Perturbation Analysis of Superconductivity in Hubbard Model

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Abstract

We discuss the origin of the superconductivity in a Hubbard model. For the superconductivity which is induced by the Coulomb interaction U, it is important to investigate the wave number dependence of the quasi particle interaction. Using the third order perturbation theory with respect to U, we treat the wave number dependence induced by the spin fluctuation and the vertex correction. We investigate the pairing states for the various lattice structures in the Hubbard model and we point out the important factors giving rise to the singlet and triplet superconductivities.

Key words: superconductivity; perturbation theory; vertex correction

In the strongly correlated systems, the origin of the superconductivity has been researched on the basis of the spin fluctuation theory. However, the triplet superconductivity of the quasi two-dimensional ruthenate [1] is recently studied with the new idea different from a spin fluctuation mechanism. Adopting the third order perturbation theory (TOPT) with respect to the Coulomb interaction U, Nomura and Yamada [1] conclude that the p-wave pairing of Sr_2RuO_4 is promoted by a wave number dependence of the third-order vertex correction rather than the spin fluctuations.

This conclusion presents a question whether the vertex correction is also generally important for the superconductor in the two- and three-dimensional various lattice structures. This problem is interesting in comparison with previous studies on the basis of the spin fluctuations. Thus, we treat the wave number dependence including both the spin fluctuations and the vertex correction in the strong coupling theory and we study the triplet and singlet superconductivities in the various lattice structures. We investigate the dominant pairing states for the two-dimensional square and the three-dimensional simple cubic (SC), FCC and BCC lattices structure. From these results, we find the important factors for the origin in common with various lattice structures.

We give the following formulation. The Hubbard Hamiltonian is given by

$$H = -t_1 \sum_{<i,j>,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + t_2 \sum_{<i,k>,\sigma} c^{\dagger}_{i,\sigma} c_{k,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}, \quad (1)$$

where σ is the spin index, $\langle i,j \rangle$ indicates taking summation over the nearest-neighbor sites and $\langle i,k \rangle$ over the next-nearest-neighbor sites. We obtain the energy dispersion for the square, SC, BCC and FCC lattices; $\mathrm{E}_k^{\mathrm{square}} = -2t_1 \sum_{l=1}^{2} \cos k_l + 4t_2 \cos(k_x)\cos(k_y)$, $\mathrm{E}_k^{\mathrm{sc}} = -2t_1 \sum_{l=1}^{3} \cos k_l + 4t_2 \sum_{l<m} \cos(k_l)\cos(k_m)$, $\mathrm{E}_k^{\mathrm{bcc}} = -8t_1 \cos k_x \cos k_y \cos k_z + 2t_2 \sum_{l=1}^{3} \cos(2k_l)$ and $\mathrm{E}_k^{\mathrm{fcc}} = -4t_1 \sum_{l<m} \cos k_l \cos k_m + 2t_2 \sum_{l=1}^{3} \cos(2k_l)$. $(l,m = 1,2,3;\ x,y,z)$ We take t_1=1.0 and $-0.5 < t_2 < 0.5$.

We obtain the bare Green's function given by $G_0(k,\epsilon_n) = \frac{1}{\mathrm{i}\epsilon_n - (E_k - \mu)}$, where $\epsilon_n = \pi T(2n+1)$ is the Matsubara frequency and μ is the chemical potential. The electron number density per spin n is given by $n = \frac{T}{N} \Sigma_{k,n} G_0(k,\epsilon_n)$.

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The effective interactions for the singlet and triplet states are given by TOPT. The effective interaction is divided into two parts, $V_{\rm TOPT}(q,k)$=$V_{\rm RPA}(q,k)$ + $V_{\rm Vertex}(q,k)$. The RPA-like term $V_{\rm RPA}$ includes the term given by the Random Phase Approximation (RPA) and $V_{\rm Vertex}$ is the vertex correction. The RPA-like term reflects the nature of the spin fluctuations. The vertex correction originates from other terms except for the spin fluctuations. For the singlet and triplet pairing states, the RPA-like part and the vertex correction part are given respectively by

$$V_{\rm RPA}^{\rm Singlet}(q,k) = U + U^2\chi_0(q-k) + 2U^3\chi_0^2(q-k), \quad (2)$$

$$V_{\rm Vertex}^{\rm Singlet}(q,k) = 2\frac{T}{N}U^3[\sum_{k'}G_0(q-k+k') \times(\chi_0(q+k') - \phi_0(q+k'))G_0(k')], \quad (3)$$

$$V_{\rm RPA}^{\rm Triplet}(q,k) = -U^2\chi_0(q-k), \quad (4)$$

$$V_{\rm Vertex}^{\rm Triplet}(q,k) = 2\frac{T}{N}U^3[\sum_{k'}G_0(q-k+k') \times(\chi_0(q+k') + \phi_0(q+k'))G_0(k')], \quad (5)$$

where k indicates $k\equiv$(k,ω_n). The bare susceptibility $\chi_0(q)$ and $\phi_0(q)$ are defined by $\chi_0(q)$ = $-\frac{T}{N}\sum_k G_0(k)G_0(q+k)$, $\phi_0(q)$=$-\frac{T}{N}\sum_k G_0(k)G_0(q-k)$, respectively. Next, we obtain the linearized Éliashberg equation at the transition temperature $T_{\rm c}$.; $\lambda\Sigma_A^\dagger(q)$=$-\frac{T}{N}\sum_k V(q,k)|G_0(k)|^2\Sigma_A^\dagger(k)$. $\Sigma_A^\dagger(k)$ is an anomalous self energy and $V(q,k)$ is given by (2 - 5). The equation is an eigenvalue equation with an eigenvalue λ and an eigenvector $\Sigma_A^\dagger$. We solve the linearized Éliashberg equation on the assumption that $\Sigma_A^\dagger$ has the pairing symmetries represented by p, d, f and g-wave pairing symmetries. The most dominant pairing symmetry has the largest value of the eigenvalues among the different pairing symmetries. Thus, we solve the equation and determine the dominant state. We carry out the calculation by taking 64×64×64 momentum meshes and $N_{\rm f}$=512 for Matsubara frequency.

We obtain the following results. In Fig. 1, we show the superconducting phase diagrams determined by the TOPT in the plane of the hopping integral t_2 and the density n and we show a most dominant pairing state which has the largest value of eigenvalues λ. The half-filling density corresponds to n = 0.5. From the phase diagrams, we point out the main factors in common with the various lattice structures.

First, we mention the effects of the spin fluctuation for the pairing state. Near the half-filling, the singlet superconductivity is realized by the spin fluctuation, such as the antiferromagnetic spin fluctuation. By the ferromagnetic spin fluctuation, the p-wave pairing is dominant in the case of the very low density for the electron or the hole ($n < 0.05$ or $n > 0.85$). The results

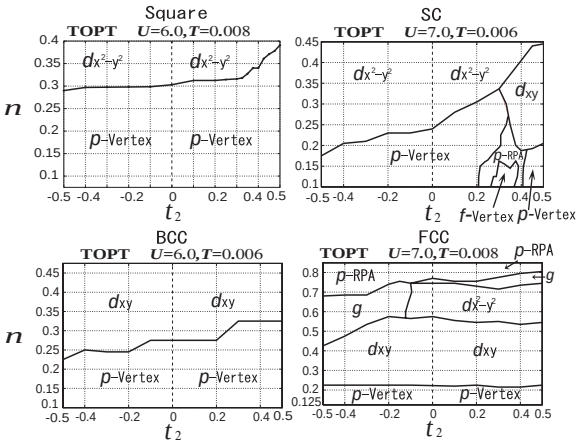

Fig. 1. The superconducting phase diagrams for the dominant pairing symmetry for the various lattice structures. t_2 and n is the next-nearest-neighbor hopping integral and the electron density, respectively. The half-filling corresponds to n=0.5.

for the p- and d-wave pairings owing to the spin fluctuations agree with the results studied with the FLEX approximation by Arita *et al.* [2]

Next, we detail that the triplet pairing is induced by the vertex correction in the intermediate density far from the half-filling ($0.05 < n < 0.3$). By adding the vertex correction, the triplet pairing can realize in the wide region of the density. The effect of the vertex correction is generally opposite to the effect of the RPA-like term. When the vertex correction gives the advantage to the triplet pairing, the RPA-like term suppresses the triplet pairing. When the RPA-like term reflecting the antiferromagnetic (ferromagnetic) spin fluctuations induces the singlet (triplet) pairing state, the vertex correction suppresses the pairing.

As the important consequence, finally, we point out that a certain intermediate density far from the half-filling is necessary for the triplet pairing induced by the vertex correction in the square, SC, BCC and FCC lattice structures. By the wave number dependence of the quasi particle interaction on the basis of Fermi liquid theory, it is possible to treat generally both the singlet and triplet superconductivities. To make clear the origin of superfluidity in ^{3}He, it is necessary to study not only the spin fluctuations but also the wave number dependence of the vertex correction. A part of two-dimensional case of this study is given in the paper [3].

References

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