# EFFECTS OF LATTICE STRUCTURES ON PAIRING SYMMETRY IN HUBBARD MODEL: THIRD ORDER PERTURBATION ANALYSIS*

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We discuss the origin of the unconventional superconductivity in a Hubbard model. The origin of the unconventional superconductivity is considered to be a wave number dependence of a quasi particle interaction, which is induced by the Coulomb interaction $U$. Using the third order perturbation theory with respect to $U$, we discuss the wave number dependence induced by spin fluctuations and vertex corrections. We investigate the pairing states for the various lattice structures in the Hubbard model and we point out the important factors in the origin of the singlet and triplet superconductivities.

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## 1. Introduction

We study the origin of the unconventional superconductivity in the Hubbard model. In the model, the origin of the superconductivity is often investigated on the basis of spin fluctuations by the FLEX approximation and a second-order perturbation with respect to the Coulomb interaction $U$. On the other hand, Nomura and Yamada [1] concluded that the triplet superconductor $Sr_2RuO_4$ is not realized by a particular peak of susceptibility representing the spin fluctuation, using the third-order perturbation theory (TOPT) with respect to $U$ [2]. From their study, the origin of the superconductivity is considered to be the wave number dependence of electron interactions which include not only spin fluctuations but also vertex corrections. In this paper, we treat the general wave number dependence by TOPT and we investigate the dominant pairing states for the various lattice structures in the Hubbard model. We discuss the origin of the superconductivity and we point out the important factors for the singlet and triplet superconductivities.

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## 2. Formulation

The Hubbard Hamiltonian is given by

$$\mathcal{H} = -t_1 \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + t_2 \sum_{\langle i,k \rangle,\sigma} c^\dagger_{i,\sigma} c_{k,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \,, \tag{1}$$

where $\sigma$ 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, simple cubic (SC), BCC and FCC lattices;

$$\begin{aligned}
E_k^{\rm Square} &= -2t_1 \sum_{l=1}^{2} \cos k_l + 4t_2 \cos(k_x)\cos(k_y) \,, \\
E_k^{\rm sc} &= -2t_1 \sum_{l=1}^{3} \cos k_l + 4t_2 \sum_{l<m} \cos(k_l)\cos(k_m) \,, \\
E_k^{\rm bcc} &= -8t_1 \cos k_x \cos k_y \cos k_z + 2t_2 \sum_{l=1}^{3} \cos(2k_l) \,, \\
E_k^{\rm fcc} &= -4t_1 \sum_{l<m} \cos k_l \cos k_m + 2t_2 \sum_{l=1}^{3} \cos(2k_l) \,,
\end{aligned}$$

where $(l,m = 1,2,3;\ x,y,z)$. We take $t_1 = 1.0$ and $-0.5 < t_2 < 0.5$. We obtain the bare Green's function given by $G_0(k,\varepsilon_n) = 1/(i\varepsilon_n - (E_k - \mu))$, where $\varepsilon_n = \pi T(2n+1)$ is the Matsubara frequency and $\mu$ is the chemical potential. The electron number (the electron density) per spin $n$ is given by $n = (T/N)\,\Sigma_{k,n} G_0(k,\varepsilon_n)$.

The effective interaction for the singlet and triplet states are given by TOPT. The effective interaction is divided into two parts,

$$V_{\rm TOPT}(q,k) = V_{\rm RPA}(q,k) + V_{\rm Vertex}(q,k) \,. \tag{2}$$

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 spin fluctuations. The vertex correction originates from the susceptibility without certain spin fluctuations. For the singlet and triplet pairing states, the RPA-like part and the vertex correction part are given respectively by

$$\begin{aligned}
V_{\rm RPA}^{\rm Singlet}(q,k) &= U + U^2 \chi_0(q-k) + 2U^3 \chi_0^2(q-k) \,, \\
V_{\rm Vertex}^{\rm Singlet}(q,k) &= 2\frac{T}{N} U^3 \Big[ \sum_{k'} G_0(q-k+k')\,(\chi_0(q+k') - \phi_0(q+k')) G_0(k') \Big] \,, \\
V_{\rm RPA}^{\rm Triplet}(q,k) &= -U^2 \chi_0(q-k) \,, \\
V_{\rm Vertex}^{\rm Triplet}(q,k) &= 2\frac{T}{N} U^3 \Big[ \sum_{k'} G_0(q-k+k')\,(\chi_0(q+k') + \phi_0(q+k')) G_0(k') \Big] \,,
\end{aligned}$$

where $k$ indicates $k \equiv (\boldsymbol{k}, \omega_n)$. 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 $T = T_{\mathrm{c}}$; $\lambda\Sigma_A^\dagger(q) = -\frac{T}{N}\sum_k V(q,k)|G_0(k)|^2\Sigma_A^\dagger(k)$. $\Sigma_A^\dagger(k)$ is an anomalous self energy and $V(q,k)$ is given by (2) and (3). The equation is an eigenvalue equation with an eigenvalue $\lambda$ 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 $p$-, $d$-, $f$-, $g$-wave pairing symmetries. The pairing symmetries degenerate due to the space 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.

## 3. Calculation and results

In Fig. 1, we show the phase diagrams for the dominant pairing state in the plane of the second-nearest-neighbor hopping integral $t_2$ and the electron density $n$. A half-filling corresponds to the density $n = 0.5$. In Fig. 2(a), the dependence of the bare susceptibility $\chi_0(\vec{q}, \omega_n = 0)$ on $n$ is shown for a quarter first-Brillouin-zone of the square lattice.

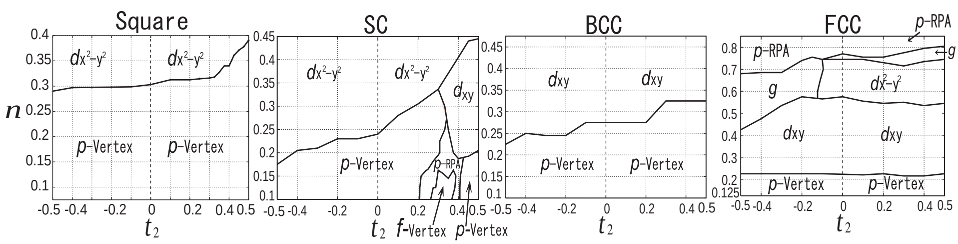


Fig. 1. Superconducting phase diagrams for the dominant pairing symmetry. The diagram has the parameters of the second-nearest-neighbor hopping integral $t_2$ and the density $n$. A half-filling corresponds to the density $n = 0.5$.

The singlet state becomes dominant by the RPA-like term reflecting the spin fluctuations. For example, the $d_{x^2-y^2}$ wave pairing state is induced by an antiferromagnetic fluctuation which has a peak of susceptibility $\chi_0$ at $(\pi, \pi)$ in the momentum space. In realizing the triplet state, the vertex correction plays the main role. The vertex correction has the wave number dependence which is induced by the third order terms.

In Fig. 2(b), (c), we show the details of the eigenvalues in the square lattice and make clear each role of the RPA-like term $V_{\mathrm{RPA}}$ and the vertex correction $V_{\mathrm{Vertex}}$. The singlet state becomes dominant by the RPA-like terms reflecting the spin fluctuations, which was shown by many previous studies.

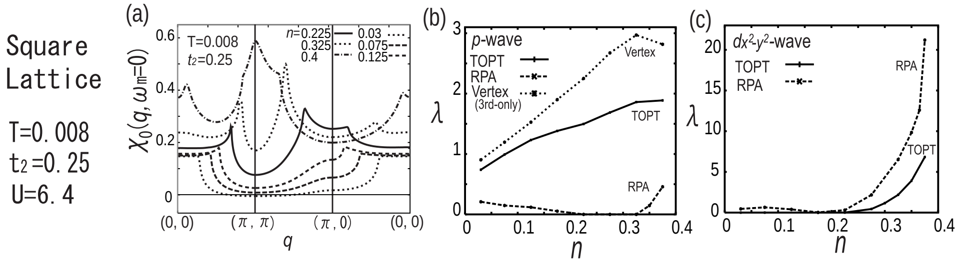


Fig. 2. (a) The dependence of the bare susceptibility $\chi_0(\vec{q}, \omega_n = 0)$ on the density $n$ in the square lattice. (b), (c) The dependence of the eigenvalue $\lambda$ on the density $n$ in the cases of the $p$- (b) and $d_{x^2-y^2}$ (c) wave pairings in the square lattice.

The vertex correction discourages the singlet pairing. Thus, the vertex correction lowers the transition temperature. For the triplet state, the vertex correction brings the advantage from low to intermediate density. The wave number dependence of the vertex correction causes the scattering near the Fermi surface, which induces the attractive force for the triplet pairing. On the other hand, the RPA-like term reflecting the spin fluctuations suppresses the triplet pairing and lowers the eigenvalue. However, the ferromagnetic spin fluctuations encourage the triplet pairing in the very low density.

## 4. Conclusion

We have studied the superconductivity in the Hubbard model by the third order perturbation theory. We have found the following important factors in common with the various lattices studied in this paper.

For the singlet pairing, the spin fluctuation is the important factor. The singlet superconductivity is realized by the spin fluctuation near the half-filling. For the triplet pairing, the vertex correction plays the vital role far from the half-filling except for the very low density. In the very low density, the triplet pairing state is dominant by the ferromagnetic spin fluctuation. Adding the vertex correction, the triplet pairing can be realized in the wide density.

Investigating the general wave number dependence of the effective interaction, we find that a sufficient high electron-density in the case far from half-filling is necessary for the triplet pairing induced by the vertex correction. A part of this study is given in paper [3].

## REFERENCES

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