

Superconductivity in e_g orbital systems with multi-Fermi-surface

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We study superconductivity in e_g orbital systems on a square lattice by applying fluctuation exchange approximation. For such a multiorbital system, even-parity spin-triplet and odd-parity spin-singlet states are allowed by constructing a pair with antisymmetrical orbitals. Indeed, it has been found that such states appear in a two-orbital Hubbard model in which Fermi surfaces for both orbitals are the same. In the e_g orbital model, the number of Fermi surfaces and their structures depend on the ratio of the Slater-Koster integrals, and exotic superconducting states peculiar to a multi-Fermi-surface system may occur. We find several superconducting states depending on the structure of the Fermi surfaces and the number of electrons per site. In particular, we find even-parity spin-triplet and odd-parity spin-singlet states with a finite total momentum like the Fulde-Ferrell-Larkin-Ovchinnikov state even without a magnetic field. Such an exotic pair can be stabilized with a finite total momentum, which connects the centers of Fermi surfaces with similar structures.

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1. Introduction

The role of orbital degree of freedom on magnetism has been studied. For example, importance of the orbital degree of freedom has been recognized for manganites [1, 2] and for f -electron systems [2, 3]. Then, it is revealed that magnetism in multi-orbital systems has a rich variety. Recently, the roles of orbital degree of freedom on superconductivity have also been studied theoretically for several materials [4, 5, 6, 7, 8, 9, 10, 11], and it has been found that orbital degree of freedom is important for determination of pairing symmetry.

To understand the effects of orbital degree of freedom on superconductivity for simple cases, two-orbital Hubbard models with the same dispersion for both orbitals have been studied by a mean-field theory [12], by a dynamical mean-field theory [13, 14], and by a fluctuation exchange (FLEX) approximation [15]. These studies have revealed that s -wave spin-triplet state and p -wave spin-singlet state, which satisfy the Pauli principle by composing an orbital state of a pair antisymmetrically, can be stabilized in the two-orbital Hubbard model.

The two-orbital Hubbard model describes a system where Fermi surfaces for both orbitals are the same. To discuss more realistic situations, we should improve the two-orbital Hubbard model. In particular, we should include effects of orbital symmetry, such as orbital dependent hopping integrals which describes a multi-Fermi-surface system and transformation property of orbitals. These properties are important for magnetism in d -electron systems [1, 2] and in f -electron systems [2, 16, 17], and should be important also for superconductivity.

In this paper, we consider an e_g orbital model on a square lattice in order to include such effects, and investigate possible superconducting states by applying FLEX approximation, which has been extended to multi-orbital models [6, 7, 9, 10, 11, 15]. We find several superconducting states depending on model parameters. In particular, we find that pairing states with a finite total momentum like the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state [18, 19] are possible in a system with multi-Fermi-surface.

2. Model

To investigate superconductivity in a multi-orbital system, we consider a tight-binding model for e_g orbitals given by

$$\begin{aligned}
 H = & \sum_{k\tau\sigma} \varepsilon_{k\tau\sigma} c_{k\tau\sigma}^\dagger c_{k\tau\sigma} + U \sum_{i,\tau} n_{i\tau\uparrow} n_{i\tau\downarrow} \\
 & + U' \sum_i n_{i1} n_{i2} + J \sum_{i,\sigma} c_{i1\sigma}^\dagger c_{i2\sigma}^\dagger c_{i1\sigma} c_{i2\sigma} \\
 & + J \sum_{i,\tau \neq \tau'} c_{i\tau\uparrow}^\dagger c_{i\tau'\uparrow}^\dagger c_{i\tau\downarrow} c_{i\tau'\downarrow} \quad (1)
 \end{aligned}$$

where $c_{i\tau\sigma}$ is the annihilation operator of the electron at site i with orbital τ ($=1$ or 2) and spin σ ($=\uparrow$ or \downarrow), $c_{k\tau\sigma}$ is the Fourier transform of it, $n_{i\tau\sigma} = c_{i\tau\sigma}^\dagger c_{i\tau\sigma}$, and

$n_{i\tau} = \sum_{\sigma} n_{i\tau\sigma}$. The coupling constants U , U' , J , and J' denote the intra-orbital Coulomb, inter-orbital Coulomb, exchange, and pair-hopping interactions, respectively. In the followings, we use the relations $U=U'+J+J'$ and $J=J'$ [20].

We consider hopping integrals for nearest neighbor sites on a square lattice, and the coefficients of the kinetic energy terms in Eq. (1) are generally given by

$$\varepsilon_{k11} = \frac{1}{2}[3(dd\sigma) + (dd\delta)](\cos k_x + \cos k_y), \quad (2)$$

$$\varepsilon_{k22} = \frac{1}{2}[(dd\sigma) + 3(dd\delta)](\cos k_x + \cos k_y), \quad (3)$$

$$\varepsilon_{k12} = \varepsilon_{k21} = -\frac{\sqrt{3}}{2}[(dd\sigma) - (dd\delta)](\cos k_x - \cos k_y), \quad (4)$$

where we have set the lattice constant unity.

3. Formulation

In this section, we derive equations for response functions, classify symmetry of superconductivity, and derive a gap equation for the anomalous self-energy for each symmetry.

First, we derive equations for the Green's function in the normal phase. For a system with orbital degree of freedom, the Green's function is defined by

$$G_{\tau_1\sigma_1;\tau_2\sigma_2}(k,\tau) = -\langle T_{\tau} c_{k\tau_1\sigma_1}(\tau) c_{k\tau_2\sigma_2}^{\dagger} \rangle, \quad (5)$$

and the anomalous Green's functions are defined by

$$F_{\tau_1\sigma_1;\tau_2\sigma_2}(k,\tau; q_{tot}) = -\langle T_{\tau} c_{k\tau_1\sigma_1}(\tau) c_{-k+q_{tot}\tau_2\sigma_2} \rangle, \quad (6)$$

where T_{τ} denotes the time-ordered product, $\langle \dots \rangle$ denotes the thermal average, and q_{tot} is the total momentum of the pair. Here we have used the Heisenberg representation for an operator O defined by

$$O(t) = e^{t(H-mN_{tot})} O e^{-t(H-mN_{tot})}, \quad (7)$$

where $N_{tot} = \sum_{i,\tau} n_{i\tau}$ is the total number operator of

electrons and μ is the chemical potential. As usual, we use the Fourier transformation with respect to imaginary time which is given by

$$O(i\varepsilon_n) = \int_0^{\beta} d\tau e^{i\varepsilon_n \tau} O(\tau), \quad (8)$$

where $\beta=1/T$ with a temperature T and $\varepsilon_n=(2n+1)\pi T$ is the Matsubara frequency for fermions with an integer n . We have set the Boltzmann constant unity.

The Dyson-Gorkov equations are given by

$$G_{\tau\sigma;\tau'\sigma'}(k) = \delta_{\sigma\sigma'} G_{\tau\tau'}^{(0)}(k) + \sum_{\tau_1\tau_2\tau_3} [G_{\tau\tau'}^{(0)}(k) \Sigma_{\tau_1\sigma;\tau_2\sigma'}(k) G_{\tau_2\sigma_2;\tau'\sigma'}(k) \quad (9)$$

$$+ G_{\tau\tau_1}^{(0)}(k) \sum_{q_{tot}} \phi_{\tau_1\sigma;\tau_2\sigma_2}(k; q_{tot}) F_{\tau_2\sigma_2;\tau'\sigma'}^t(k, q_{tot})], \quad (10)$$

$$F_{\gamma\sigma;\gamma'\sigma'}(k; q_{tot}) \quad (10)$$

$$= \sum_{\tau_1\tau_2\sigma_2} [G_{\tau\tau_1}^{(0)}(k) \Sigma_{\tau_1\sigma;\tau_2\sigma_2}(k) F_{\tau_2\sigma_2;\tau'\sigma'}(k; q_{tot})$$

$$- G_{\tau\tau_1}^{(0)}(k) \phi_{\tau_1\sigma;\tau_2\sigma_2}(k; q_{tot}) G_{\tau'\sigma';\tau_2\sigma_2}(-k + q_{tot}, -i \in_n)] \quad (11)$$

where $\Sigma_{\tau\sigma;\tau'\sigma'}(k)$ is the self-energy and $\phi_{\tau\sigma;\tau'\sigma'}(k; q_{tot})$ is the anomalous self-energy. We have used the abbreviation $k=(k, i\varepsilon_n)$. The non-interacting Green's function

$G^{(0)}(k, i\varepsilon_n)$ in a matrix form is given by

$$G^{(0)}(k, i\varepsilon_n) = [i\varepsilon_n - \varepsilon_k + \mu]^{-1}. \quad (12)$$

Here we consider the normal phase. In the normal phase, the Green's function and self-energy do not depend on spin, that is, $G_{\tau\sigma;\tau'\sigma'}(k) = \delta_{\sigma\sigma'} G_{\tau\tau'}(k)$ and $\Sigma_{\tau\sigma;\tau'\sigma'}(k) = \delta_{\sigma\sigma'} \Sigma_{\tau\tau'}(k)$. Then the Dyson-Gorkov equation is given by

$$G_{\tau\tau'}(k) = G_{\tau\tau'}^{(0)}(k) + \sum_{\tau_1\tau_2} G_{\tau\tau_1}^{(0)}(k) \Sigma(k)_{\tau_1\tau_2} G_{\tau_2\tau'}(k). \quad (13)$$

In the FLEX approximation, the self-energy is given by

$$\Sigma_{\tau\tau'}(k) = \frac{T}{N} \sum_{q, \tau_1, \tau_2} \chi_{\tau\tau_1;\tau'\tau_2}(q) G_{\tau_1\tau_2}(k-q), \quad (14)$$

where N is the number of lattice sites, $q=(q, i\omega_m)$, and $\omega_m=2m\pi T$ is the Matsubara frequency for bosons with an integer m . The matrix $V(q)$ is given by

$$V(q) = \frac{3}{2} [U^S \chi^S(q) - U^S \chi^{(0)}(q) U^S / 2 + U^S] \quad (15)$$

$$+ \frac{1}{2} [U^C \chi^C(q) U^C / 2 - U^C]$$

The matrix elements of U^S and U^C , which describe interactions for the spin part and the charge part, respectively, are given by

$$U_{11;11}^S = U_{22;22}^S = U_{11;11}^C = U_{22;22}^C = U, \quad (16)$$

$$U_{11;22}^S = U_{22;11}^S = J, \quad (17)$$

$$U_{11;22}^C = U_{22;11}^C = 2U - J, \quad (18)$$

$$U_{12;12}^s = U_{21;21}^s = U', \quad (19)$$

$$U_{12;12}^c = U_{21;21}^c = -U' + 2J, \quad (20)$$

$$U_{12;21}^s = U_{21;12}^s = U_{12;21}^c = U_{21;12}^c = J', \quad (21)$$

and zero for the other elements of these matrices. The susceptibilities $\chi^s(q)$ for the spin part and $\chi^c(q)$ for the charge part are given by

$$\chi^s(q) = \chi^{(0)}(q)[1 - U^s \chi^{(0)}(q)]^{-1}, \quad (22)$$

$$\chi^c(q) = \chi^{(0)}(q)[1 - U^c \chi^{(0)}(q)]^{-1}, \quad (23)$$

in matrix forms, where the matrix elements of $\chi^{(0)}(q)$ are given by

$$\chi_{\tau_1\tau_2;\tau_3\tau_4}^{(0)}(q) = -\frac{T}{N} \sum_k G_{\tau_1\tau_3}(k+q) G_{\tau_4\tau_2}(k). \quad (24)$$

We solve Eqs. (13)-(15) and (22)-(24) self-consistently. Then, we can calculate response functions by using obtained $\chi^s(q)$ and $\chi^c(q)$. The response function corresponding to an operator O_i^A is given by

$$\chi^A(q, i\omega_m) = \sum_i \int_0^\beta d\tau e^{-iq \cdot r_i + i\omega_m \tau} \langle T_\tau O_i^A(\tau) O_o^A \rangle, \quad (25)$$

where o denotes the origin. A one-electron operator O_i^A in the second-quantized form is generally written as

$$O_i^A = \sum_{t,s,s'} c_{its}^\dagger O_{ts;s'}^A c_{its'}. \quad (26)$$

For a two-orbital model, the matrix elements $O_{\tau\sigma;\tau'\sigma'}^A$ are given by

$$O_{\tau\sigma;\tau'\sigma'}^{charge} = \delta_{\tau\tau'} \delta_{\sigma\sigma'}, \quad (27)$$

$$O_{\tau\sigma;\tau'\sigma'}^{\sigma^x} = \delta_{\tau\tau'} \delta_{\sigma\sigma'}, \quad (28)$$

$$O_{\tau\sigma;\tau'\sigma'}^{\sigma^y} = \delta_{\tau\tau'} \delta_{\sigma\sigma'}, \quad (29)$$

$$O_{\tau\sigma;\tau'\sigma'}^{\sigma^z} = \delta_{\tau\tau'} \delta_{\sigma\sigma'}, \quad (30)$$

for charge, spin, orbital, and spin-orbital coupled operators, respectively, where σ^v is the Pauli matrix for v ($=x, y, \text{ or } z$) component. Due to the rotational symmetry in

the spin space, the relations $\chi^{\sigma^x}(q) = \chi^{\sigma^y}(q) = \chi^{\sigma^z}(q)$ and $\chi^{\tau^v\sigma^x}(q) = \chi^{\tau^v\sigma^y}(q) = \chi^{\tau^v\sigma^z}(q)$ hold.

The response functions in the FLEX approximation are given by

$$\chi^{charge}(q) = 2 \sum_{\tau_1, \tau_2, \tau_3, \tau_4} \delta_{\tau_2\tau_1} \delta_{\tau_3\tau_4} \chi_{\tau_1\tau_2;\tau_3\tau_4}^c(q), \quad (31)$$

$$\chi^{\sigma^z}(q) = 2 \sum_{\tau_1, \tau_2, \tau_3, \tau_4} \delta_{\tau_2\tau_1} \delta_{\tau_3\tau_4} \chi_{\tau_1\tau_2;\tau_3\tau_4}^s(q), \quad (32)$$

$$\chi^{\tau^v}(q) = 2 \sum_{\tau_1, \tau_2, \tau_3, \tau_4} \hat{\sigma}_{\tau_2\tau_1}^z \hat{\sigma}_{\tau_3\tau_4}^z \chi_{\tau_1\tau_2;\tau_3\tau_4}^c(q), \quad (33)$$

$$\chi^{\tau^v\sigma^z}(q) = 2 \sum_{\tau_1, \tau_2, \tau_3, \tau_4} \hat{\sigma}_{\tau_2\tau_1}^z \hat{\sigma}_{\tau_3\tau_4}^z \chi_{\tau_1\tau_2;\tau_3\tau_4}^s(q), \quad (34)$$

Now, we derive a gap equation for superconductivity. First, we categorize the anomalous self-energy by symmetry. The anomalous self-energy for a spin-singlet state is given by

$$f_{it}^{singlet}(k; q_{tot}) = \frac{1}{2} [f_{t,-t}(k; q_{tot}) - f_{t,-t}(k; q_{tot})], \quad (35)$$

and the anomalous self-energy for a spin-triplet state is given by

$$\phi_{\tau\tau'}^{triplet}(k; q_{tot}) = \frac{1}{2} [\phi_{\tau\uparrow;\tau'\downarrow}(k; q_{tot}) + \phi_{\tau\downarrow;\tau'\uparrow}(k; q_{tot})]. \quad (36)$$

The spin-triplet states with $\phi_{\tau\tau'}^{triplet}(k; q_{tot})$, with $\phi_{\tau\uparrow;\tau'\uparrow}(k; q_{tot})$, and with $\phi_{\tau\downarrow;\tau'\downarrow}(k; q_{tot})$ are degenerate due to the rotational symmetry in the spin space. The linearized gap equation for the anomalous self-energy is written as

$$\begin{aligned} & \lambda(\Gamma, \xi) \phi_{\tau\tau'}^\xi(k; q_{tot}) \\ &= \frac{T}{N} \sum_{k', \tau_1, \tau_2} V_{\tau\tau_1; \tau_2\tau'}^\xi(k - k') F_{\tau_1\tau_2}^\xi(k'; q_{tot}) \\ &= -\frac{T}{N} \sum_{k', \tau_1, \tau_2, \tau_3, \tau_4} V_{\tau\tau_1; \tau_2\tau'}^\xi(k - k') \\ & \times G_{\tau_1\tau_3}(k') \phi_{\tau_3\tau_4}^\xi(k', q_{tot}) G_{\tau_2\tau_4}(-k' + q_{tot}, -i \in_n) \end{aligned} \quad (37)$$

with $\lambda(\Gamma, \xi) = 1$, where Γ denotes a representation of tetragonal symmetry C_{4v} which $\phi_{\tau\tau'}^\xi(k; q_{tot})$ obeys, and $F_{\tau\tau'}^\xi(k; q_{tot})$ is defined by the same way as $\phi_{\tau\tau'}^\xi(k; q_{tot})$.

Thus, the superconducting transition temperature is given by the temperature where an eigenvalue $\lambda(\Gamma, \xi)$ of Eq. (37) becomes unity. The effective pairing interactions $V^{\xi}(q)$ are given as

$$V^{\text{singlet}}(q) = \frac{3}{2}[U^s \chi^s(q)U^s + U^s/2] \quad (38)$$

$$-\frac{1}{2}[U^c \chi^c(q)U^c - U^c/2]$$

$$V^{\text{triplet}}(q) = -\frac{1}{2}[U^s \chi^s(q)U^s + U^s/2] \quad (39)$$

$$-\frac{1}{2}[U^c \chi^c(q)U^c - U^c/2]$$

4. Results

In this section, we show results for a 64×64 lattice. In the calculation, we use 2048 Matsubara frequencies. We normalize $(dd\sigma)$ and $(dd\delta)$ so as to make the band-width 8, e.g., $(dd\delta)=(dd\sigma)=1$ for $(dd\delta)/(dd\sigma)=1$. In this study, we fix the value of the intra-orbital Coulomb interaction $U=6$ and vary J ($=J$). Then the inter-orbital Coulomb interaction is given by $U'=U-2J$.

The calculations have been done for $(dd\delta)/(dd\sigma)=1, 0$, and -1 . For $(dd\delta)/(dd\sigma)=1$, the model is equivalent to the two-orbital Hubbard model with the same hopping integral for both orbitals, except for orbital symmetry. For the two-orbital Hubbard model, it is usual to assume orbital symmetry is s orbital one. From the results of the two-orbital Hubbard model [15], we immediately find that $d_{x^2-y^2}$ -wave spin-triplet and p -wave spin-singlet states with $q_{\text{tot}}=(0,0)$ appear in the e_g orbital model with $(dd\delta)/(dd\sigma)=1$. For $(dd\delta)/(dd\sigma)=0$, we cannot find any superconducting state within $T \geq 0.005$. Thus, we show results only for $(dd\delta)/(dd\sigma)=-1$ in the followings.

In Fig. 1, we show Fermi surfaces for $(dd\delta)=-1$.

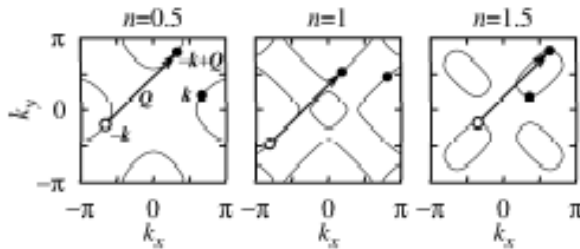


Fig. 1. Fermi surfaces for $(dd\delta)=-1$.

For the electron number $n=\langle N_{\text{tot}} \rangle/N=2$ per site, the Fermi surfaces disappear. As is shown in Fig. 1, if an electron with the momentum $-k$ is on a Fermi surface, the electron with $-k+Q$ is on another Fermi surface, where

$Q=(\pi, \pi)$. Thus it is possible to form a superconducting pair with total momentum $q_{\text{tot}}=Q$ by electrons with k and $-k+Q$ for $(dd\delta)=-1$. Thus we consider superconducting states with $q_{\text{tot}}=Q$ in addition to the ordinary ones with $q_{\text{tot}}=(0,0)$.

In Fig. 2, we show static susceptibilities $\chi^A(q)=\chi^A(q, i\omega_m=0)$ for $J=0, 1$, and 2 at $T=0.005$ and $n=1.5$.

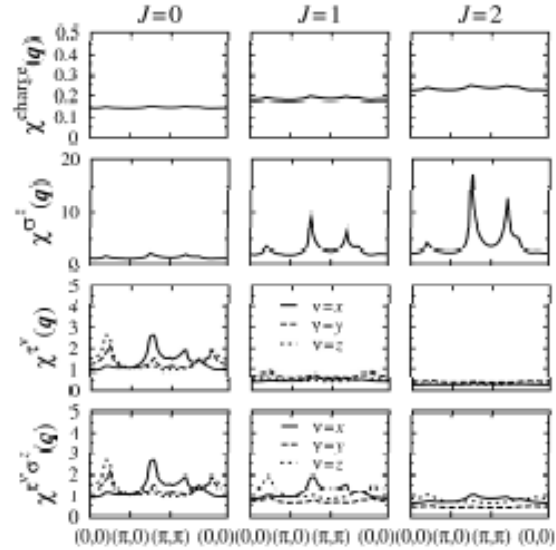


Fig. 2. q dependence of the susceptibilities for $J=0, 1$, and 2 at $T=0.005$, $(dd\delta)=-1$, $n=1.5$, and $U=6$.

Among all the susceptibilities, the spin susceptibility $\chi^{\tau^z}(q)$ becomes large by increasing J , that is, magnetic fluctuations are enhanced by the Hund's rule coupling. On

the other hand, the orbital susceptibility $\chi^{\tau^v}(q)$ and the spin-orbital susceptibility $\chi^{\tau^v\sigma^z}(q)$ are suppressed by the Hund's rule coupling. The charge susceptibility $\chi^{\text{charge}}(q)$ is enhanced a little by the Hund's rule coupling, but its value is very small. Thus, among various fluctuations, the spin fluctuations for a large J are important in the present model at least within the FLEX approximation.

Figure 3 shows the spin susceptibility at $q=q_{\text{max}}$ where

q_{max} is defined as the wave vector at which $\chi^{\sigma^z}(q)$ takes the maximum value, and the eigenvalue λ for p -wave spin-singlet and $d_{x^2-y^2}$ -wave spin-triplet with $q_{\text{tot}}=Q=(\pi, \pi)$.

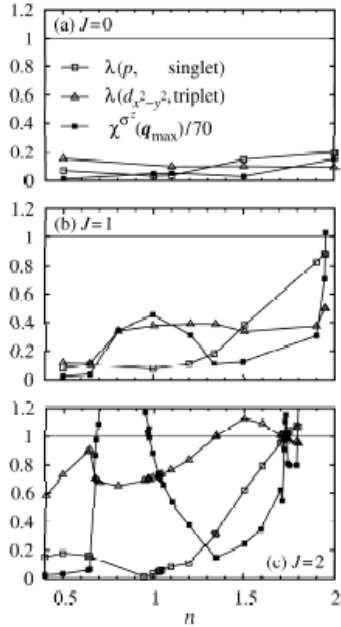


Fig. 3. Eigenvalues λ for p -wave spin-singlet and $d_{x^2-y^2}$ -wave spin-triplet for $q_{\text{tot}}=Q=(\pi,\pi)$, and the spin susceptibility $\chi^{\sigma_z}(q_{\max})$ as functions of n for (a) $J=0$, (b) $J=1$, and (c) $J=2$ at $T=0.005$, $(dd\delta)=-(dd\sigma)$, and $U=6$.

For other pairing states, λ does not become larger than unity at least for parameters we have used. For $J=0$, the spin susceptibility does not enhance so much even at $n=2$, and λ also remains small. For $J=1$, the spin susceptibility enhances around $n=2$, and $\lambda(p, \text{singlet})$ also becomes large. However, the spin susceptibility enhances more rapidly than $\lambda(p, \text{singlet})$, and the ground state is probably an antiferromagnetic state around $n=2$. For $J=2$, the spin susceptibility becomes very large around $n=0.8$ and $n=2$. Between these regions, $\lambda(p, \text{singlet})$ and $\lambda(d_{x^2-y^2}, \text{triplet})$ become larger than unity, thus superconductivity for these symmetry takes place with transition temperatures higher than 0.005. These superconducting states appear for a large J and thus these states should be composed mainly of orbital-antisymmetric components for which the anomalous ξ self-energy is given by $[\phi_{12}^{\sigma}(k; q_{\text{tot}}) - \phi_{21}^{\sigma}(k; q_{\text{tot}})]/2$. These components satisfy the Pauli principle for even-parity spin-triplet and for odd-parity spin-singlet within even-frequency states.

5. Summary

We have studied an e_g orbital model on a square lattice. We pointed out that a pairing state with the total momentum $q_{\text{tot}}=Q=(\pi,\pi)$ is possible for $(dd\delta)=-(dd\sigma)$ from the Fermi surface structure. First we have calculated susceptibilities for charge, spin, orbital, and spin-orbital components. Then, we have found that the

spin fluctuations are the most important ones in the model. For $(dd\delta)=(dd\sigma)$, $U=6$, and $J=2$, we find p -wave spin-singlet and $d_{x^2-y^2}$ -wave spin-triplet states with $q_{\text{tot}}=(0,0)$. We also find that near the region where the spin susceptibility enhances, p -wave spin-singlet and $d_{x^2-y^2}$ -wave spin-triplet states appear for $(dd\delta)=-(dd\sigma)$, $U=6$, and $J=2$ with superconducting pairs which have the finite total momentum Q like the FFLO state.

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