

Stability of $s + id$ -Wave Pairing State in the 2-D Extended Hubbard Model

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(Received October 20, 1994)

Coexistence of the s and $d_{x^2-y^2}$ -wave (d -wave) pairing is investigated in the two-dimensional (2-D) extended Hubbard model with on-site repulsive and inter-site attractive interactions using the mean-field approximation at $T=0$ K. The next-nearest-neighbor hopping effect can induce the coexistence of the s and d -wave pairing. It is found that in such a case, $s + id$ -wave pairing state becomes most stable.

[superconductivity, Hubbard model, anisotropic pairing, Hartree Fock approximation]

§1. Introduction

Symmetries of the pair potentials of superconductivity are one of the important problem of superconductivity. As for anisotropic Cooper pairing, a variety of studies have been done concerning with ^3He , heavy-fermion systems and high- T_c materials.^{1,2)} Recently symmetry of the pair potentials of high T_c superconductors is one of the hottest issues in the solid state physics.³⁻¹⁰⁾ However it is not clarified yet whether the symmetry of the pairing of high T_c superconductors is d -wave or s -wave. At this stage, we have a very fundamental question whether s -wave and d -wave pairing coexist or not? Apart from high- T_c physics, it is a very fundamental problem in solid state physics. The possibility of the mixed state of s -wave and d -wave pairing has not been discussed sufficiently.¹⁰⁾

In this paper, we will reveal the condition

when above coexistence can be attainable. For this purpose, we will investigate the extended Hubbard model that describes the anisotropic pairings in the simplest form. It is known that the extended Hubbard model becomes an effective Hamiltonian of many bands systems.¹¹⁾ This model especially expresses the narrow band feature of an electron's motion. The phase diagram of this Hamiltonian in one-dimensional case is determined recently by the exact diagonalization.¹²⁾ However, at this stage, it is difficult to obtain rigorous properties in two-dimension by numerical simulations. In the following, we will investigate this model within the mean field approximation level by the selfconsistent numerical calculations.

§2. Formulation

The Hamiltonian, H , of the two-dimensional extended Hubbard model is given as,

$$H = \sum_{ij\sigma} (t_{ij} - \mu \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{W}{2} \sum_{\langle ij \rangle \sigma \sigma'} n_{i\sigma} n_{j\sigma'}, \quad n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}, \quad (1)$$

with on-site repulsive interaction U and inter-site attractive interaction W ($U, W > 0$). We consider this model on a two-dimensional square lattice with N sites. In eq. (1), $c_{i\sigma}^\dagger$, μ , and t_{ij} are the creation operator for spin $\sigma = \uparrow$ at site i , chemical potential, and transfer integral, respectively. Within the mean field approximation, extensive investigations have been done by Micnas *et al.*¹³⁻¹⁵⁾ They studied mutual stability of anisotropic pairing state, i.e., s , p , and d -wave pairing

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However in their calculations, the renormalization of band width that is not fully taken into account. Further the coexistence of s -wave and d -wave is to be studied.

We calculate the free energy of the s , d , and s/d mixed wave pairings using the Bogoliubov approximation at $T=0$ K more thoroughly. Hereafter, we will follow the notation

of Bogoliubov approximation, the mean-field Hamiltonian for the system is given by

$$H = \sum_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} - \sum_k (\Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + h.c.) - \frac{N}{4} (U - 2W_0) n^2 + \sum_{k'\sigma} W_{k-k'} \langle n_{k'\sigma} \rangle \langle n_{k\sigma} \rangle + \sum_k \Delta_k \langle c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \rangle \quad (2)$$

$$W_{k-q} \langle c_{q\sigma}^\dagger c_{q\sigma} \rangle = \bar{\mu}, \quad \bar{\mu} = \mu - n \left(\frac{U}{2} + W_0 \right), \quad (3)$$

$$\gamma(\cos k_x + \cos k_y), \quad \Delta_k = -\frac{1}{N} \sum_q (U - W_{k-q}) \langle c_{-q\downarrow} c_{q\uparrow} \rangle, \quad (4)$$

electron per lattice site. The gap equation can be expressed in the following form

$$(U - W_{k-q}) \Delta_q F_q, \quad F_q = \frac{1}{2E_q} \tanh \frac{\beta E_q}{2}, \quad E_q = \sqrt{\bar{\epsilon}_q^2 + |\Delta_q|^2}. \quad (5)$$

where Δ_k has the form of Δ_k as

$$\Delta_k = \Delta_0 + \Delta_s \gamma_k + \Delta_d \eta_k \quad (6)$$

$$r_q F_q \equiv r_0 \exp(i\theta_0), \quad \Delta_s = \frac{W}{4N} \sum_q \gamma_q \Delta_q F_q \equiv r_s \exp(i\theta_s), \quad (7)$$

$$\Delta_d F_q \equiv r_d \exp(i\theta_d), \quad \eta_k = 2(\cos k_x - \cos k_y). \quad (8)$$

From the above equations, we obtain the following six equations,

$$r_s \cos \theta_1 \left(-\frac{U}{N} \sum_q \gamma_q F_q \right) + r_d \cos \theta_2 \left(-\frac{U}{N} \sum_q \eta_q F_q \right), \quad (9a)$$

$$r_s \sin \theta_1 \left(-\frac{U}{N} \sum_q \gamma_q F_q \right) + r_d \sin \theta_2 \left(-\frac{U}{N} \sum_q \eta_q F_q \right), \quad (9b)$$

$$r_s \cos \theta_1 \left(\frac{W}{4N} \sum_q \gamma_q^2 F_q \right) + r_d \cos \theta_2 \left(\frac{W}{4N} \sum_q \gamma_q \eta_q F_q \right), \quad (9c)$$

$$r_s \sin \theta_1 \left(\frac{W}{4N} \sum_q \gamma_q^2 F_q \right) + r_d \sin \theta_2 \left(\frac{W}{4N} \sum_q \gamma_q \eta_q F_q \right), \quad (9d)$$

$$r_s \cos \theta_1 \left(\frac{W}{4N} \sum_q \gamma_q \eta_q F_q \right) + r_d \cos \theta_2 \left(\frac{W}{4N} \sum_q \eta_q^2 F_q \right), \quad (9e)$$

$$r_s \sin \theta_1 \left(\frac{W}{4N} \sum_q \gamma_q \eta_q F_q \right) + r_d \sin \theta_2 \left(\frac{W}{4N} \sum_q \eta_q^2 F_q \right), \quad (9f)$$

s and d -wave pairing states, by choosing $r_d=0$, $\theta_1=0$ and s -wave pairing state $[(\theta_1, \theta_2)=(0, 0)]$ and $s+id$ -wave pairing state in the following. Under the coexistence of two kinds of pairing states, we use two kinds of Fock parameters,

$$p_1 = \frac{1}{N} \sum_q \bar{\epsilon}_q \eta_q F_q, \quad (10)$$

in the case of $s+d$ -wave pairing state, where the square lattice band structure of this model is given by

$$\epsilon_k = -\mu(n-1) + \frac{n^2}{4} (U-2W_0) + |\Delta_k|^2 F_k, \quad (11)$$

The magnitude of f is not affected by U at all and has a maximum at the center of the band. As compared from Fig. 1 to 2, since the magnitude of f is enhanced for different values of n , the coexistence of s and d -wave pairing is not expected to occur at all.¹³⁾ To realize mixed states with the same values of W and U as in Figs. 1 and 2, it is necessary to transform the band structure. The effect of the next-nearest-neighbor hopping is expressed as follows,

$$\epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y. \quad (13)$$

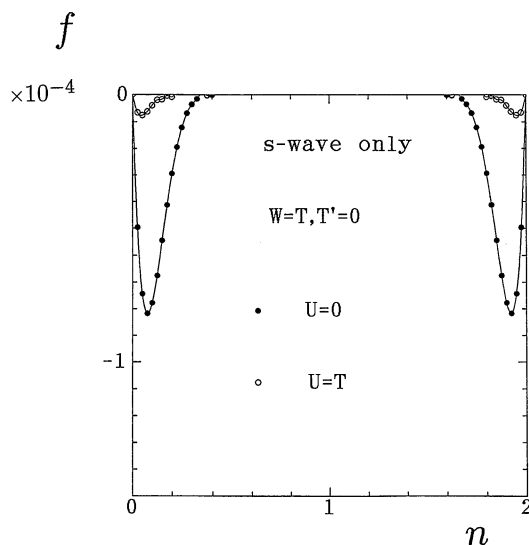


Fig. 1. Normalized Free energy is plotted as a function of carrier concentration n for s -wave pairing state for various U with $W=T$ and $T'=0$.

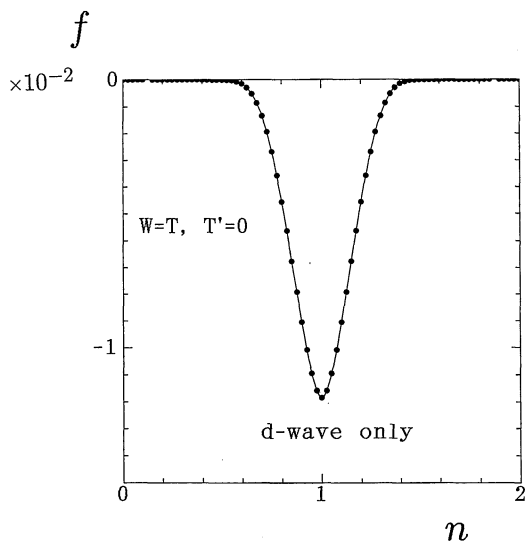


Fig. 2. Plots similar to Fig. 1, for d -wave pairing state with $W=T$ and $T'=0$.

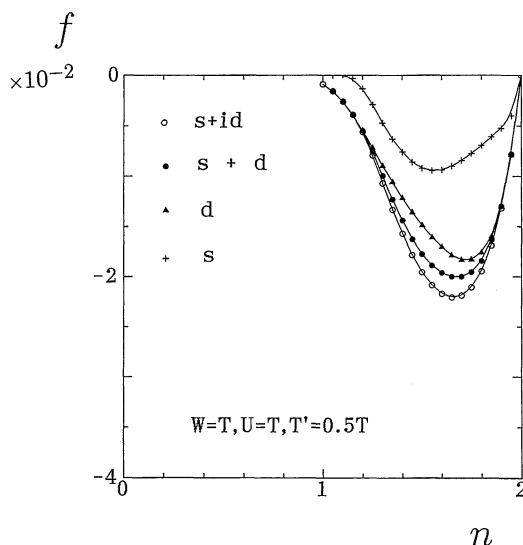


Fig. 4. Plots similar to Fig. 3, for $W=T$, $T'=0.5T$ and $U=T$.

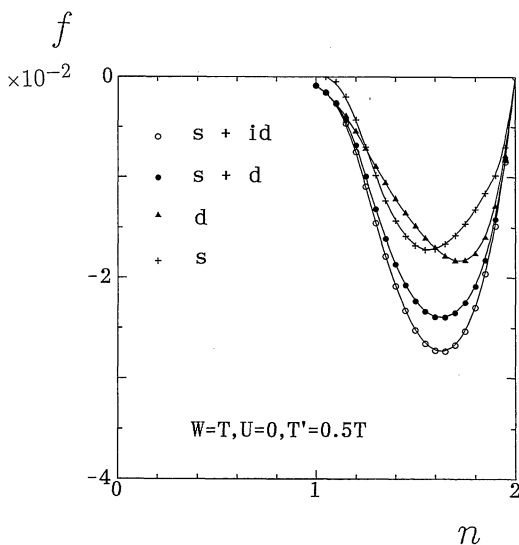


Fig. 3. Free energy of four kinds of pairing states for $W=T$, $T'=0.5T$ and $U=0$.

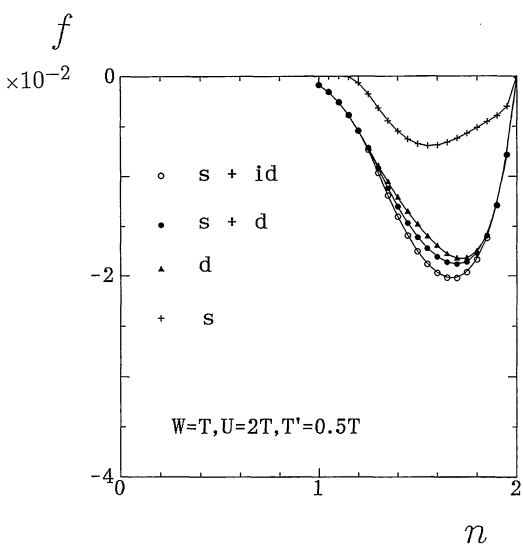


Fig. 5. Plots similar to Fig. 3, for $W=T$, $T'=0.5T$ and $U=2T$.

In the following, we set $t'=0.5t$. In the present case, electron-hole symmetry is broken, and density of states in the non-ordered state is an increasing function of n . As seen in Figs. 3 to 5, f vanishes in the electron doping region ($n < 1$) for all pairing states. For s -wave pairing state, as compared from Fig. 1, the magnitude of f is much enhanced.

However with the increase of U , the magnitude of f is reduced as in Fig. 1. For d -wave pairing state, the order of f is almost the same as that in Fig. 2, and f is independent of U/t . Let us see the mixed state. In every case, the magnitude of f for mixed state is larger than that of d -wave and s -wave pairing state. The mixing of two kinds of pair potentials lowers

the Free energy. Among the mixed state, $s+id$ -wave pairing state is most stable for any n and U . In this state, the square lattice symmetry is also preserved in the energy spectrum of the quasiparticles. With increasing U/t , the free energy of mixed states approach those of d -wave pairing states, since the s -wave components of the pair potentials are reduced.

§4. Conclusions

In this paper, we have established a numerical calculation method to obtain the Free energy taking account of the chemical potential, the renormalization factors of the band width, and the pair potentials fully selfconsistently. It is revealed that the coexistence of the s and d -wave pair potentials can be attainable by the transformation of the energy band. The mixing of two kinds of pair potentials lowers the Free energy. In such a case, $s+id$ -wave pairing state becomes most stable.

In the present calculation, we have used the mean-field approximation. This approximation is only valid in the weak coupling limit. Therefore, we can never exclude the possibility that another pairing state with more stable Free energy. Further it is necessary to compare the free energies with various ordered states except for superconductivity, *e.g.*, SDW and phase separation. This vagueness calls for more rigorous studies beyond mean field approximations. Our calculation is limited at $T=0$ K. It is easy to extend our results to finite temperature within the present formalism. These results will be published elsewhere.

Acknowledgement

The authors would like to thank to Profes-

sors H. Aoki, M. Ogata, H. Kaga and Dr. K. Kuroki for valuable discussions. They would like to thank to Professors M. Azuma, A. Hasegawa and M. Kobayashi for encouragement of this work. This work is supported by a Grant-in-Aid for Scientific Research on Priority Areas, Computational Physics as a New Frontiers of Education and Science. One of the author Y. T. would like to thank the Computer Center, Institute for Molecular Science, Okazaki National Research Institutes for the use of the NEC SX-3R.

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