Journal of the Physical Society of Japan
Vol. 64, No. 3, March, 1995, pp. 922–926

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

Hiroki TSUCHIURA*, Yukio TANAKA and Yasunari USHIJIMA

Department of Physics, Faculty of Science, Niigata University, Ikarashi, Niigata 950-21

(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 ^{3}He, 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,

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

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), $c^{\dagger}_{i\sigma}$, 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

* Present address: Department of Applied Physics, Osaka University, Suita 565.

state, comparing their T_C. However in their calculations, the renormalization of band width that originates from Fock term is not fully taken into account. Further the coexistence of *s*-wave and *d*-wave pairing still remains to be studied.

In this paper, we calculate the free energy of the *s*, *d*, and *s*/*d* mixed wave pairings using the mean-field approximation at $T=0$ K more thoroughly. Hereafter, we will follow the notation used by Micnas *et al.*

Using the Hartree–Fock–Bogoliubov approximation , the mean-field Hamiltonian for the singlet superconductivity is given by

$$H_0=\sum_{k\sigma}\bar{\varepsilon}_k c^\dagger_{k\sigma}c_{k\sigma}-\sum_k(\Delta_k c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}+h.c.)-\frac{N}{4}(U-2W_0)n^2$$
$$-\frac{1}{2N}\sum_{kk'\sigma}W_{k-k'}\langle n_{k\sigma}\rangle\langle n_{k'\sigma}\rangle+\sum_k\Delta_k\langle c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}\rangle \tag{2}$$

where

$$\bar{\varepsilon}_k=\varepsilon_k+\frac{1}{N}\sum_q W_{k-q}\langle c^\dagger_{q\sigma}c_{q\sigma}\rangle-\bar{\mu},\quad \bar{\mu}=\mu-n\left(\frac{U}{2}+W_0\right), \tag{3}$$

$$W_k=W\gamma_k=2W(\cos k_x+\cos k_y),\quad \Delta_k=-\frac{1}{N}\sum_q(U-W_{k-q})\langle c_{-q\downarrow}c_{q\uparrow}\rangle, \tag{4}$$

and n is the number of electron per lattice site. The gap equation can be expressed in the following form,

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

Since $\Delta_k=\Delta_{-k}$, we obtain a form of Δ_k as

$$\Delta_k=\Delta_0+\Delta_s\gamma_k+\Delta_d\eta_k \tag{6}$$

from eq. (5), with

$$\Delta_0=-\frac{U}{N}\sum_q\Delta_q F_q\equiv r_0\exp(i\theta_0),\quad \Delta_s=\frac{W}{4N}\sum_q\gamma_q\Delta_q F_q,\equiv r_s\exp(i\theta_s), \tag{7}$$

$$\Delta_d=\frac{W}{4N}\sum_q\eta_q\Delta_q F_q\equiv r_d\exp(i\theta_d),\quad \eta_k=2(\cos k_x-\cos k_y). \tag{8}$$

Equation (6) is separated into following six equations,

$$r_0=r_0\left(-\frac{U}{N}\sum_q F_q\right)+r_s\cos\theta_1\left(-\frac{U}{N}\sum_q\gamma_q F_q\right)+r_d\cos\theta_2\left(-\frac{U}{N}\sum_q\eta_q F_q\right), \tag{9a}$$

$$0=r_s\sin\theta_1\left(-\frac{U}{N}\sum_q\gamma_q F_q\right)+r_d\sin\theta_2\left(-\frac{U}{N}\sum_q\eta_q F_q\right), \tag{9b}$$

$$r_s\cos\theta_1=r_0\left(\frac{W}{4N}\sum_q\gamma_q F_q\right)+r_s\cos\theta_1\left(\frac{W}{4N}\sum_q\gamma_q^2 F_q\right)+r_d\cos\theta_2\left(\frac{W}{4N}\sum_q\gamma_q\eta_q F_q\right), \tag{9c}$$

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

$$r_d\cos\theta_2=r_0\left(\frac{W}{4N}\sum_q\eta_q F_q\right)+r_s\cos\theta_1\left(\frac{W}{4N}\sum_q\gamma_q\eta_q F_q\right)+r_d\cos\theta_2\left(\frac{W}{4N}\sum_q\eta_q^2 F_q\right), \tag{9e}$$

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

where $\theta_1 \equiv \theta_s - \theta_0$, $\theta_2 \equiv \theta_d - \theta_0$. We can obtain s and d-wave pairing states, by choosing $r_d=0$, $\theta_1=0$ and $r_0=r_s=0$, respectively. Further, $s+d$-wave pairing state $[(\theta_1, \theta_2)=(0, 0)]$ and $s+id$-wave pairing state $[(\theta_1, \theta_2)=(0, \frac{\pi}{2})]$ will be considered in the following. Under the coexistence of two kinds of pair potentials, it is necessary to introduce two kinds of Fock parameters,

$$p_1=-\frac{1}{N}\sum_q \bar{\varepsilon}_q \gamma_q F_q, \quad p_2=-\frac{1}{N}\sum_q \bar{\varepsilon}_q \eta_q F_q. \tag{10}$$

The quantity p_2 does not vanish only in the case of $s+d$-wave pairing state, where the square lattice symmetry is broken. The free energy of this model is given by

$$\frac{F}{N}=-\frac{2}{\beta N}\sum_k \ln\left[2\cosh\frac{\beta E_k}{2}\right]+\bar{\mu}(n-1)+\frac{n^2}{4}(U-2W_0) -\frac{W}{4}(p_1^2+p_2^2)+\frac{1}{N}\sum_k |\Delta_k|^2 F_k, \tag{11}$$

with

$$n-1=-\frac{2}{N}\sum_q \bar{\varepsilon}_q F_q,$$
$$\bar{\varepsilon}_k=\varepsilon_k-\bar{\mu}+\frac{W}{4}(p_1\gamma_k+p_2\eta_k). \tag{12}$$

§3. Numerical Calculation

The procedure of the numerical calculation is composed of three folds loops for given n, U and W. In the most inner loop, pair potentials r_0, r_s and r_d are determined selfconsistently for a given μ, p_1 and p_2. In the middle loop, the renormalization factors of band width p_1, p_2 are determined. The most outer loop is to determine the chemical potential μ checking carrier concentration per site (n). The total number of calculations which is necessary for the most inner loop is about one hundred thousands. Above procedure is taken for the s, d, $s+d$, $s+id$-wave pairing state and the non-ordered state for each n.

For the first step, we investigate the case, where $\varepsilon_k=-t\gamma_k$ is satisfied. In Fig. 1, normalized Free energy $f=(F-F_N)/Nt$ is plotted as a function of n for various U/t and W/t, where F_N is the free energy of the non-ordered state ($\Delta_k=0$). The quantity f becomes finite at the edge of the band,[13] and the magnitude of f is reduced by the on site repulsive interaction U. The s-wave pairing state is very sensitive to the on site repulsion. In Fig. 2, f for d-wave pairing state is plotted. The pair potential r_d is independent of U as seen from eq. (9). 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,

$$\varepsilon_k=-2t(\cos k_x+\cos k_y)-4t' \cos k_x \cos k_y. \tag{13}$$

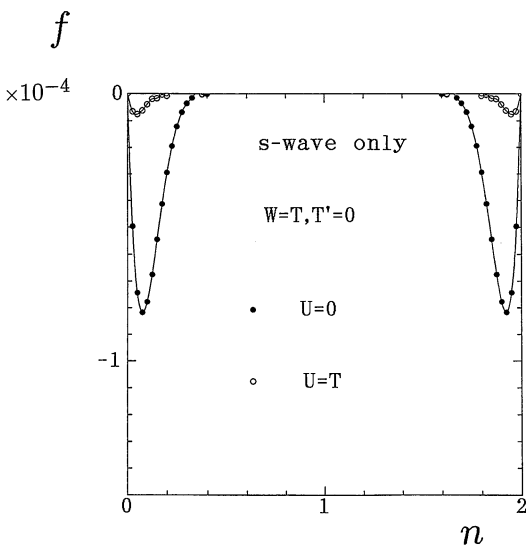

Fig. 1. Normalized Free energy is plotted as a function of carrier concentration n for s-wave pairing state for various U with $W=T$ and $T'=0$.

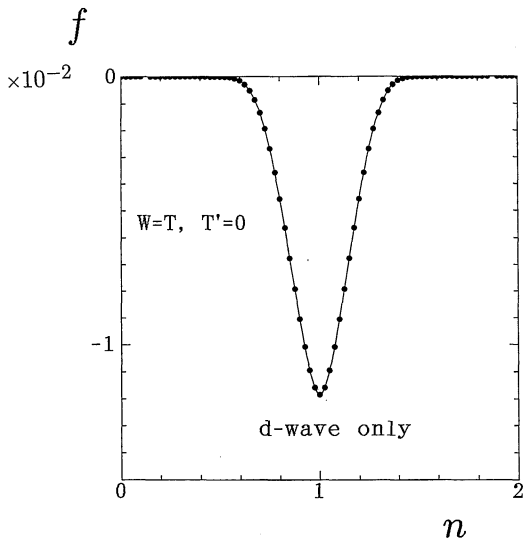

Fig. 2. Plots similar to Fig. 1, for d-wave pairing state with $W=T$ and $T'=0$.

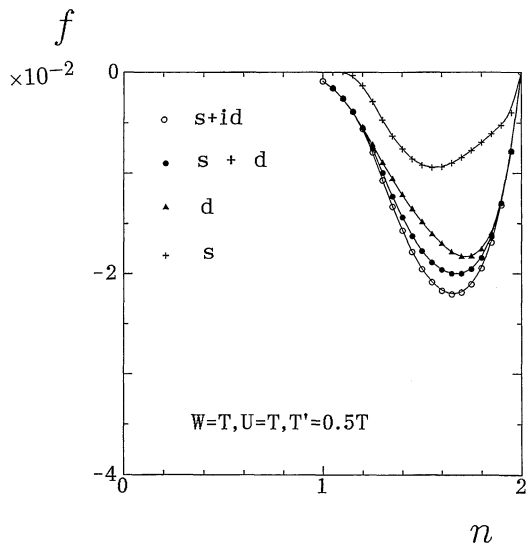

Fig. 4. Plots similar to Fig. 3, for $W=T$, $T'=0.5T$ and $U=T$.

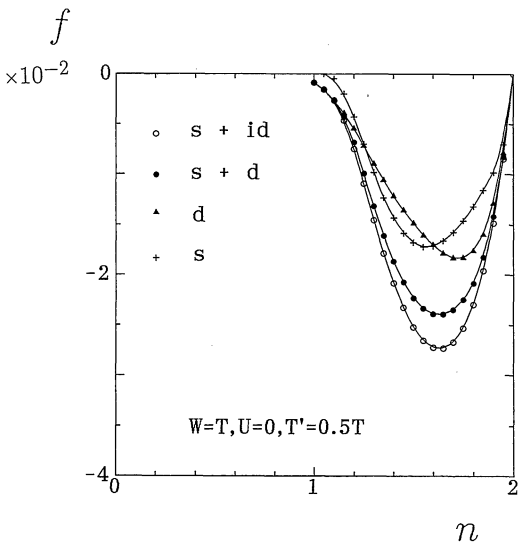

Fig. 3. Free energy of four kinds of pairing states for $W=T$, $T'=0.5T$ and $U=0$.

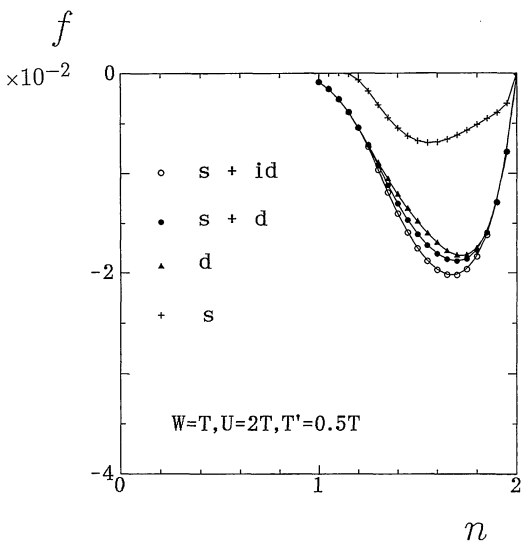

Fig. 5. Plots similar to Fig. 3, for $W=T$, $T'=0.5T$ and $U=2T$.

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 Professors 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.

References

1) A. J. Leggett: Rev. Mod. Phys. **47** (1975) 331.
2) K. Miyake, T. Matsuura, H. Jichu and Y. Nagaoka: Prog. Theor. Phys. **72** (1984) 1065.
3) Z.-X. Shen *et al.*: Phys. Rev. Lett. **70** (1993) 1553.
4) T. Moriya, Y. Takahashi and K. Ueda: Physica C **185** (1991) 114.
5) D. A. Wollman, D. J. V. Harlingen, W. C. Lee, D. M. G. Ginsberg and A. J. Legett: Phys. Rev. Lett. **71** (1993) 2134.
6) I. Iguchi and Z. Wen: Phys. Rev. B **49** (1994) 12388.
7) Y. Tanaka: Phys. Rev. Lett. **72** (1994) 3871.
8) T. Hasegawa and K. Kitazawa: J. Phys. Chem. Solids. **54** (1993) 1351.
9) P. Chaudhari and S.Y. Lin: Phys. Rev. Lett. **72** (1994) 1084.
10) Y. Tanaka and A. Hasegawa: Physica B **194–196** (1994) 1411.
11) K. Kuroki and H. Aoki: Phys. Rev. Lett. **69** (1992) 3820; Phys. Rev. B **48** (1993) 7598.
12) K. Sano and Y. Ōno: J. Phys. Soc. Jpn. **63** (1994) 1250.
13) R. Micnas, J. Ranninger, S. Robaszkiewicz and S. Tabor: Phys. Rev. B **37** (1988) 9410.
14) R. Micnas, J. Ranninger and S. Robaszkiewicz: Phys. Rev. B **39** (1989) 11653.
15) R. Micnas, J. Ranninger and S. Robaszkiewicz: Rev. Mod. Phys. **62** (1990) 113.