Phase diagram of the $t-U^2$ Hamiltonian of the weak coupling Hubbard model

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Abstract. We determine the symmetry of Cooper pairs, on the basis of the perturbation theory in terms of the Coulomb interaction $U$, for the two-dimensional Hubbard model on the square lattice. The phase diagram is investigated in detail. The Hubbard model for small $U$ is mapped on to an effective Hamiltonian with the attractive interaction using the canonical transformation: $H_{\text{eff}} = e^S H e^{-S}$. The gap equation of the weak coupling formulation is solved without numerical ambiguity to determine the symmetry of Cooper pairs. The superconducting gap crucially depends on the position of the van Hove singularity. We show the phase diagram in the plane of the electron filling $n_e$ and the next nearest-neighbor transfer $t'$. The d-wave pairing is dominant for the square lattice in a wide range of $n_e$ and $t'$. The d-wave pairing is also stable for the square lattice with anisotropic $t'$. The three-band d–p model is also investigated, for which the d-wave pairing is stable in a wide range of $n_e$ and $t_{pp}$ (the transfer between neighboring oxygen atoms). In the weak coupling analysis, the second-neighbor transfer parameter $-t'$ could not be so large so that the optimum doping rate is in the range of $0.8 < n_e < 0.85$. 
1. Introduction

Since the discovery of high-temperature superconductors, the strongly correlated electron systems have been studied intensively. The effect of the strong correlation between the electrons is important for many quantum critical phenomena such as unconventional superconductivity (SC). High-temperature superconductors [1]–[3] as well as heavy fermions [4]–[7] are known as the typical correlated electron systems. These systems are modeled by the Hamiltonian with the electronic interaction of the on-site Coulomb repulsion. Recently, the mechanisms of SC in high-temperature superconductors have been extensively studied using the two-dimensional (2D) Hubbard model [8]–[16].

The SC of the Hubbard model has been questioned for many years. It is extremely difficult to show the existence of superconducting phase for the Hubbard model in a reasonable way. At present we cannot answer this long-standing question. Instead of examining the possibility of SC, it is possible to investigate possible symmetries of Cooper pairs for an effective Hamiltonian with the attractive interaction. For this purpose effective Hamiltonians have been obtained for the Hubbard model. The $t$–$J$ model is the well-known effective Hamiltonian derived in the limit of the large on-site repulsion $U$, using the canonical transformation $H_{t-J} = e^S H e^{-S}$ with $S \propto t/U$. On the other hand, in the limit of small $U$, the perturbation theory also leads to an effective Hamiltonian with the attractive interaction [17]–[20], where we have $S \propto U/t$. The phase diagram with respect to the Cooper pair symmetry can be determined if we solve the gap equation.

We must notice that we should compare the energy with other electronic states to show that the superconducting state is indeed stable. For the half-filled band with vanishing $t' = 0$ in two space dimensions, the antiferromagnetic order parameter for small $U$ is [21]

$$\Delta_{AF} = \frac{8tc}{U} \exp \left( -\frac{4\pi^2 t_c}{U} \right),$$

(1)

where $c = 3 - \sqrt{3}$. It is, however, obvious that the antiferromagnetically ordered state is unstable away from half filling if the Coulomb repulsion $U$ is small. Thus, we focus on the...
The purpose of the paper is to determine the gap symmetry for the square lattice using the small-$U$ gap equation derived for the effective Hamiltonian. Although the real SC in correlated electron systems should be described by a theory of strong-coupling SC, the phase diagram can be determined in detail using the weak coupling formulation. Precise calculations are sometimes not easy at low temperatures in the strong-coupling formulation due to the Matsubara frequency summation and the wave number summation. It is important to examine the detailed phase diagram for materials belonging to strongly correlated systems such as the cuprate high-temperature superconductors, the organic superconductors, the ruthenate superconductor Sr$_2$RuO$_4$.

The paper is organized as follows. In section 2, the effective Hamiltonian is derived using the canonical transformation. We show that we can derive the attractive effective Hamiltonian using some approximations. In section 3, the gap equation is shown and the results are presented in section 4. We give a summary in section 5.

2. Effective Hamiltonian

The Hubbard Hamiltonian is

$$H = -t \sum_{\langle ij \rangle} (c_{i \sigma}^\dagger c_{j \sigma} + \text{h.c.}) - t' \sum_{\ll j \ell \gg} (c_{j \sigma}^\dagger c_{\ell \sigma} + \text{h.c.}) + U \sum_i n_{i \uparrow} n_{i \downarrow}, \quad (2)$$

where $\langle ij \rangle$ and $\ll j \ell \gg$ denote the nearest-neighbor and next-nearest-neighbor pairs, respectively. $U$ is the on-site Coulomb repulsion. The unit of energy is given by $t$ in this paper. The total number of sites and the number of electrons are denoted as $N$ and $N_e$, respectively. The half-filled band corresponds to $n_e = N_e/N = 1$.

The effective Hamiltonian is derived using the perturbation theory for small $U$. The canonical transformation also maps the Hubbard model to an effective Hamiltonian with the attractive interaction [2]. Since no instability except SC occurs for small $U$ away from half filling, we assume that the pairing interaction is the most singular. The procedure of mapping is as follows. The Hamiltonian is written as

$$H = H_0 + H_1 + H_2 + H_3, \quad (3)$$

where

$$H_0 = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma}, \quad (4)$$

$$H_1 = \frac{U}{N} \sum_{k \neq k'} c_{k'\uparrow}^\dagger c_{-k'\downarrow}^\dagger c_{-k\downarrow} c_{k\uparrow}, \quad (5)$$

$$H_2 = \frac{U}{N} \sum_{k \neq k', q \neq 0} c_{k'\uparrow}^\dagger c_{-k'-q\downarrow} c_{-k-q\downarrow} c_{k\uparrow}, \quad (6)$$

$$H_3 = \frac{U}{N} \sum_{kk'} c_{k\uparrow}^\dagger c_{k\downarrow} c_{k'\uparrow}^\dagger c_{k'\downarrow}. \quad (7)$$

The dispersion relation $\epsilon_k$ for the square lattice is

$$\epsilon_k = -2t (\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y, \quad (8)$$
where $\mu$ is the chemical potential. We set $\xi_k = \epsilon_k - \mu$. Using a canonical transformation, $\tilde{\psi} = e^\varphi \psi$, we look for the solution of the Schrödinger equation $H_{\text{eff}} \tilde{\psi} = \tilde{E} \tilde{\psi}$. The effective Hamiltonian reads

$$H_{\text{eff}} = e^S H e^{-S} = H + [S, H] + \frac{1}{2} [S, [S, H]] + \cdots$$

$$= H_0 + H_1 + H_2 + H_3 + [S, H_0] + H_1 + H_2 + H_3 + \frac{1}{2} [S, [S, H_0]] + \cdots. \quad (9)$$

We determine $S$ so as to satisfy $H_2 + [S, H_0] = 0$. We find

$$S = \frac{U}{N} \sum_{k \neq k', q \neq 0} \frac{1}{\xi_{k' + q} + \xi_k - \xi_{k + q} - \xi_k} c_{k'q}^\dagger c_{-k'q}^\dagger c_{-k-q} c_{-k-q}^\dagger. \quad (10)$$

Since $[S, H_3] = 0$, we obtain up to the order of $U^2$,

$$H_{\text{eff}} = H_0 + H_1 + H_3 + [S, H_1] + \frac{1}{2} [S, H_2]. \quad (11)$$

The commutator $[S, H_2]$ is evaluated as

$$[S, H_2] = \left(\frac{U}{N}\right)^2 \sum_{k \neq k', q \neq 0} \sum_{p \neq p', q \neq 0} S_{kk'}^{qq'} (-\delta_{pq} c_{p'q}^\dagger c_{-p'q}^\dagger c_{-p-q} c_{-k-q} c_{-k-q}^\dagger c_{k^\dagger} c_{-p-q} c_{-p-q})$$

$$+ \delta_{p+q', k+q} c_{k'}^\dagger c_{-q} c_{-p-q} c_{-k-q} c_{-k-q}^\dagger c_{k^\dagger} c_{-p-q} c_{-p-q} c_{p^\dagger}$$

$$+ \delta_{p+q', k+q} c_{k'}^\dagger c_{-q} c_{-p-q} c_{-k-q} c_{-k-q}^\dagger c_{k^\dagger} c_{-p-q} c_{-p-q} c_{p^\dagger}), \quad (12)$$

where

$$S_{kk'}^{qq'} = \frac{1}{\xi_{k' + q} + \xi_k - \xi_{k + q} - \xi_k}. \quad (13)$$

Since the purpose of this paper is to investigate the pairing symmetry, we need only the first term and the last term of $[S, H_2]$. We find that the average of the second and third terms with respect to the Bardeen–Cooper–Schrieffer (BCS) wavefunction vanish. Due to the same reason $[S, H_1]$ can be neglected. Then the effective Hamiltonian is

$$H_{\text{eff}} = \sum_{k \sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{U}{N} \sum_{k \neq k'} c_{k\uparrow}^\dagger c_{-k\downarrow} c_{-k\downarrow}^\dagger c_{k\uparrow} + \frac{1}{2} \frac{U^2}{N^2} \sum_{k \neq k', q \neq 0} \frac{1}{\xi_{k' + q} + \xi_k - \xi_{k + q} - \xi_k}$$

$$\times \left(\delta_{p+q', k+q} c_{k'}^\dagger c_{-q} c_{-p-q} c_{-k-q} c_{-k-q}^\dagger c_{k^\dagger} c_{-p-q} c_{-p-q} c_{p^\dagger} - \delta_{pq} c_{p^\dagger} c_{-p-q} c_{-p-q} c_{-k-q} c_{-k-q}^\dagger c_{k^\dagger} c_{-p-q} c_{-p-q} c_{p^\dagger}\right). \quad (14)$$

If we set $k = p + q'$ and $p' = k' + q$, the first term of $[S, H_2]$ is approximated as

$$H_{2a} \equiv -\left(\frac{U}{N}\right)^2 \sum_{k \neq k', q \neq 0, p \neq p', q \neq 0} S_{kk'}^{qq'} S_{p+q', k+q}$$

$$\approx \left(\frac{U}{N}\right)^2 \sum_{k \neq k', q \neq 0} c_{k'q}^\dagger c_{-k'q}^\dagger c_{-k-q} c_{-k-q}^\dagger$$

$$\approx \left(\frac{U}{N}\right)^2 \sum_{k \neq k', q \neq 0} c_{k'q}^\dagger c_{-k'q}^\dagger$$

$$= \left(\frac{U}{N}\right)^2 \sum_{k' + q \neq 0, k \neq 0} \sum_{q \neq 0} c_{k'q}^\dagger c_{-k'q}^\dagger \frac{\xi_{k' + q} + \xi_k - \xi_{k + q} - \xi_k}{c_{-k-q} c_{-k-q}^\dagger}. \quad (15)$$
where \( f_k \) is the Fermi distribution function,
\[
f_k = \frac{1}{e^{\beta \xi_k} + 1}. \tag{16}\]

Since the summation is restricted to the small region near the Fermi surface, we obtain assuming \( \xi_{-k} = \xi_k \)
\[
H_{2a} \approx \left( \frac{U}{N} \right)^2 \sum_{k \neq -q, k' \neq -q} \frac{f_q}{\xi_{k+k+q} - \xi_q} c_{k+q}^\dagger c_{-k+q} c_{-k} c_k^\dagger. \tag{17}\]

Similarly the last term of \( [S, H_2] \) is written as
\[
H_{2b} \approx \left( \frac{U}{N} \right)^2 \sum_{k \neq -q, k' \neq -q} \frac{f_{k+k+q}}{\xi_{k+k+q} - \xi_q} c_{k+q}^\dagger c_{-k+q} c_{-k} c_k^\dagger. \tag{18}\]

The resulting effective Hamiltonian is
\[
H_{\text{eff}} = e^S H e^{-S} \equiv H_{t-U^2} = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k'k} V_{kk'} c_{k'}^\dagger c_{-k} c_k, \tag{19}\]

where
\[
V_{kk'} = \left( \frac{U}{N} \right)^2 \frac{U^2}{N} \chi(k+k'). \tag{20}\]

\( \chi(k+k') \) is the magnetic susceptibility defined as
\[
\chi(k+k') = \frac{1}{N} \sum_q \frac{f_{k+k+q} - f_q}{\xi_q - \xi_{k+k+q}}. \tag{21}\]

Thus, we have reached the effective Hamiltonian up to the order of \( U^2 \) using the canonical transformation.

### 3. Gap equation

The gap equation for the \( t-U^2 \) model was investigated in \[19\]. Since the equation was considerably simplified for small \( U \), the gap equation was solved without numerical ambiguity. We define the order parameter,
\[
\Delta_k = \sum_{k'} V_{kk'} \langle c_{-k'} c_{k} \rangle. \tag{22}\]

Using the mean-field theory, the gap equation for the Hamiltonian \( H_{t-U^2} \) is
\[
\Delta_k = -\sum_{k'} V_{kk'} \Delta_{k'} \frac{1 - 2f(E_k)}{2E_{k'}}, \tag{23}\]

where \( E_k = \sqrt{\xi_k^2 + \Delta_k^2} \). We assume the anisotropic order parameter given as
\[
\Delta_k = \Delta \cdot z_k, \tag{24}\]

where \( z_k \) denotes the \( k \)-dependence of \( \Delta_k \). At \( T = 0 \), the gap equation is written as
\[
\Delta_k = -\frac{1}{2} \sum_{k'} V_{kk'} \Delta_{k'} \frac{\Delta_{k'}}{E_{k'}}, \tag{25}\]

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For small $U$, the gap equation for anisotropic pairing is extremely simplified retaining only the logarithmic term \[ 19 \]:

$$z_k = \log \left( \frac{\Delta}{2\omega_0} \right) U^2 \frac{1}{N} \sum_{k'} \chi(k+k')\delta(\xi_{k'})z_{k'},$$

(26)

where $\omega_0$ is the cut-off energy. The critical temperature $T_c$ is determined by

$$z_k = -\sum_{k'} V_{kk'}z_{k'} \frac{1 - 2f(|\xi_{k'}|)}{2|\xi_{k'}|} \quad \text{for } T = T_c.$$

(27)

For small $U$, the critical temperature $T_c$ is extremely small. In this case, we can use the following approximation,

$$I \equiv \int_0^{\omega_0} d\xi g(\xi) \frac{\tanh(\beta_c \xi/2)}{\xi} \approx g(\omega_0) \log \omega_0 - \frac{\beta_c}{2} \int_0^{\omega_0} d\xi \log \xi g(\xi) \frac{1}{(\cosh(\beta_c \xi/2))^2} = g(\omega_0) \log \omega_0 - \int_0^{\beta_c \omega_0/2} dx \log \left( \frac{2x}{\beta_c} \right) g\left( \frac{2x}{\beta_c} \right) \frac{1}{(\cosh x)^2} = g(\omega_0) \log \omega_0 - g(0) \int_0^{\beta_c \omega_0/2} dx \log \left( \frac{2x}{\beta_c} \right) \frac{1}{(\cosh x)^2} \approx g(0) \log \left( \frac{2e^{\gamma} \omega_0}{\pi k_B T_c} \right),$$

(28)

where we assume that $g(\xi)$ is a slowly varying function and $g'(\xi)$ is negligible. The equation is written as

$$z_k = -\log \left( \frac{2e^{\gamma} \omega_0}{\pi k_B T_c} \right) \sum_{k'} V_{kk'}z_{k'} \delta(\xi_{k'}).$$

(29)

Since $T_c$ is very small, the summation over $k'$ can be restricted to the average over near the Fermi surface. If we solve the eigenequation

$$\frac{2}{N} \sum_{k'} \chi(k+k')z_{k'}\delta(\xi_{k'}) = -xz_k,$$

(30)

the critical temperature is obtained as

$$k_B T_c = 1.13 \omega_0 \exp \left( -\frac{2t^2}{xU^2} \right),$$

(31)

where the energy unit is given by $t$. Since $\Delta$ is given as

$$\Delta = 2\omega_0 \exp \left( -\frac{2t^2}{xU^2} \right),$$

(32)

the ratio $2\Delta / k_B T_c$ equals the BCS universal value $2\pi/e^{\gamma} = 3.53$.  

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4. Pairing symmetry

4.1. Method of solving the eigenvalue equation

We express $z_k$ and $V_{kk'}$ in terms of the polar coordinates $\xi$, $\theta$:

$$z_k = z(\xi, \theta),$$  \hspace{1cm}  (33)

$$\chi(\mathbf{k} + \mathbf{k'}) = \chi(\xi, \theta, \xi', \theta'),$$  \hspace{1cm}  (34)

where $\mathbf{k}$ is expressed using the polar angle $\theta$: $\mathbf{k} = (\xi, \theta)$ in terms of the polar coordinates.

We consider the gap function on the Fermi surface $z(\theta) \equiv z(0, \theta)$. If we define $\chi(\theta, \theta') = \chi(0, \theta, 0, \theta')$, the gap equation is

$$2 \int_{0}^{2\pi} d\theta' \rho_F(\theta') \chi(\theta, \theta') z(\theta') = -xz(\theta),$$  \hspace{1cm}  (35)

where $\rho_F(\theta)$ is the density of states at the Fermi surface:

$$\rho_F(\theta) = \frac{1}{(2\pi)^2} k_F(\theta) \frac{1}{|\partial \xi / \partial k(k = k_F(\theta))|},$$  \hspace{1cm}  (36)

where $k_F(\theta)$ is the Fermi wave number of the polar coordinate $\theta$ and $\partial \xi / \partial k$ is the derivative with respect to $k = |\mathbf{k}|$. If we expand $z(\theta)$ as

$$z(\theta) = \sum_n z_n e^{in\theta},$$  \hspace{1cm}  (37)

the gap equation is given as

$$\sum_n \chi_{mn} z_n = -xz_m,$$  \hspace{1cm}  (38)

where $\chi_{mn}$ are the matrix elements of $\chi(\theta, \theta')$:

$$\chi_{mn} = \frac{1}{\pi} \int_{0}^{2\pi} d\theta \int_{0}^{2\pi} d\theta' \rho_F(\theta') e^{-im\theta} \chi(\theta, \theta') e^{in\theta'}. $$  \hspace{1cm}  (39)

The number of basis functions kept in solving the eigenequation is 30–40 in this paper. The $\mathbf{k}$-space is divided into $200 \times 20$ points on equally spaced mesh in the numerical calculations of $\chi(\theta, \theta')$.

4.2. Simple square lattice

Let us investigate the phase diagram for the square lattice (figure 1). The basis functions $\{e^{in\theta}\}$ ($n = 0, \pm 1, \pm 2, \ldots$) are classified into irreducible representations according to the symmetry group. The eigenfunctions are specified by one of irreducible representations of the square lattice (see table 1). It is convenient to use real basis functions $\cos(n\theta)$ and $\sin(n\theta)$ for this purpose. The gap function in each representation is [19]

$$z(\theta) = \sum_{\ell=1}^{4} z_{4\ell} \cos(4\ell\theta) \quad A_1,$$  \hspace{1cm}  (40)

$$z(\theta) = \sum_{\ell=1}^{4} z_{4\ell} \sin(4\ell\theta) \quad A_2,$$  \hspace{1cm}  (41)
Figure 1. Square lattice with next-nearest transfer $t'$.

$$z(\theta) = \sum_{\ell=1} z_{4\ell-2} \cos(4\ell - 2)\theta \quad B_1,$$

$$z(\theta) = \sum_{\ell=1} z_{4\ell-2} \sin(4\ell - 2)\theta \quad B_2.$$  

$$z(\theta) = \sum_{\ell=1} z_{2\ell-1} \cos(2\ell - 1)\theta \quad E,$$

or $\sin(2\ell - 1)\theta$  

In [19], the representations $A_1$–$B_2$ were investigated. Here, the $E$ symmetry for triplet pairing is also examined. The eigenvalue $x$ for $t' = 0$ is shown in figure 2 as a function of the electron density $n_e$. For $n_e > 0.6$ the paired state with $d_{x^2-y^2}$ symmetry is most stable for $t' = 0$. Since the exponent $x$ sensitively depends on the van Hove singularity, $x$ is an increasing function of $n_e$ near half-filling for $t' = 0$.

The exponent $x$ for $t' = -0.1$, $-0.2$ and $-0.3$ is shown in figures 3–5, respectively. The exponents for small electron filling are not shown here because the high numerical accuracy is required for exponentially small exponents. As is shown in the figures, the $d$-wave state is most stable near half-filled case for $t'$ in the range of $0 \leq t' \leq 0.4$. The position of the van Hove singularity depends on $t'$, and the peak of $x$ shifts as $-t' > 0$ increases (figure 6). $x$ has a sharp peak showing a logarithmic increase due to the van Hove singularity:

$$x \sim -\log|\mu - \mu_{vH}|,$$

where $\mu_{vH}$ is the chemical potential corresponding to the van Hove singularity. The figure suggests higher $T_c$ for small $-t'$. The antiferromagnetism, however, may compete and suppress
SC near half filling. Hence, we must have a bell-shape critical temperature as a function of the electron filling.

It was pointed out from the electronic states calculations that the Fermi surface is much deformed for Tl$_2$Ba$_2$CuO$_6$ [23] and HgBa$_2$CuO$_4$ [24] for which the band parameter values must be assigned as $t' \sim -0.4$ and $t'' \sim 0.1$ (third-neighbor transfer). Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212) also

Figure 2. The exponent $x$ as a function of the electron density for $t' = 0$. (See [19]. We have included $x$ for the E representation.) Since the line for A$_1$ mostly coincides with that for B$_2$, the A$_1$ line is omitted.

Figure 3. The exponent $x$ as a function of the electron density for $t' = -0.1$. 

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Figure 4. The exponent $x$ as a function of the electron density for $t' = -0.2$.

Figure 5. The exponent $x$ as a function of the electron density for $t' = -0.3$.

has deformed Fermi surface so that $t' \sim -0.3$ and $t'' \sim 0.2$ [25]. For these values the optimum doping rate must be larger than that for La$_{1-x}$Sr$_x$CuO$_4$ (LSCO) for which $t' \sim -0.1$ and $t'' \sim 0$. Experiments, however, indicated that the optimum doping rate is almost the same for Bi2212 and LSCO [26]. This may be a flaw of the weak coupling formulation, which, however, may not be completely remedied by the strong coupling treatment since the van Hove singularity still has a large effect on the critical temperature. This suggests that we must re-examine the structure of
the Fermi surface of high-temperature cuprates. In particular, the band parameters for Bi2212 will be modified if we take into account the double layer structure [27, 28]. The band structure reported by recent studies [28, 29] is well fitted using smaller $t'$ such as [30]

$$t' \sim -0.2.$$  (46)

The phase diagram in the $n_e$–$t'$ plane is shown in figure 7 for $t' \leq 0$ and in figure 8 for $t' \geq 0$. For $n_e \sim 0.5$ and $-t' \sim 0.4$, there is a possibility that the p-wave SC is realized. For example, the ruthenate superconducting material Sr$_2$RuO$_4$ [31] is sometimes modeled by the one-band Hubbard model for the $\gamma$ orbital with $t' \sim -0.4$ and $n_e \simeq 0.67$ after the electron–hole transformation. The state of these parameters just corresponds to the point within the singlet region near the boundary to p-wave regions in figure 7. In order to obtain the stable p-wave pairing for the parameters corresponding to Sr$_2$RuO$_4$, we may need to consider the multi-band structure including $\alpha$ and $\beta$ orbitals [32]. For $t' > 0$, we have a large d-wave region.

If $t'$ is large and negative, i.e. if $-t' > 0.5$, we have the case with two Fermi surfaces; one is a large Fermi surface (FS1) and the other is a small Fermi surface (FS2) inside of the larger one. In this case, we must examine the coupled equation of two gap functions $z^1_k$ and $z^2_k$ corresponding to two Fermi surfaces:

$$\frac{2}{N} \sum_{k:F S 1} \chi^{11}(\mathbf{k} + \mathbf{k}') z^1_k \delta(\xi_k) + \frac{2}{N} \sum_{k:F S 2} \chi^{12}(\mathbf{k} + \mathbf{k}') z^2_k = -xz^1_k,$$  (47)

$$\frac{2}{N} \sum_{k:F S 1} \chi^{21}(\mathbf{k} + \mathbf{k}') z^1_k \delta(\xi_k) + \frac{2}{N} \sum_{k:F S 2} \chi^{22}(\mathbf{k} + \mathbf{k}') z^2_k = -xz^2_k,$$  (48)

\[3\] We thank K Yamaji for stimulating discussions on this point.
Figure 7. Phase diagram in the $n_e$-$t'$ plane for $t' \leq 0$. $s$ denotes the pairing state with extended, s-wave symmetry. In the s-wave region for small $|t'|$, the s- and p-wave states are sometimes nearly degenerate. Small regions near boundaries are not shown.

Figure 8. Phase diagram in the $n_e$-$t'$ plane for $t' \geq 0$. s, g and d pairing states are almost degenerate in the low carrier region for large $t'$. 
Table 1. Irreducible representations of $C_{4v}$ for the square lattice. One of basis functions are also shown.

| Representation | Symmetry | Bases               |
|----------------|----------|---------------------|
| $A_1$          | s        | $1$                 |
| $A_2$          | g        | $xy(x^2 - y^2)$     |
| $B_1$          | $d_{x^2-y^2}$ | $\cos(k_x) - \cos(k_y)$ |
| $B_2$          | $d_{xy}$ | $\sin(k_x)\sin(k_y)$ |
| $E$            | p        | $x, y$              |
|                |          | $\cos(\theta), \sin(\theta)$ |

Figure 9. Square lattice with anisotropic next-nearest transfer $t'$ (anisotropic triangular lattice) which is the lattice of organic conductors.

where the symbol $\sum_{k':FS_j}^k$ indicates the summation over the Fermi surface $FS_i$ and $\chi_{ij}(k+k')$ is the susceptibility for $k$ on $FS_i$ and $k'$ on $FS_j$. The stable pairing symmetry is also obtained using the electron–hole transformation for $t' > 0$ for which we have almost only one Fermi surface even in the electron-doped case.

4.3. Square lattice with anisotropic $t'$

The Hubbard model on the square lattice with anisotropic next-nearest-neighbor transfer $t'$ (figure 9) has been investigated intensively as a model for organic conductors such as BDET-TTF(ET) molecules [33]–[35]. The model for organic conductors is well known as the Hubbard model with anisotropic next-nearest-neighbor transfer $t'$ (which is sometimes called the anisotropic triangular lattice). The dispersion relation is

$$\xi_k = -2t(\cos k_x + \cos k_y) - 2t'\cos(k_x + k_y) - \mu.$$  (49)
This model has the two-fold rotational symmetry and we classify the irreducible representation using the $C_{2v}$ point group (table 2). The exponent $x$ is in figures 10 and 11 as a function of the electron density $n_e$ for $t' = -0.1$ and $t' = -0.5$, respectively. As apparent from the figures, the d-wave state is stable over the whole region, which is consistent with the FLEX prediction [36]. The phase diagram in the $n_e-t'$ plane is presented in figure 12 for $t' < 0$ and in figure 13 for $t' > 0$. For this model, we conclude that the d-wave pairing is stable over the whole range of parameters.
Figure 12. Phase diagram for the square lattice with anisotropic $t' < 0$ (lattice of organic conductors).

Figure 13. Phase diagram for the square lattice with anisotropic $t' > 0$ (lattice of organic conductors).
Table 2. Irreducible representations of $C_{2v}$ for the square lattice with anisotropic next-nearest-neighbor transfer.

| Representation | Symmetry | Bases  |
|----------------|----------|--------|
| $A_1$          | $d_{x^2-y^2}$ | $x^2, y^2, \cos(2\theta)$ |
| $A_2$          | $d_{xy}$   | $xy, \sin(2\theta)$ |
| $B_1$          | $p_x$     | $x, \cos(\theta)$ |
| $B_2$          | $p_y$     | $y, \sin(\theta)$ |

4.4. Three-band $d$–$p$ model

The formulation is also applied to the three-band model for the CuO$_2$ plane [37]. We are interested in the relation between the single-band Hubbard model and the three-band $d$–$p$ model. The pairing symmetry in the electron-doped cuprates is still controversial between the $d$-wave and $s$-wave order parameter [38]–[40]. The Hamiltonian is

$$H_{dp} = \epsilon_d \sum_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + \epsilon_p \sum_{i\sigma} (p_{i+\hat{x}/2}\sigma p_{i-\hat{x}/2}\sigma + p_{i+\hat{y}/2}\sigma p_{i-\hat{y}/2}\sigma)$$

$$+ t_{dp} \sum_{i\sigma} [d_{i\sigma}^\dagger (p_{i+\hat{x}/2}\sigma + p_{i+\hat{y}/2}\sigma - p_{i-\hat{x}/2}\sigma - p_{i-\hat{y}/2}\sigma) + \text{h.c.}]$$

$$+ t_{pp} \sum_{i\sigma} [p_{i+\hat{x}/2}\sigma p_{i+\hat{y}/2}\sigma - p_{i+\hat{y}/2}\sigma p_{i-\hat{x}/2}\sigma - p_{i-\hat{y}/2}\sigma p_{i+\hat{x}/2}\sigma$$

$$+ p_{i-\hat{y}/2}\sigma p_{i+\hat{x}/2}\sigma + \text{h.c.}] + U_d \sum_i d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow}. \quad (50)$$

In this subsection, the energy is measured in units of $t_{dp}$. The energy levels of the non-interacting Hamiltonian is written as in a concise form [37]:

$$\epsilon_k^\alpha = \frac{2}{\sqrt{3}} h \cos \left( \frac{\phi_k + 2\pi \alpha}{3} \right) + \epsilon_d - \epsilon_p \quad (51)$$

for $\alpha = 0$, 1, and 2, where

$$t_k = \sqrt{|\eta_k^\uparrow|^2 + |\eta_k^\downarrow|^2 + (\eta_k^p)^2 + (\epsilon_d - \epsilon_p)^2/3}, \quad (52)$$

$$\phi_k = \frac{\pi}{2} + \text{sign}(s_k) \left( \frac{\pi}{2} - \arctan \sqrt{1 - 4t_k^\rho/(27s_k^2)} \right), \quad (53)$$

$$s_k = (\epsilon_d - \epsilon_p) \left( \frac{(\epsilon_d - \epsilon_p)^2}{27} - \frac{t_k^2}{3} + (\eta_k^p)^2 \right) + \eta_k^p (\eta_k^\rho s_k^\sigma + \eta_k^s s_k^\rho), \quad (54)$$

where $\eta_k^\rho = 2it_{dp} \sin(k_x/2)$, $\eta_k^\sigma = 2it_{dp} \sin(k_y/2)$, and $\eta_k^p = -4t_{pp} \sin(k_x/2) \sin(k_y/2)$. $\epsilon_k^\alpha$ for $\alpha = 0$, 1, 2 is the dispersion relation of the upper, lower and middle band, respectively. We examine the doped case within the hole picture where the lowest band is occupied up to the Fermi energy $\mu$. The effective interaction is

$$V_{kk'} = \frac{U_d}{N} + \frac{U_d^2}{N} \chi^{dd}(k+k'), \quad (55)$$
\begin{align}
\chi_{dd}(q) &= \frac{1}{N} \sum_p \sum_{\alpha\beta} w_{q+p}^{\alpha} f_{q+p}^{\alpha} - f_{q+p}^{\beta} w_{p}^{\beta}, 
\end{align}

where \( f_k^{\alpha} \) is the Fermi distribution function,
\begin{align}
f_k^{\alpha} &= (e^{\beta(\epsilon_k^{\alpha} - \mu)} + 1)^{-1}.
\end{align}

The weighting factor of d electrons \( w_k^{\alpha} \) is defined as
\begin{align}
w_k^{\alpha} &= \frac{(n_k^\beta - \epsilon_k^{\alpha})(n_k^\gamma + \epsilon_k^{\alpha})}{(\epsilon_k^{\beta} - \epsilon_k^{\alpha})(\epsilon_k^{\alpha} - \epsilon_k^{\gamma})},
\end{align}
where \( \alpha, \beta \) and \( \gamma \) are different from each other. The gap equation is
\begin{align}
\Delta_k &= -\sum_{k'} w_{k} V_{kk'}^{dd} w_{k'} \Delta_{k'} \frac{1}{2E_{k'}},
\end{align}

where \( w_k = w_k^1 \) and \( E_k = \sqrt{\xi_k^2 + \Delta_k^2} \) for the lowest-band dispersion \( \xi_k = \epsilon_k^1 - \mu \).

The d-wave pairing is predominant over the whole range in the parameter space as is shown in figure 14. In particular, \( d_{x^2-y^2} \)-wave pairing is stable near half-filling. Although the extended s-wave pairing is possible in the narrow region near half filling in the Gutzwiller variational Monte Carlo study [14], we have no chance of s-wave SC within the weak-coupling perturbation theory. The phase diagram for the d–p model is shown in figure 15.
Figure 15. Phase diagram for the three-band d–p model in the plane of the carrier number $n$ and $t_{pp}$ in the range of $0 \leq t_{pp} \leq 0.4$. We set $\epsilon_p - \epsilon_d = 2$ and $t_{dp} = 1$. $n = 0$ indicates half filling, and the positive and negative $n$ are for hole doping and electron doping, respectively.

5. Summary

We have examined the phase diagram with respect to pairing symmetry on the basis of the 2D Hubbard model. The weak coupling formulation is convenient to investigate the phase diagram in detail. The results are almost consistent with the strong-coupling perturbation theory. We summarize the results as follows.

1. The d-wave pairing is stable near half filling for the square lattice and the anisotropic square lattice.

2. The gap function has a maximum at the van Hove singularity. As the second neighbor transfer $t'$ increases, the energy of the van Hove singularity decreases. For large $t' = -0.3$ to $-0.4$, the optimal doping is more than 25% doping, i.e. $n_e < 0.75$. For small third neighbor transfer $t''$ the situation remains the same. The large $-t'$ is assigned to several high-temperature cuprates to fit the angle resolved photoemission spectroscopy (ARPES) data or the Fermi surface obtained by the band structure calculations. Most of them, however, have optimum critical temperature in the range of $0.8 < n_e < 0.85$. Thus, the weak coupling analysis suggests that we must consider other electronic or lattice interactions, or reexamine the band parameters $t'$ and $t''$. Recent ARPES studies have reported the band structure which is well fitted using rather smaller $t'$ such as $t' \sim -0.2$ by our analysis.

3. The predictions of the weak-coupling theory are almost consistent with the variational Monte Carlo method. An effective interaction to induce SC is possibly the simple $\chi(q)$ with renormalization in the Gutzwiller variational theory.
4. For the d–p model, the d-wave pairing is predominant in a wide range and the phase diagram is almost symmetric between electron and hole dopings. Although the pairing symmetry in the electron-doped cuprates is controversial, only the d-wave pairing is possible near half-filling in the weak-coupling formulation.

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Appendix. Higher-order corrections

In the appendix, we examine higher-order corrections to \( x \). If the third-order terms have an effect to reduce the exponent \( x \), the results obtained using the second-order perturbation have a possibility to become unstable as \( U \) increases. It is not an easy task to derive an effective Hamiltonian up to the third order of the interaction using the canonical transformation. The gap equation up to the third order of \( U \) has been obtained using the perturbative expansion for the Hubbard model [41, 42]. The Green’s functions satisfy the Dyson equations:

\[
G(\mathbf{k}, i\epsilon_n) = G_0(\mathbf{k}, i\epsilon_n) + G_0(\mathbf{k}, i\epsilon_n)\Sigma_n(\mathbf{k}, i\epsilon_n)G(\mathbf{k}, i\epsilon_n) + G_0(\mathbf{k}, i\epsilon_n)\Sigma_a(\mathbf{k}, i\epsilon_n)F^*(\mathbf{k}, i\epsilon_n), \quad (A.1)
\]

\[
F(\mathbf{k}, i\epsilon_n) = G_0(\mathbf{k}, i\epsilon_n)\Sigma_n(\mathbf{k}, i\epsilon_n)F(\mathbf{k}, i\epsilon_n) - G_0(\mathbf{k}, i\epsilon_n)\Sigma_a(\mathbf{k}, i\epsilon_n)G(-\mathbf{k}, -i\epsilon_n), \quad (A.2)
\]

where \( \epsilon_n = (2n + 1)\pi k_B T \) is the Matsubara frequency, and \( \Sigma_n (\Sigma_a) \) is the normal (anomalous) self-energy. \( G_0 \) is the free-electron Green’s function: \( G_0(\mathbf{k}, i\epsilon_n) = (i\epsilon_n - \xi_k)^{-1} \). Since we are interested in the third-order contributions, \( \Sigma_n \) (of the order of \( U^2 \)) is neglected as follows:

\[
G(\mathbf{k}, i\epsilon_n) = -\frac{i\epsilon_n + \xi_k}{\epsilon_n^2 + \xi_k^2 + |\Sigma_a(\mathbf{k}, i\epsilon_n)|^2}, \quad (A.3)
\]

\[
F(\mathbf{k}, i\epsilon_n) = -\frac{\Sigma_n(\mathbf{k}, i\epsilon_n)}{\epsilon_n^2 + \xi_k^2 + |\Sigma_a(\mathbf{k}, i\epsilon_n)|^2}. \quad (A.4)
\]

The equation for the anomalous self-energy is

\[
\Sigma_a(\mathbf{k}, i\epsilon_n) = \frac{1}{\beta N} \sum_{\mathbf{k}', \epsilon_n'} [U + U^2\chi_0(\mathbf{k} + \mathbf{k}', i\epsilon_n + i\epsilon_n') + 2U^3\chi_0(\mathbf{k} + \mathbf{k}', i\epsilon_n + i\epsilon_n')^2]F(\mathbf{k}', i\epsilon_n') + U^3\frac{1}{\beta^2 N^2} \sum_{\mathbf{k}', \epsilon_n', \mathbf{p}, \epsilon_\ell} G_0(\mathbf{k}', i\epsilon_n')[\chi_0(\mathbf{k} + \mathbf{k}', i\epsilon_n + i\epsilon_n')]F(\mathbf{p}, i\epsilon_\ell)
\]

\[-\phi_0(\mathbf{k} + \mathbf{k}', i\epsilon_n + i\epsilon_n')G_0(\mathbf{k} + \mathbf{k}' + \mathbf{p}, i\epsilon_n + i\epsilon_n' + i\epsilon_\ell)F(\mathbf{p}, i\epsilon_\ell)
\]

\[+ U^3\frac{1}{\beta^2 N^2} \sum_{\mathbf{k}', \epsilon_n', \mathbf{p}, \epsilon_\ell} G_0(\mathbf{k}', i\epsilon_n')[\chi_0(-\mathbf{k} + \mathbf{k}', -i\epsilon_n + i\epsilon_n') \phi_0(-\mathbf{k} + \mathbf{k}', -i\epsilon_n + i\epsilon_n')]G_0(-\mathbf{k} + \mathbf{k}' - \mathbf{p}, -i\epsilon_n + i\epsilon_n' - i\epsilon_\ell)F(\mathbf{p}, i\epsilon_\ell), \quad (A.5)
\]
for $\beta = 1/k_BT$. The second and third terms originate from the vertex corrections. $\chi_0(q, i\omega_m)$ and $\phi_0(q, i\omega_m)$ are defined as

$$\chi_0(q, i\omega_m) = -\frac{1}{N} \sum_k \frac{f(\xi_k) - f(\xi_{k+q})}{i\omega_m + \xi_k - \xi_{k+q}}, \quad (A.6)$$

$$\phi_0(q, i\omega_m) = -\frac{1}{N} \sum_k \frac{f(\xi_k) - f(-\xi_{-k+q})}{i\omega_m - \xi_k - \xi_{-k+q}}, \quad (A.7)$$

where $\omega_m = 2\pi mk_BT$. We assume that $\Sigma_a$ is small and that we can neglect the $\epsilon$-dependence since we consider the small-$U$ limit. We set $\Delta_k = \Sigma_a(k, \epsilon_n = 0)$, then the equation for $\Delta_k$ is derived. We show the results in figure A1 for $U/t = 0.1$ on the square lattice. The exponent $x$ slightly decreases due to the third-order corrections. There is a cancellation among the third-order terms. As has been shown in the literature [41], the vertex corrections reduce the exponents $x$ and $T_c$ compared to those without vertex corrections.

References

[1] Dagotto E 1994 Rev. Mod. Phys. 66 763
[2] Scalapino D J 1990 High Temperature Superconductivity—the Los Alamos Symposium—1989 Proceedings ed K S Bedell, D Coffey, D E Deltzer, D Pines and J R Schrieffer (Redwood City, CA: Addison-Wesley) p 314
[3] Anderson P W 1997 The Theory of Superconductivity in the High-$T_c$ Cuprates (Princeton, NJ: Princeton University Press)
[4] Stewart G R 1984 Rev. Mod. Phys. 56 755

New Journal of Physics 10 (2008) 023014 (http://www.njp.org/)
[5] Lee P A, Rice T M, Serene J W, Sham L J and Wilkins J W 1986 Comments Condens. Matter Phys. 12 99
[6] Ott H R 1987 Prog. Low Temp. Phys. 11 215
[7] Maple M B 2000 Handbook on the Physics and Chemistry of Rare Earths vol 30 (Amsterdam: North-Holland, Elsevier)
[8] Loh E Y, Gubernatis J E, Scalettar R T, White S R, Scalapino D J and Sugar R L 1990 Phys. Rev. B 41 9301
[9] Moreo A, Scalapino D J and Dagotto E 1991 Phys. Rev. B 56 11442
[10] Wheatley J 1993 Solid State Commun. 88 593
[11] Nakanishi T, Yamaji K and Yanagisawa T 1997 J. Phys. Soc. Japan 66 294
[12] Yamaji K, Yanagisawa T, Nakanishi T and Koike S 1998 Physica C 304 225
[13] Neumayr A and Metzner W 2003 Phys. Rev. B 67 035112
[14] Yanagisawa T, Koike S and Yamaji K 2001 Phys. Rev. B 64 184509
Yanagisawa T, Koike S and Yamaji K 2003 Phys. Rev. B 67 132408
[15] Yanagisawa T, Koike S and Yamaji K 2002 J. Phys.: Condens. Matter 14 21
[16] Miyazaki M, Yamaji K and Yanagisawa T 2004 J. Phys. Soc. Japan 73 1643
[17] Miyake K, Schmidt-Rink S and Varma C M 1986 Phys. Rev. B 34 6554
[18] Scalapino D J, Loh E and Hirsch J E 1986 Phys. Rev. B 34 8190
[19] Kondo J 2001 J. Phys. Soc. Japan 70 808
[20] Hubina R 1999 Phys. Rev. B 59 9600
[21] Schauerte T and van Dongen P G J 2002 Phys. Rev. B 65 081105
[22] Kondo J private communication
[23] Singh D J and Pickett W E 1992 Physica C 203 193
[24] Singh D J 1993 Physica C 212 228
[25] Tohyama T and Maekawa S 2000 Supercond. Sci. Technol. 13 17
[26] Harris J M, Shen Z X, White P J, Marshall D S and Schabel M C 1996 Phys. Rev. B 54 R15665
[27] McElory K, Simmonds R W, Hoffman J E, Lee D-H, Orenstein J, Eisaki H, Uchida S and Davis J C 2003 Nature 422 592
[28] Feng D L et al 2001 Phys. Rev. Lett. 86 5550
[29] Hussey N E, Abdel-Jawad M, Carrington A, Mackenzie A P and Ballcas L 2003 Nature 425 814
[30] Yamaji K 2007 private communication
[31] Maeno Y, Hashimoto H, Yoshida K, Nishizaki S, Fujita T, Bednorz J G and Lichtenberg F 1994 Nature 372 532
[32] Koikegami S, Yoshida Y and Yanagisawa T 2003 Phys. Rev. B 67 134517
[33] McKenzie R H 1997 Science 278 820
[34] McKenzie R H 1998 Comments Condens. Matter Phys. 18 309
[35] Miyangaka K, Kanoda K and Kasamoto A 2004 Chem. Phys. 104 5635
[36] Kondo H and Moriya T 2004 J. Phys. Soc. Japan 73 812
[37] Koikegami S and Yanagisawa T 2001 J. Phys. Soc. Japan 70 3499
Koikegami S and Yanagisawa T 2002 J. Phys. Soc. Japan 71 671
[38] Yanagisawa T, Koikegami S, Shibata H, Kimura S, Kashiwaya S, Sawa A, Matsubara N and Takita K 2001 J. Phys. Soc. Japan 70 2833
[39] Sato T, Kamiyama T, Takahashi T, Kurahashi K and Yamada K 2001 Science 291 1517
[40] Chen C-T, Seneor P, Yeh N-C, Vasquez R P, Bell L D, Jung C U, Kim J Y, Park M-S, Kim H-J and Lee S-I 2002 Phys. Rev. Lett. 88 227002
[41] Jujo T, Koikegami S and Yamada K 1999 J. Phys. Soc. Japan 68 1331
[42] Nomura T and Yamada K 2001 J. Phys. Soc. Japan 70 2694

New Journal of Physics 10 (2008) 023014 (http://www.njp.org/)