in the linearized form as

\[
F_{\mu\nu}(i\omega_n) = -\sum_k \sum_{\mu',\nu'} G_{\mu\nu'}(k, i\omega_n) G_{\nu\mu'}(-k, -i\omega_n) \phi_{\mu'\nu'}(i\omega_n),
\]

where \( G \) denotes normal Green’s function, given by

\[
[G(k, i\omega_n)]^{-1} = [G(0)(k, i\omega_n)]^{-1} - \Sigma_{\mu\nu}(i\omega_n).
\]

Here \( G_0 \) is non-interacting electron Green’s function, given in the matrix form as

\[
G^{(0)}(k, i\omega_n) = \begin{pmatrix}
i\omega_n + \mu - \varepsilon_{kaa} & -\varepsilon_{kab} \\
-\varepsilon_{kba} & i\omega_n + \mu - \varepsilon_{kbb}
\end{pmatrix}^{-1},
\]

where \( \mu \) is a chemical potential determined from the relation of \( n = 2T \sum_n \sum_k \text{Tr} G(k, i\omega_n) \) and \( n \) is electron number per site. The normal self-energy \( \Sigma_{\mu\nu}(i\omega_n) \) is given in the second-order perturbation theory in terms of \( g_2 \) and \( g_3 \) as

\[
\Sigma_{\mu\nu}(i\omega_n) = -T \sum_{n'} \sum_{\mu',\nu'} \sum_k V_{\mu\mu',\nu\nu'}(i\omega_n - i\omega_{n'}) G^{(0)}_{\mu\nu'}(k', i\omega_{n'}).
\]

In order to obtain \( T_c \), first we calculate the normal self-energy \( \Sigma \) in eq. (9). Next we solve the gap equation eqs. (3) and (6) by using \( G \) in eq. (7). Then, we obtain \( T_c \) as a temperature at which the positive maximum eigenvalue of eq. (3) becomes unity. Throughout this paper, the energy unit \( t \) is taken as \( t = |(dd\sigma)| \). Note that we set \( (dd\sigma) = -t \) in this paper. For the sum on the imaginary axis, we use 131,072 Matsubara frequencies. In order to accelerate the sum of large amount of Matsubara frequencies in eqs. (3) and (9), we exploit the fast-Fourier-transformation algorithm. For the evaluation of the eigenvalue of the gap equation eq. (3), we use the power method. As for the phonon energy, we set \( \omega_2/t = \omega_3/t = 0.2 \). We define the non-dimensional electron-phonon coupling constants as \( \lambda_2 = 2g_2^2/(t\omega_2) \) and \( \lambda_3 = 2g_3^3/(t\omega_3) \), which are set as \( \lambda_2 = \lambda_3 = 0.8 \). Concerning the electron number density, we set \( n = 1.5 \) in this paper.

3. Calculated Results

In Fig. 1, we show the change of the Fermi surfaces, when we control the Slater-Koster integral \( (dd\delta)/t \) from \(-2.0 \) to \( 2.0 \) for \( (dd\sigma)/t = -1.0 \). We note that the term of “Fermi surface” is conventionally used here, although we consider the two-dimensional system. Note also that the normal self-energy effect is included in the determination of the chemical potential \( \mu \) when we fix the electron number density \( n \) as \( n = 1.5 \). The temperature is set as \( T/t = 10^{-4} \) in Fig. 1.

For \( (dd\delta) < 0 \), we find a couple of Fermi surfaces, except for the case of \( (dd\delta)/t = -1.0 \), at which two Fermi surfaces accidentally coincide with each other, as understood from the electron dispersion of eq. (2). For the cases of \( (dd\delta)/t = -1.5 \) and \( -0.66 \), we observe that the Fermi surface touches the X and Y points. Namely, for such cases, the van Hove singularities will appear at the Fermi level in the density of states.

At \( (dd\delta) = 0 \), the center of one Fermi surface exists on the \( \Gamma \) point, while another has the center at the \( M \) point. Note that the nesting vectors are approximately given by \( (\pi, 0) \) and
(0, π) in this case, leading to the stabilization of the metallic phase in contrary to the cooperative Jahn-Teller distortion with the ordering vector of (π, π) [28].

When we increase the value of \((ddδ)/t\) from zero, the Fermi-surface topology is the same as that of the case of \((ddδ)/t = 0\) for a while, although the shape of Fermi surfaces is gradually changed. For \((ddδ)/t\) between 0.2 and 0.3, the Fermi surface with the center at the Γ point disappears and we obtain single Fermi surface.

For \((ddδ)/t ≈ 0.6\), there appears another Fermi surface with the center at the M point. At \((ddδ)/t = 1.0\), there occurs the reconstruction of the Fermi-surface structure and we find four pocket-like Fermi surfaces around the points of \((±π/2, ±π/2)\) and \((±π/2, ±π/2)\). This pocket-like Fermi-surface structure continues to exist for a while, but for \((ddδ)/t ≈ 1.3\), the four pocket-like Fermi surfaces are connected so as to form a star-like Fermi surface. At \((ddδ)/t ≈ 1.5\), in addition to the large-size star-like Fermi surface, we find a small-size Fermi surface with the center at the Γ point. This small-size Fermi surface disappears at \((ddδ)/t ≈ 1.6\). Then, for \((ddδ)/t ≥ 1.6\), we observe the single Fermi surface.

Let us summarize the change of the number \(N_F\) of the Fermi surfaces: \(N_F = 2\) for \(-2.0 ≤ (ddδ)/t ≤ 0.25\), \(N_F = 1\) for \(0.25 ≤ (ddδ)/t ≤ 0.6\), \(N_F = 2\) for \(0.6 ≤ (ddδ)/t ≤ 0.8\), \(N_F = 4\) for \(0.8 ≤ (ddδ)/t ≤ 1.3\), \(N_F = 2\) for \(1.3 ≤ (ddδ)/t ≤ 1.6\), and \(N_F = 1\) for \(1.6 ≤ (ddδ)/t ≤ 2.0\). Note that we consider the extended zone when we count \(N_F\).

Now we consider the change of \(T_c\) depending on the Fermi-surface topology. In Fig. 2, we show \(T_c/t\) vs. \((ddδ)/t\) in the range of \(-2.0 ≤ (ddδ)/t ≤ 2.0\). In the region of negative \((ddσ)\), we observe the overall tendency of the increase of \(T_c\) with the increase of \((ddδ)/t\) from \(-2.0\) to \(0.0\), except for the cusps at \((ddδ)/t = -1.5\) and \(-0.7\). As easily understood from the Fermi-surface structure, those cusps originate from the van Hove singularities. The overall tendency of the increase of \(T_c\) is explained by the increase of the density of states. When we decrease \((ddδ)\) in

![Figure 1. Variation of the Fermi surfaces for \((ddσ)/t = -1.0\) depicted in the first Brillouin zone of \(-π ≤ k_x ≤ π\) and \(-π ≤ k_y ≤ π\) with Γ = (0, 0), X = (π, 0), Y = (0, π), and M = (π, π).](image-url)
in the present paper, since the perfectly degenerate Fermi surfaces are unrealistic. It may be interesting to pursue such exotic solutions, but we do not consider them.

\[ \text{dd}\delta \]

has no singular behavior around at \((\text{dd}\delta)/t = 0\). The Fermi-surface topology is abruptly changed again, leading to the van Hove singularity.

This is understood from the discussion of \(N_F\). Since the Fermi-surface topology is not so drastically changed in the region of \((\text{dd}\delta)/t < 0\), as understood from the density of states and the van Hove singularity. Note that \(T_c\) is continuously changed at \((\text{dd}\delta)/t = -1.0\), in which two Fermi surfaces are perfectly degenerate. In this paper, we consider only the spin-singlet s-wave solution, which has no singular behavior around at \((\text{dd}\delta)/t = -1.0\). However, when two Fermi surfaces are degenerate, in general, it is possible to consider other solutions such as odd-frequency and spin-triplet pairs. It may be interesting to pursue such exotic solutions, but we do not consider them in the present paper, since the perfectly degenerate Fermi surfaces are unrealistic.

When we increase \((\text{dd}\delta)\) from zero, \(T_c\) is monotonically increased for \(0 \leq (\text{dd}\delta)/t \lesssim 0.2\). This is also understood from the increase of the density of states. At \((\text{dd}\delta)/t = 0.2\), we find a cusp which originates from the van Hove singularity due to the abrupt change of the Fermi-surface topology, i.e., the disappearance of the Fermi surface with the center at the \(\Gamma\) point. For \(0.2 \lesssim (\text{dd}\delta)/t \lesssim 0.6\), there appears the single Fermi surface and \(T_c\) is totally low, since the density of states is suppressed in this region. However, when we increase \((\text{dd}\delta)\), \(T_c\) is rapidly increased. Around at \((\text{dd}\delta)/t = 0.6\), there occurs a new Fermi surface and the Fermi-surface topology is abruptly changed again, leading to the van Hove singularity.

For \(0.6 \lesssim (\text{dd}\delta)/t \lesssim 1.6\), \(T_c\) depends on the values of \((\text{dd}\delta)\), but we observe that the magnitude of \(T_c\) is kept high as \(T_c/t = 0.005 \sim 0.01\), even though the Fermi-surface topology is changed in this region. We emphasize that we always find the plural numbers of the Fermi surfaces in the corresponding region. We imagine that the value of \(T_c\) is heavily decreased, when \(N_F\) is reduced to 1. In fact, for \((\text{dd}\delta)/t \gtrsim 1.6\) with the single Fermi surface, we observe the rapid decrease of \(T_c\), which cannot be simply explained by the decrease of the density of states. Note that for \(1.6 \lesssim (\text{dd}\delta)/t \leq 2.0\), \(T_c\) is totally low and it is difficult to obtain \(T_c\) with enough precision in this region, since \(T_c\) approaches the lower limit which we can safely calculate.

The enhancement of \(T_c\) in the case of the plural numbers of the Fermi surfaces is explained by the enhancement of the pair-hopping attraction between Cooper pairs on different Fermi surfaces due to Jahn-Teller phonons [27]. This pair-hopping attraction does not work for the case of the single Fermi surface. Thus, \(T_c\) in the case of the plural numbers of the Fermi surfaces is enhanced in comparison with the case of \(N_F = 1\). This enhancement mechanism still works even for the case of small-size pocket-like Fermi surfaces.

![Figure 2](image-url)

**Figure 2.** Superconducting transition temperature \(T_c/t\) vs. \((\text{dd}\delta)/t\) for \((\text{dd}\sigma)/t = -1.0, \omega_2/\omega_3 = 0.2, \lambda_2 = \lambda_3 = 0.8,\) and \(n = 1.5\) in the range of \(-2.0 \leq (\text{dd}\delta)/t \leq 2.0\).
4. Discussion and Summary
In this paper, we have ignored the effect of Coulomb interaction. Here it is interesting to consider a possibility that the pair-hopping attraction due to Jahn-Teller phonons is changed to be repulsive by the effect of inter-band Coulomb interaction. If we include the breathing-mode phonons and the intra-band pair interaction is kept negative, we obtain the superconductivity even if the pair-hopping amplitude is repulsive. Note that in such a case, we may provide an alternative scenario for $s_\pm$-wave pairing, which has been proposed for iron pnictides [21, 22, 23, 24]. It is one of our future problems to treat both Jahn-Teller phonons and inter-band Coulomb repulsion.

In summary, we have found that in the two-band system coupled with Jahn-Teller phonons, $T_c$ becomes relatively high for the case of the plural numbers of the Fermi surfaces. This result is understood by the pair-hopping attraction between different Fermi surfaces enhanced by Jahn-Teller phonons.

Acknowledgments
This work has been supported by a Grant-in-Aid for Scientific Research (C) (No. 24540379) of Japan Society for the Promotion of Science and a Grant-in-Aid for Scientific Research on Innovative Areas “Heavy Electrons” (No. 20102008) of The Ministry of Education, Culture, Sports, Science, and Technology, Japan. The computation in this work has been done using the facilities of the Supercomputer Center of Institute for Solid State Physics, University of Tokyo.

References
[1] J. G. Bednorz and K. A. Müller: Z. Phys. B 64 (1986) 189.
[2] T. Moriya and K. Ueda: Adv. Phys. 49 (2000) 555.
[3] T. Moriya and K. Ueda: Rep. Prog. Phys. 66 (2003) 1290.
[4] Y. Yanase, T. Jujo, T. Nomura, H. Ikeda, T. Hotta, and K. Yamada: Phys. Rep. 387 (2003) 1.
[5] Y. Maeno, H. Hashimoto, K. Yoshida, S. Nishizaki, T. Fujita, J. G. Bednorz, and F. Lichtenberg: Nature (London) 372 (1994) 532.
[6] J. Nagamatsu, N. Nakagawa, Y. Muranaka, Y. Zenitani, and J. Akimitsu: Nature (London) 410 (2001) 63.
[7] K. Takada, H. Sakurai, E. Takayama-Muromachi, F. Izumi, R. A. Dilanian, and T. Sasaki: Nature (London) 422 (2003) 53.
[8] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono: J. Am. Chem. Soc. 130 (2008) 3296.
[9] K. Ishida, Y. Nakai, and H. Hosono: J. Phys. Soc. Jpn. 78 (2009) 062001.
[10] J. Bardeen, L. N. Cooper, and J. R. Schrieffer: Phys. Rev. 108 (1957) 1175.
[11] H. Suhl, B. T. Matthias, and L. R. Walker: Phys. Rev. Lett. 2 (1959) 552.
[12] T. Takimoto: Phys. Rev. B 62 (2000) 14641.
[13] A. Bussmann-Holder, M. Gulacsi, and A. R. Bishop: Phil. Mag. B 82 (2002) 1749.
[14] T. Nomura and K. Yamada: J. Phys. Soc. Jpn. 71 (2002) 404.
[15] T. Takimoto, T. Hotta, and K. Ueda: Phys. Rev. B 69 (2004) 104504.
[16] Y. Yanase, M. Mochizuki, and M. Ogata: J. Phys. Soc. Jpn. 74 (2005) 430.
[17] Y. Yang: Physica D 200 (2005) 60.
[18] K. Yada and H. Kontani: J. Phys. Soc. Jpn. 75 (2006) 033705.
[19] O. V. Dolgov and A. A. Golubov: Phys. Rev. B 77 (2008) 214526.
[20] C. Bersier, A. Floris, P. Cudazzo, G. Profeta, A. Sanna, P. Bernardini, M. Monni, S. Pittalis, S. Sharma, H. Glawe, A. Continenza, S. Massidda, and E. K. U. Gross: J. Phys.: Condens. Matter 21 (2009) 164209.
[21] I. I. Mazin, D. J. Singh, M. D. Johannes, and M. H. Du: Phys. Rev. Lett. 101 (2008) 057003.
[22] K. Kuroki, S. Onari, R. Arita, H. Usui, Y. Tanaka, H. Kontani, and H. Aoki: Phys. Rev. Lett. 101 (2008) 087004.
[23] H. Ikeda: J. Phys. Soc. Jpn. 77 (2008) 123707.
[24] T. Nomura: J. Phys. Soc. Jpn. 78 (2009) 034716.
[25] E. Dagotto, T. Hotta, and A. Moreo: Phys. Rep. 344 (2001) 1.
[26] T. Hotta: Rep. Prog. Phys. 69 (2006) 2061.
[27] T. Hotta: J. Phys. Soc. Jpn. 79 (2010) 023709.
[28] T. Hotta: Phys. Rev. B 67 (2003) 104428.