Superconductivity of Carriers Doped into the Static Charge Density Wave State in 2-Dimensional Square Lattice

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(Received December 14, 1994)

On the purpose of studying the effect of long-range Coulomb-interaction in strongly correlated electronic systems we bring in as its representative the nearest-neighbor repulsion ($v$) in addition to the on-site repulsion ($u$) and shall investigate the possibility of the superconducting transition of carriers doped into the charge-density wave (CDW) state expected for $v > u/4$ in 2-dimensional square lattice. We shall see that strongly correlated hopping processes of doped carriers make the systems superconducting. The favored superconducting phase is of extended s-wave symmetry, and $T_c \sim 100$ K is shown to easily be attained near the half-filling.

§.1. Introduction

In studying strong correlation among electrons culminating in high $T_c$ cuprates, heavy fermion systems or organic conductors, one of the most intricate problems in condensed-matter physics currently, we call for the Hubbard model and its derivatives like the $t$-$J$ model. It is true that we have learnt much from these models but it is not at all certain whether the learning survives, even qualitatively, when the neglected long-range Coulomb interactions are restored. This is mainly because these models are, in spite of being simple, not tractable analytically, even in perturbation theory. To say the least of it we still do not know what the ground state of the two-dimensional Heisenberg antiferromagnet is, the most important starting point toward real understanding of high $T_c$ copper oxides as commonly believed.

In viewing the status it is worthwhile putting the problem other way around, namely, taking into account the long-rangeness of the Coulomb interaction, to some extent, from the beginning. The new "Problemstellung" is physically fitter, especially for cuprates, because of their ionic character. For this purpose we have proposed a model in which the nearest neighbor Coulomb repulsion, $v$, is brought in as a representative of the

\[ \begin{align*}
A & \quad s_0 \\
B & \quad \alpha_0 \\
A & \quad \alpha_0 \\
B & \quad \alpha_0
\end{align*} \]

Fig. 1. The static CDW configuration at the half-filling having alternate doubly occupied sites (A-sublattice) and empty sites (B-sublattice). Arrows stand for electrons of corresponding spin direction, and $\alpha_0$ and $a = \sqrt{2} \alpha_0$ respectively are the lattice constants of the original square lattice and A- or B-sublattice.
long-range Coulomb repulsion, in addition to the on-site repulsion, $u$ and the nearest neighbor hopping integral, $t$:

$$H = -t \sum_{\langle i,j \rangle} (c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}) + u \sum_i n_{i,\uparrow} n_{i,\downarrow} + v \sum_{\langle i,j \rangle} n_{i,\sigma} n_{j,\sigma'}. \quad (1.1)$$

where $c_{i,\sigma}^\dagger (c_{i,\sigma})$ is the creation (annihilation) operator of an electron of spin $\sigma$ at site $i$, $n_{i,\sigma}$ is the corresponding number operator with $n_i$ the total electron number at the site and $\langle i,j \rangle$ stands for a nearest neighbor combination. We shall call this model the $t$-$(u,v)$ model.* With the model we have discussed\(^1\) the possibility of the Cooper-pair formation in 2-dimensional square lattice when doped and $v > u/4 \gg |t|$. As shown there, an advantage of the model is that the ground state is known, in contrast to the conventionally assumed case of antiferromagnetic (AF) uniform charge distribution ($v < u/4$), to be the static, nonmagnetic charge-density wave (CDW) state in which lattice sites are separated into A-sublattice with two electrons in a spin singlet pair and B-sublattice with no electron (Fig. 1). The observation is confirmed later numerically by the quantum Monte Carlo simulation\(^5\) and by the exact diagonalization method.\(^3\) Indeed at the absolute zero the ground state at half filling can be identified as an antiferromagnetic spin-density wave (SDW) state for $w = u/v > 4$ while for $w < 4$, as the CDW state as predicted. Further, for $w < 4$, the CDW phase is shown to be rather rigid against doping\(^2,3\) even up to quarter filling.\(^4\) Recently it is also shown\(^5\) that the true ground state at half filling is the CDW state modified by the condensed charge fluctuation due to the hopping, just like the ground states of spin ordered states renomalized by spin waves. The single particle as well as collective excitations is found to be gapped with rather wide openings (about $8v - u$ for the former and $7v - u$ for the latter). Thus, as long as $|t| \ll v$ or $u$, the thermal fluctuations do not disturb the ground state at temperatures even as high as $v/k_B$.

It is true that the system described by the model for $w < 4$ is nonmagnetic, charge-density wave ordered and exhibiting a small Fermi surface when doped, not necessarily in accord with experimental observations up to now, thus seems not relevant to high $T_c$ cuprates, as it stands. But, as mentioned above, it has definite advantages, namely, the well-defined ground state being rigid against doping and thermal fluctuation, so that it is worth further theoretical investigation.

As such we would like to pursue the line set by Ref. 1) and study in this paper superconductivity of the model when doped. Since the model is particle-hole symmetric we shall only consider the hole doping of $N_h = 2N - N_e$ holes where $N_e$ is the total electron number and $2N$ is the number of whole sites. In § 2 we present the effective Hamiltonian for the doped holes given in Ref. 1) based on the second-order perturbation theory. Elimination of on-site processes is carried out systematically by introducing pseudo-spin operators in terms of on-site-avoiding hole operators (construction of the pseudo-spin operator is done in Appendix A). As a result of the elimination the Bloch energy of a hole and the hole-hole interaction are modified.

* We thought it better to avoid calling it "extended Hubbard model" as sometimes done, since the same calling is often used for ones, e.g., including the hopping term to the next nearest neighbors, $t'$, the one which may be called the $(t,t')$-$u$ model instead. In the same token the Hubbard model itself might be called the $t$-$u$ model.
Pairing of holes is favored, especially near the CDW-AF phase boundary, for the spin-singlet and s-wave like state as in the ordinary BCS mechanism.

Due to the symmetry character of the gap function \((\Gamma_1\) of the point group \(D_4\)), the corresponding gap equation is brought into a \(3\times3\) matrix form in § 3 (its elements will explicitly be given in Appendix B). We shall solve the gap equation iteratively and present the results for the transition temperature, \(T_c\), as a function of hole concentration, \(n_h=N_h/2N\) for various values of \(w\): It shows a maximum around \(n_h\sim0.05\) and can reach a value \(k_BT_c\sim1/10\) near the CDW-AF phase boundary \((w=4)\) with \(J=t^2/4u\), the exchange integral adopted by the ordinary Hubbard model, thus \(T_c\) can easily be \(\sim100\) K. We also calculate the superconducting correlation function and the specific heat. It is found that the superconducting correlation length is about \(2.8a_0\) where \(a_0\) is the lattice constant of the original square lattice.

Finally in § 4 we give conclusions and discussion.

Fig. 2. (a) Classification of the hopping integrals. The hole to hop is marked by a circle, while the doubly encircled hole is a spectator: (b) An example of processes leading to the correlated hopping integral, \(\tilde{T}\). The dark arrows are for background electrons and the hatched ones for holes. By consecutive hoppings of a background electron (No. 3 in the figure) via a neighboring empty site, a hole (No. 1) in the initial configuration \((\vert i\rangle\) is effectively moved to the final one \((\vert f\rangle\) through the intermediate one \((\vert m\rangle\)).
§ 2. Possibility of Cooper pair formation

Based on Ref. 1) we shall study the possibility of superconductivity of doped carriers (holes) in this section.

As noted there, when doped, holes occupy the A-sublattice sites (corresponding to Cu⁺, in case of CuO₂ system) while B-sublattice (corresponding to Cu³⁺, ditto) remains intact unless doped heavily. Hopping integrals and potentials of holes to the second order in \( t^2 \) are summarized in terms of \( w = u/v \) and \( g = t^2/v \) in the following:

A) Hopping integrals: (Fig. 2(a)) There are two free hopping integrals

\[
\begin{align*}
T_1 &= -2g/(6-w), \\
T_2 &= T_1/2, \\
\end{align*}
\]

(2·1)

and also two for correlated hopping*)

\[
\begin{align*}
\bar{T}_1 &= -g(1/(5-w)+1/(6-w)), \\
\bar{T}_2 &= -g/(5-w). \\
\end{align*}
\]

(2·2)

See Fig. 2(b) for a typical correlated hopping process.

B) Hole-hole potentials: The potential energy \( V_m \) for holes of \( m \)-th neighbor apart is

\[
\begin{align*}
V_1 &= -8g\{1/60+1/(5-w)-3/(6-w)+2/(7-w)\} \quad \text{for } m = 1, \\
V_2 &= V_1/2 \quad \text{for } m = 2, \\
V_m &= 0 \quad \text{for } m \geq 3. \\
\end{align*}
\]

(2·3)

To the above we must add, at least formally, hopping integrals and potentials including on-site repulsion, namely, \( \bar{T}_{1(\text{on})} \), \( \bar{T}_{2(\text{on})} \) and \( V_0 \). All of them are of order of \( u \) and should properly be eliminated, as will be seen.

Taking all the above into account and performing Fourier-transform over A-sublattice sites we get Hamiltonian for the doped hole system in the following form:

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1, \quad \quad (2·4a)
\]

\[
\mathcal{H}_0 = \sum_{k,\sigma} \varepsilon(k)b_{k,\sigma}b_{k,\sigma}^\dagger, \quad \quad (2·4b)
\]

\[
\mathcal{H}_1 = (2N)^{-1} \sum_{k, k', \sigma, \sigma'} C V(k, k') b_{k,\sigma} b_{k'+\sigma,\sigma'} b_{k'+\sigma',\sigma} b_{k,\sigma'}, \quad \quad (2·4c)
\]

where \( N \) is the number of A-sublattice sites. Further \( b_{k,\sigma}(b_{k,\sigma}^\dagger) \) denotes the creation (annihilation) operator of a hole defined by

* Correlated hopping mechanism first presented in Ref. 1) is analogous to the superexchange mechanism of the attractive interaction between two localized spins which leads the system to the antiferromagnetic ordering. In both mechanisms an intermediate state with higher energy plays an essential role and produces effective attraction between two carriers.
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Fig. 3. (a) The contour of the Bloch energy of doped carriers, \( \varepsilon(k) \), in the first Brillouin zone for \( w = 3.9 \); (b) The chemical potential, \( \mu_\nu \), of doped carriers for \( w = 3.9 \). Energy is in units of the band width, \( W = 16g/(6-w) = 7.6g \).

\[
\begin{align*}
\mathbf{b}_k,\sigma &= N^{-1/2} \sum_{R_i \in A} e^{-ik \cdot R_i} c_{k,-\sigma} , \\
\mathbf{b}_k,\sigma &= N^{-1/2} \sum_{R_i \in A} e^{ik \cdot R_i} c_{k,-\sigma} ,
\end{align*}
\]

(2·5)

where \( c_{k,-\sigma}(c_{k,-\sigma}^\dagger) \) is the creation (annihilation) operator of an electron which appeared in (1·1) and \( A \) represents the set of all the A-sublattice sites. In (2·4b) \( \varepsilon(k) \) is the tight-binding Bloch-energy relative to the band bottom (Fig. 3(a))

\[
\begin{align*}
\varepsilon(k) &= -2 T_1(3 - \cos k_x a - \cos k_y a - \cos k_x a \cos k_y a) \\
&= -\frac{W}{4} (3 - \cos k_x a - \cos k_y a - \cos k_x a \cos k_y a) ,
\end{align*}
\]

(2·6)

where \( a = \sqrt{2}a_0 \) (\( a_0 \) is the lattice constant of the original square-lattice) denotes the lattice constant of the A-sublattice and \( W \) stands for the band width defined by

\[
W = 8|T_1| = 16g/(6-w) .
\]

(2·7)

Notice that the band bottom lies at \( 6 T_1 \) relative to the energy of a localized single hole. Finally the hole-hole interaction, \( CV_h \), in (2·4c) can be given by the aforementioned hopping integrals and potentials as

\[
CV_h(k, k') = V(k, k') + 2\bar{T}(k, k') ,
\]

(2·8a)

where \( V(k, k') \) and \( \bar{T}(k, k') \) are respectively given by

\[
V(k, k') = V_0 + 2 V_1(\cos(k'_x - k_x)a + \cos(k'_y - k_y)a) \\
+ 4 V_2\cos(k'_x - k_x)a\cos(k'_y - k_y)a ,
\]

(2·8b)
The tilded hopping integrals are defined by subtracting from the correlated ones the corresponding free hopping integrals, namely, \( \tilde{T}_i = T_i - T_i\), since the latter are already taken into account in defining the Bloch energy. Thus, for example, \( \tilde{T}_1 = \tilde{T}_2 = -g\{1/(5-w)-1/(6-w)\}\).

In order to discuss the possibility of superconductivity in the doped carrier system it is convenient to introduce pairing operators defined by

\[
\tau_0(k) = \frac{-1}{2} \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) + \frac{i}{2} \left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right),
\]

where \(\sigma_a\) is the 2\(\times\)2 unit matrix and \(\sigma_a\) for \(a=1,2,3\) are conventional Pauli-matrices. Needless to say \(\tau_0(k)\) corresponds to the singlet pairing while \(\tau(k)\) governs the triplet pairing. Further they satisfy

\[
t_0(-k) = t_0(k) \quad \text{and} \quad t(-k) = -t(k).
\]

In terms of the pairing operators the reduced Hamiltonian corresponding to \(\mathcal{H}_i\) can be written as

\[
\mathcal{H}_i = \mathcal{H}_{\text{ISP}} + \mathcal{H}_{\text{ITP}},
\]

\[
\mathcal{H}_{\text{ISP}} = (2N)^{-1} \sum_{k,k'} CV(k, k')\tau_0(k')\tau_0(k),
\]

\[
\mathcal{H}_{\text{ITP}} = (2N)^{-1} \sum_{k,k'} CV(k, k')\tau(k')\cdot\tau(k),
\]

where \(\mathcal{H}_{\text{ISP}}\) and \(\mathcal{H}_{\text{ITP}}\) are the reduced interactions respectively for singlet and triplet pairings and

\[
CV_\pm(k, k') = CV(k, k') \pm CV(-k, -k')/2.
\]

We now concern ourselves with the elimination of "on-site" terms. In the case of triplet pairing we are automatically free from them owing to the exclusion principle so that we can use \(\mathcal{H}_{\text{ITP}}\) as it stands with \(CV_-(k, k')\) of (2·10d) given by

\[
CV_-(k, k') = CV^{(p)}(k, k')
\]

\[
= 2V_1(\sin k_x\sin k_y a + \sin k_x\sin k_y' a)
\]

\[
+ 4V_2(\sin k_x\cos k_y a + \cos k_x\sin k_y a)
\]

\[
+ 8\tilde{T}_1(\sin k_x\sin k_y a + \sin k_x\sin k_y' a)
\]

\[
+ 8\tilde{T}_2(\sin k_x\cos k_y a + \cos k_x\sin k_y' a).
\]

For singlet pairing, on the other hand, we have to restrict the Hilbert-space to the states of no doubly occupied sites. By so doing we can discard the terms explicitly
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pertaining to on-site quantities like $V_0$, $\tilde{T}_i^{(on)}$. Further we have to eliminate the on-site processes inherent in the Fourier-transformed operators. To do so we replace, in a conventional manner, the hole operators by

$$
\tilde{b}_{k,\sigma} = N^{-1} \sum_{R_i \in A} e^{-ik \cdot R_i} \tilde{b}_{i,\sigma}, \\
\tilde{b}_{k,\sigma} = N^{-1} \sum_{R_i \in A} e^{ik \cdot R_i} \tilde{b}_{i,\sigma},
$$

(2.12a)

where $\tilde{b}_{i,\sigma}$ and $\tilde{b}_{i,\sigma}$ are the on-site-avoiding operators defined respectively by

$$
\tilde{b}_{i,\sigma} = b_{i,\sigma}(1 - \tilde{n}_{i,-\sigma}), \\
\tilde{b}_{i,\sigma} = (1 - \tilde{n}_{i,-\sigma}) b_{i,\sigma},
$$

(2.12b)

where $\tilde{n}_{i,\sigma} = b_{i,\sigma}^\dagger b_{i,\sigma} = c_{i,-\sigma} c_{i,-\sigma}$ denotes the number operator of holes at site $i$ of spin $\sigma$. Then $H_0$ of (2.4b) should be replaced by

$$
\hat{\mathcal{R}}_0 = \sum_{k,\sigma} \varepsilon(k) \tilde{b}_{k,\sigma} \tilde{b}_{k,\sigma},
$$

(2.13a)

and $H_{ISP}$ by

$$
\hat{\mathcal{R}}_{ISP} = N^{-1} \sum_{k,k'} CV_+(k, k') \tilde{t}_0^\dagger(k) \tilde{t}_0(k'),
$$

(2.13b)

with $\tilde{t}_0(k)$ defined by the on-site-avoiding operators through (2.9a) and with $CV_+(k, k')$ given as

$$
CV_+(k, k') = CV^{(a)}(k, k') + CV^{(d)}(k, k'),
$$

(2.13c)

where

$$
CV^{(a)}(k, k') = 2 V_1 (\cos k_x \cos k'_x + \cos k_y \cos k'_y) \\
+ 4 V_2 \cos k_x \cos k'_x \cos k_y \cos k'_y \\
+ 8 \tilde{T}_1 (\cos k_x \cos k'_x \cos k'_y + \cos k_y \cos k'_x \cos k'_y \\
+ \cos k_x \cos k'_y \cos k'_x + \cos k'_x \cos k'_y \cos k'_x) \\
+ 8 \tilde{T}_2 (\cos k_x \cos k'_x + \cos k_y \cos k'_x) - 2 (6 T_1 + \varepsilon(k) + \varepsilon(k'))
$$

(2.13d)

and

$$
CV^{(d)}(k, k') = 4 V_2 \sin k_x \sin k'_x \sin k_y \sin k'_y.
$$

(2.13e)

Note that the last term on the r.h.s. of (2.13d) comes from the fact that in eliminating the on-site potential term

$$
N^{-1} V_0 \sum_k \tilde{t}_0^\dagger(k) \sum_{k'} t_0(k') = N^{-1} V_0 \sum_{R_i \in A} \tilde{b}_{i,\sigma} \tilde{b}_{i,\sigma} \sum_{R_j \in A} b_{i,\sigma} b_{j,\sigma},
$$


$V_0$ should be replaced by the Bloch energy of two localized holes, $2 \times 6 T_1$, and similarly in eliminating the on-site hopping term the term with $\bar{T}^{(on)}(k)$ but not with $\bar{T}^{(on)}(k')$ should be taken out, namely,

$$2N^{-1} \sum_k \bar{T}^{(on)}(k) t_{kl}(k) \sum_k t_{kl}(k') ,$$

thus, in effect $-2(\epsilon(k) + 6 T_1)$ is left.\(^1\)

It is rather clear from the definition that the pairing interaction $\mathcal{C}^{(p)}$ is of $p$-wave character while $\mathcal{C}^{(s)}$ and $\mathcal{C}^{(d)}$ are of $s$- and $d$-wave character, respectively. In Figs. 4(a)~(c) we illustrate the pairing interactions in the first Brillouin zone for $w = u/v = 3.9$. As seen from them $\mathcal{C}^{(s)}$ develops rather a wide and deep valley around the center of the Brillouin zone, but the attractive valley of $\mathcal{C}^{(d)}$ is off the center and shallow ($|\mathcal{C}^{(d)}|/\mathcal{C}^{(s)} \sim 10^{-1}$), so that the $s$-wave like pairing seems favored. This is mainly because the correlated hopping processes, which give rise to large attraction in $\mathcal{C}^{(s)}$, are absent in $\mathcal{C}^{(d)}$. As for the $p$-wave type pairing $\mathcal{C}^{(p)}$ can be as large as $\mathcal{C}^{(s)}$ in magnitude, thanks to the correlated hopping integral, but the former exhibits alternating valleys and hills around the center of the Brillouin zone, as can be seen from Fig. 4(b) so that the transition temperature higher than that of $s$-wave is
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unlikely. Thus we shall study in the following the possibility of superconductivity for the s-wave pairing alone. It is worth noting here that the attractive valley of $C_{\text{CDW-AF}}$ becomes the deeper and wider the closer $w$ is to 4, the CDW-AF boundary: This is mainly due to the correlated hopping terms in (2.13d) which are seen from (2.2) most attractive at $w=4$ for $w \leq 4$.

Now the reduced Hamiltonian to be investigated is

$$\mathcal{H}(s) = \mathcal{H}_0 + N^{-1} \sum_{k,k'} C_{\text{CDW}}^{(s)}(k, k') \tilde{\tau}_0(k) \tilde{\tau}_0(k').$$ (2.14a)

For a consistent treatment of the Hamiltonian, the pseudo-spin formalism is most suited. Its application is, however, not immediate since the hole operators were modified as to avoid on-site double occupation. As we shall show in Appendix A we can construct appropriate pseudo-spin operators from the modified operators, by making use of local mean field approximation for the commutators among the modified pairing operators, $\tilde{b}_{-k,\downarrow} \tilde{b}_{k,\uparrow}, \tilde{b}_{k,\uparrow} \tilde{b}_{-k,\downarrow}$ and $\tilde{n}_c(k) = \tilde{b}_{k,\uparrow} \tilde{b}_{k,\uparrow}$, as below:

$$\begin{align*}
\tilde{\tau}^{(z)}(k) &= \frac{1}{2(1 - \frac{n_h}{2})} (\tilde{n}_s(k) + \tilde{n}_s(-k) - 1), \\
\tilde{\tau}^{(+)}(k) &= \frac{1}{1 - \frac{n_h}{2}} \tilde{b}_{k,\uparrow} \tilde{b}_{-k,\downarrow}, \\
\tilde{\tau}^{(-)}(k) &= \frac{1}{1 - \frac{n_h}{2}} \tilde{b}_{-k,\downarrow} \tilde{b}_{k,\uparrow}.
\end{align*}$$ (2.15)

The pseudo-spin operators satisfy usual $SU(2)$ commutation relations:

$$\begin{align*}
[ \tilde{\tau}^{(+)}(k), \tilde{\tau}^{(-)}(k')] &= 2 \delta_{k,k'} \tilde{\tau}^{(z)}(k), \\
[ \tilde{\tau}^{(z)}(k), \tilde{\tau}^{(z)}(k')] &= \pm \delta_{k,k'} \tilde{\tau}^{(\pm)}(k). 
\end{align*}$$ (2.16)

In terms of the pseudo-spin, the reduced Hamiltonian (2.14a) including the chemical potential term can be rewritten as:

$$\mathcal{H}(s) = \sum_k (\bar{\varepsilon}(k) - \bar{\mu}_h)(2 \tilde{\tau}^{(z)}(k) + 1) + N^{-1} \sum_{k,k'} \mathcal{C}_{\text{CDW}}(k, k') \tilde{\tau}^{(+)}(k) \tilde{\tau}^{(-)}(k'),$$ (2.14b)

where $\bar{\varepsilon}(k), \bar{\mu}_h$ and $\mathcal{C}_{\text{CDW}}(k, k')$ respectively are the Bloch energy, the chemical potential (Fig. 3(b)) and the s-wave like pairing-interaction modified by the introduction of the on-site avoiding pseudo-spin and are given by

$$\bar{\varepsilon}(k) = \left(1 - \frac{n_h}{2}\right) \varepsilon(k) = \tilde{W}(3 - \cos k_x a - \cos k_y a - \cos k_x a \cos k_y a)$$ (2.17a)

with

$$\tilde{W} = \left(1 - \frac{n_h}{2}\right) W,$$ (2.17b)

$$N_h = \left(1 - \frac{n_h}{2}\right) \sum_k e^{\bar{\varepsilon}(k) - \bar{\mu}_h} + 1$$ (2.18)
and
\[ C_{\text{eff}}^{(s)}(k, k') = \left(1 - \frac{n_{h}}{2}\right)^{2} C_{\text{eff}}^{(s)}(k, k'). \] (2.19)

We can then readily write down the gap equation at a temperature \( T \):
\[ \Delta^{(s)}(k, T) = -N^{-1} \sum_{k' \in C^{<}} C_{\text{eff}}^{(s)}(k, k') \Delta^{(s)}(k', T) \Theta(k') \] (2.20a)

with
\[ \Theta(k) = \frac{1}{2E(k)} \tanh \left( \frac{\beta E(k)}{2} \right) \] (2.20b)
for the gap defined by
\[ \Delta^{(s)}(k, T) = -N^{-1} \sum_{k' \in C^{<}} C_{\text{eff}}^{(s)}(k, k') \langle \bar{\tau}^{(s)}(k') \rangle, \] (2.20c)

where \( \langle \cdots \rangle \) denotes the thermal average
\[ \langle \cdots \rangle = \frac{\text{Tr}(e^{-\beta S^{(s)}})}{\text{Tr}(e^{-\beta S^{(s)}})}, \] (2.21)

and \( \bar{\tau}^{(s)} = (1/2)(\bar{\tau}^{(+)} + \bar{\tau}^{(-)}) \). We have taken the phase convention that \( \langle \bar{\tau}^{(s)}(k) \rangle = 0 \) with \( \bar{\tau}^{(s)} = (1/2i)(\bar{\tau}^{(+)} - \bar{\tau}^{(-)}) \). Further \( E(k) \) stands for Bogoliubov’s quasi-particle energy
\[ \begin{cases} E(k) = \sqrt{\xi^{2}(k) + \Delta^{(s)}(k, T)^{2}} \\ \text{with} \quad \xi^{2}(k) = \bar{\xi}(k) - \bar{\mu}_{h}. \end{cases} \] (2.22)

In (2.20a) and (2.20c) \( C^{<} \) stands for the region in the first Brillouin zone where the modified Bloch energy is less than an appropriate cutoff. We shall deal with the cutoff in the next section.

§ 3. Properties of the superconducting phase

Based on the formalism given in the preceding section we shall solve the gap equation to determine the transition temperature and the energy gap, then study the superconducting correlation and the specific heat. We shall omit the superscript \( (s) \) since we restrict ourselves to the \( s \)-wave like pairing alone.

The transition Temperature and the Energy Gap: Without any loss of generality we can factorize the gap function as
\[ \Delta(k, T) = d(T) c(k, T). \] (3.1a)

We note that \( d(T) \) depends only on temperature and \( c(k, T) \) depends both on temperature and wave vector. The wave-vector part, \( c(k, T) \), represents the symmetry of the gap and directly reflects the lattice symmetry and the anisotropy of the hole-hole interaction. Then the gap equation (2.20a) can be reduced to
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\[ c(\mathbf{k}, T) = \frac{-1}{N} \sum_{\mathbf{k} \in c} \mathcal{D}_{\text{eff}}(\mathbf{k}, \mathbf{k}') c(\mathbf{k}', T) \Theta(\mathbf{k}') , \quad (3.2) \]

where \( \mathcal{D}_{\text{eff}}(\mathbf{k}, \mathbf{k}') \) is given by (2·19) and (2·13d). The transition temperature is determined by the condition

\[ d(T_c) = 0 . \quad (3·3a) \]

From the hole-hole interaction (2·13d) the wave-vector dependent part, \( c(\mathbf{k}, T) \), should take the following form:**

\[ c(\mathbf{k}, T) = c_0(T) + c_1(T)(\cos k_x a + \cos k_y a) + c_2(T)\cos k_x \cos k_y a . \quad (3·4) \]

Before going into the detailed study of the gap equation, we should note that, although the irreducible representations appearing on the right-hand side of (3·4), \( 1, \cos k_x a + \cos k_y a, \) and \( \cos k_x \cos k_y a, \) are independent and orthogonal to each other, we cannot decouple (3·2) into each of these representations due to the presence of the thermal factor, \( \Theta(\mathbf{k}') \). We can only bring the gap equation into the \( 3 \times 3 \) matrix form as

\[ M(T) c(T) = 0 , \quad (3·5a) \]

where

\[ c(T) = \begin{pmatrix} c_0(T) \\ c_1(T) \\ c_2(T) \end{pmatrix} , \quad (3·6) \]

\[ M(T) = \begin{pmatrix} P(T) & Q(T) & R(T) \\ S(T) & T(T) & U(T) \\ V(T) & W(T) & Z(T) \end{pmatrix} . \quad (3·7) \]

All the matrix elements appeared in \( M(T) \) are listed in Appendix B.

It should be noted here that there is an arbitrariness in the factorization, (3·1a): Indeed an overall factor for \( c(\mathbf{k}, T) \) may be factored out and be absorbed into \( d(T) \). Let us define the gap function at the center of the first Brillouin zone (\( \Gamma \) point) as

\[ \Delta_\Gamma(T) = d(T)(c_0(T) + 2c_1(T) + c_2(T)) . \quad (3·8a) \]

Now one way for the factorization is to factor out \( (c_0 + 2c_1 + c_2) \) from \( c(\mathbf{k}, T) \) and use \( \Delta_\Gamma(T) \) in place of \( d(T) \). Instead we factor out \( c_0 \) from \( c(\mathbf{k}, T) \), for the sake of numerical simplicity, and redefine relevant quantities as

\[ \begin{aligned}
D(T) &= c_0(T) d(T) , \\
C_\mathbf{k}(\mathbf{k}, T) &= c(\mathbf{k}, T)/c_0(T) = 1 + C_1(T)(\cos k_x a + \cos k_y a) + C_2(T)\cos k_x \cos k_y a \\
\text{with } C_i &= c_i/c_0 , \\
\Delta(\mathbf{k}, T) &= \Delta_\Gamma(T) C(\mathbf{k}, T) \\
&= \bar{D}(T)\{1 + C_1(T)(\cos k_x a + \cos k_y a) + C_2(T)\cos k_x \cos k_y a\} .
\end{aligned} \quad (3·9) \]

** The form of the gap consists of irreducible representations of \( \Gamma_1 \) of the point group \( D_\Gamma \). Indeed (3·4) corresponds to the superposition of the s-(1) and extended \( s \)-wave solutions \( (\cos k_x a + \cos k_y a, \cos k_x \cos k_y a). \) There is no symmetry-related distinction among these representations.33

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Then $\Delta r(T)$ is given by
\[
\Delta r(T) = \bar{D}(T)(1 + 2C_1(T) + C_2(T)) . \tag{3\cdot8b}
\]
The gap equation, (3\cdot5a), remains the same formally, but due to the above-mentioned arbitrariness in the vector $(c)$, should turn out to be
\[
\text{det}M(T) = 0 , \tag{3\cdot5b}
\]
although $M$ contains $C_i$ in a nonlinear manner through $E(k)$. The coefficients, $C_i$, are self-consistently determined by
\[
\begin{cases}
C_1 = \frac{RS - PU}{QU - RT} , \\
C_2 = \frac{PT - QS}{QU - RT} .
\end{cases} \tag{3\cdot5c}
\]
Needless to say the transition temperature is determined from (3\cdot3), or $\Delta r(T_c) = 0$, in other words, by
\[
\text{det}M(T_c)|_{\Delta r(T_c) = 0} = 0 \tag{3\cdot10}
\]
for a given set of hole concentration, $n_h$, and $w$.

To solve the gap equation we resort to the iterative procedure: To begin with we solve (3\cdot10) and determine the transition temperature, $T_c$. Then at a temperature lower than $T_c$ we put the zeroth order solution for $C_i(T)$ as
\[
\begin{cases}
C_1^{(0)}(T) = C_1(T_c)|_{\Delta r(T_c) = 0} , \\
C_2^{(0)}(T) = C_2(T_c)|_{\Delta r(T_c) = 0} ,
\end{cases} \tag{3\cdot11}
\]
where $C_i(T_c)$ are determined by (3\cdot5c) by setting $T = T_c$ and $\Delta r(T_c) = 0$. We next write down the first iteration for $\Delta(k, T)$ as
\[
\Delta^{(1)}(k, T) = \bar{D}^{(1)}(T)(1 + C_1^{(0)}(T)(\cos k_x a + \cos k_y a) + C_2^{(0)}(T)\cos k_x a \cos k_y a) , \tag{3\cdot12}
\]
and solve (3\cdot5b) for $\bar{D}^{(1)}(T)$. By using the solution we calculate the r.h.s. of (3\cdot5c) to obtain the first iteration to $C_i(T)$. By repeating the procedure for higher iterations until the desired accuracy is attained we can reach the solution for the gap function at an arbitrary temperature below $T_c$.

We shall now present the numerical results for the transition temperature as well as the gap function. As for the energy cutoff, $\bar{\varepsilon}_c$, we take the energy contour corresponding to the Fermi surface at the hole concentration of $n_{hc} = 0.25$: This value is chosen because above which the rigidity of the CDW ground-state for the $t\cdot(u, v)$ model is shown demolished, as stated before for CuO$_2$ system.\(^4\) Then we have
\[
\bar{\varepsilon}_c = 0.58 \bar{W} . \tag{3\cdot13}
\]
We shall call this the natural cutoff.

First in Fig. 5(a) we give $T_c$ as a function of $n_h$ for several values of $w$. As seen there it increases as $\sqrt{n_h}$ as $n_h$ increases from 0, then develops maximum at $n_h = 0.054$
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Fig. 5. (a) The transition temperature, $T_c$, divided by $g=(t^2/v)$ and (b) the gap-anisotropy parameters, $C_1$ and $C_2$, as functions of hole concentration, $n_h$, respectively for $w=4.0, 3.9$ and $3.8$. The energy cutoff corresponds to the chemical potential at the natural cutoff for the hole concentration, $n_{hc}=0.25$.

for $w=4.0$; at $n_h=0.048$ for $w=3.9$; at $n_h=0.043$ and $n_h=0.192$ for $w=3.8$, respectively. It vanishes at $n_{hc} \approx n_{hc}$ around the cutoff, as $\sqrt{n_{hc} - n_h}$. Further, as $w$ approaches 4, the curve of $T_c$ grows up in accordance with the observation stated before that the pairing interaction becomes most attractive at the CDW-AF phase boundary. The maximum value of the transition temperature reaches $\sim 10^{-1} g$, where the coupling constant $g=t^2/v$ corresponds to the conventional exchange energy, i.e., $4t^2/u$, of the Hubbard-model near $w=4$ and can be of order of $\sim 10^3$ K. Hence our mechanism easily explains the transition temperature as high as $\sim 100$ K. We have also shown in Fig. 5(b) the anisotropy parameters, $C_1$ and $C_2$, at $T_c$ as functions of $n_h$ for the same
set of values for $w$. Notice that

$$C_1 \sim C_2$$  \tag{3.14} \]

for all the values of $w$ considered. Further they are rather large at low hole concentrations, at the CDW-AF boundary decrease as $n_h$ increases and become small at high concentrations.

As is pointed out just in the above, the transition temperature is dependent on the choice of the cutoff. To illustrate this we give $T_c$ in Fig. 6(a) and $C_i$ in Fig. 6(b) as functions of $n_h$ at $w=3.9$ for several choices of the cutoff. The cutoff dependence can clearly be seen in Fig. 6(a). Further, as seen in Fig. 6(b) the anisotropy is conspicuous.
Fig. 7. The gap function, $\Delta(k, T)$, divided by $g$ in the first Brillouin zone at $T=0$ for $\nu=3.9$, $n_h=0.05$ and the natural cutoff.

Fig. 8. (continued)
at a low cutoff: This is because the main source of the pairing interaction is the correlated hopping terms in (2·13d), which are inherently anisotropic and give strong attraction around the center of the first Brillouin zone, the region most important for a smaller cutoff.

Next we provide the solution to the gap equation at temperatures below $T_c$ at the natural cutoff. To be specific we have chosen $\omega$ to be 3.9. To obtain an overall view of the gap in $k$ space we plot in Fig. 7 $\Delta(k, T)$ at the absolute zero and $n_h=0.05$. As seen from the figure the gap function is very much similar to the sign-reversed Bloch energy. This is owing to the approximate relation (3·14) which is seen holding also at $T<T_c$ as shown in Fig. 8(a). Thanks to this relation we can approximately express the gap function (3·9) in terms of the modified Bloch energy (2·17a) as

$$
\Delta(k, T) = \bar{D}(T) \left[ 1 + 3 C_1(T) - 4 C_1(T) \left( \frac{\bar{E}(k)}{W} \right) \right].
$$

\[ (3·15a) \]
In other words, the gap function has a constant value on a Bloch contour. We shall thus define from (3·15a) the energy gap, say, \( \Delta_r(T) \) of our model as the gap on the Fermi surface, \( \varepsilon(\vec{k}) = \tilde{\mu}_n \), which is explicitly given by

\[
\Delta_r(T) = \tilde{D}(T) \left[ 1 + 3C_1(T) - 4C_1(T) \left( \frac{\tilde{\mu}_n}{\tilde{W}} \right) \right] = \Delta_r(0) \left[ 1 - \left( \frac{4C_1(T)}{1 + 3C_1(T)} \right) \left( \frac{\tilde{\mu}_n}{\tilde{W}} \right) \right].
\]

(3·15b)

In Fig. 8(b) we have plotted \( \Delta_r(T) \) as a function of temperature for several values of hole concentration. The results for the gaps reveal general features of the mean field approximation, namely, all of them vanish as \( \sqrt{1 - T/T_c} \) at \( T_c \) and develop wide plateau at low temperatures. Further in accord with the behavior of \( T_c \) as a function of \( n_h \), shown in Fig. 5(a) the gap becomes the widest at \( n_h = 0.05 \) at which \( T_c \) is the largest for \( w = 3.9 \). Further we have presented in Fig. 8(c) \( \Delta_r(0) \) and \( \Delta_s(0) \), together with \( \Delta(0) \), the gap function at the absolute zero averaged over the 2-dimensional Fermi sea, as functions of \( n_h \). Also shown in Fig. 8(d) are the ratios \( 2\Delta_r(0)/k_BT_c, 2\Delta_s(0)/k_BT_c \) and \( 2\Delta(0)/k_BT_c \) as functions of hole concentration for \( w = 3.9 \). We can see that the gap on the Fermi contour gives the ratio close to the BCS value, 3.52.

From (3·15b) we may find the condition for the gap on the Fermi surface to vanish, namely,

\[
\frac{\tilde{\mu}_n}{\tilde{W}} = \frac{1 + 3C_1(T)}{4C_1(T)} = \frac{3}{4} + \frac{1}{4C_1(T)} > \frac{3}{4}.
\]

(3·15c)

From the above it is clear that the lower bound for \( \langle \mu_n/\tilde{W} \rangle \) exceeds the natural cutoff set by (3·13) so that in our model the gap function never vanishes on the Fermi contour. For a hole concentration of our interest, i.e., \( n_h \leq n_{hc} \) the Fermi surface is much smaller than the contour on which the gap vanishes.

**Superconducting Correlation:** As is already clear so far the gap function shows strong anisotropy reflecting the lattice symmetry and the anisotropic pairing interaction. It is then of great interest to know how this anisotropy affects the superconducting correlation. The superconducting correlation function for the s-wave like pairing can be calculated at \( T = 0 \) by

\[
\chi_s(r) = \frac{1}{2Na^2} \sum_{k \in C} \frac{\mathcal{A}(\vec{k}, 0) \cos k_x x \cos k_y y}{\sqrt{\xi(\vec{k})^2 + \mathcal{A}(\vec{k}, 0)^2}},
\]

(3·16)

where \( r = (x, y) \) denotes the relative distance between paired holes in the A-sublattice coordinates. Recall that the coordinates are rotated by 90 degree with respect to the coordinates of the original lattice, say \( (X, Y) \), so that the \( x = y \)-line in the former corresponds to the \( Y \)-axis in the latter and the \( x \)-axis, to the \( X = Y \)-line. In Fig. 9(a) we have plotted the correlation function along the \( X = Y \)-line, respectively for \( n_h = 0.03, 0.05 \) and \( 0.20 \) at \( w = 3.9 \). It indicates the superconducting correlation falls rather rapidly as distance increases and reveals a clear correlation length, \( \xi \), almost independent of hole concentration, which is estimated to be about \( (\xi/a_0) \approx 2.8 \) from the plot of maxima of \( \chi_s \)(see Fig. 9(b)). We have also found that the superconducting correlation in other directions is quite similar to the above, thus the superconducting...
Fig. 9. (a) The superconducting correlation function and (b) the logarithm of its local maxima along the line $X = Y$ for $n_a = 0.03$, 0.05 and 0.20 at $w = 3.9$.

Fig. 10 The specific heat in the superconducting ($C_s$) and normal ($C_N$) phases normalized by $C_s(T_c)$ for $w = 3.9$ and $n_a = 0.05$ at the natural cutoff.
correlation extends about $\xi \sim 2.8 \, a_0$ in every direction.

**Electronic Specific Heat**: Electronic specific heat in the superconducting phase is given by the standard expression,

$$C_s = \frac{1}{k_BT^2} \sum_{\mathbf{k}} \left[ E_{\mathbf{k}}^2 + \beta \Delta(\mathbf{k}, T) \frac{d\Delta(\mathbf{k}, T)}{d\beta} \right].$$  \hspace{1cm} (3·17)

We have evaluated this quantity as a function of temperature and shown the result for $w=3.9$ and $n_h=0.05$ in Fig. 10. As a comparison we have also plotted there the heat capacity in the normal phase, $C_N$. The jump $(C_s - C_N)/C_N$ at $T= T_c$ becomes 1.67 for $w=3.9$ and $n_h=0.05$, a value little larger than the BCS value, 1.43.

§ 4. Conclusions and discussion

Based on the 2-dimensional $t$-$\sigma$ model we have shown that the static, nonmagnetic CDW state, consisting of alternate doubly occupied sites (A-sublattice) and empty sites (B-sublattice), is eligible for superconductivity with $T_c$ as high as $10^2$ K when the system is,

1. doped near the half-filling and
2. close to the phase boundary to AF.

Main source of pairing interaction between doped carriers, say, holes which necessarily reside on A-sublattice (in case electrons, on B-sublattice), comes from the correlated hopping caused by consecutive hoppings of the background electrons via a nearby empty site (e.g., Fig. 2(b)). We have paid special attention to elimination of the on-site processes by making use of the pseudo-spin formalism. In accord with the elimination, the Hamiltonian of the doped system has to be modified. We have shown that the effective hole-hole interaction especially enhances the $s$-wave type attraction and results in the highest superconducting-transition temperature at the CDW-AF phase boundary, $w=4$.

Throughout this paper we have assumed that the background CDW configuration remains rigid against hole doping for $n_h$ less than $n_{hc}=0.25$, the critical dose set by the numerical study for CuO$_2$ system.\(^{41}\) If more holes are doped, the CDW configuration will make a transition to a metallic phase.

As noted in the Introduction the CDW ground-state is shown\(^{51}\) modified by the condensed charge fluctuations: There is in effect a fraction of charges on the originally empty sites, although the CDW state remains stable even at temperatures as high as $\nu/k_B$. The finding is at the half-filling, thus it is of due interest to know how doping affects the ground state and the interaction among doped carriers. By doing so we can shed light on the strongly correlated electronic system starting from the localized configuration, a picture complementary to the conventional ones.

Lastly a few remarks should be made whether our model is relevant to real superconductors. CDW configurations similar to ours are known to occur in substances such as polyacetylene (1D), NbSe$_2$(2D) and BaBiO$_6$(3D). In these systems the CDW instability is driven by the Fermi-surface instability. For example, BaBiO$_6$ system is a semiconductor with the 3-dimensional CDW-configuration Ba$_2$Bi$_{3+}^{3+}$Bi$_{3+}^{5+}$O$_6$.\(^{46}\)
If Bi is substituted by Pb the system shows superconductivity at the Pb concentration of 65% or higher. The behavior of this compound can be explained in terms of the modified $t$-$(u,v)$ model, although the Cooper-pair formation seems mediated by the electron-phonon interaction. As for cuprate high-$T_c$ superconductors it is believed that the ground state is in some AF phase, even doped, and no clue is yet found for any static CDW configuration. If, however, $w$ is very close to 4, where our mechanism is most efficient for high $T_c$, the spin fluctuation might well emerge and play some role in the ground state as well as in the superconducting phase, since the boundary to AF phase is immediate. This possibility is to be investigated as a future problem together with the charge fluctuation mentioned above.

Acknowledgements

One of the authors (H. N.) would like to express his sincere thanks to Professor Y. Mizuno from Science University of Tokyo for his valuable discussions and continual interests in the early stage of this work.

Appendix A

We shall construct the pseudo-spin operator in terms of the on-site avoiding creation and annihilation operators of $(2 \cdot 12b)$. First we define $\tau$-operators by

$$
\begin{align*}
\tau^{(+)}(k) &= b_{k,+,l}^\dagger b_{k,+,l}, \\
\tau^{(-)}(k) &= b_{-k,+,l}^\dagger b_{k,+,l} = N^{-1} \sum_{R_i,R_j \in A} e^{i(k \cdot (R_i-R_j))} b_{R_i,+,l}^\dagger b_{R_j,+,l}^\dagger,
\end{align*}
\hspace{1cm} (A \cdot 1)
$$

Then we calculate the commutation relation of $\tau$-operators, i.e.,

$$
[\tau^{(+)}(k), \tau^{(-)}(k')] = \sum_{R_i,R_j,R_i,R_m \in A} e^{i(k \cdot (R_i-R_j) - i(k' \cdot R_{i,m} - R_{j,m}}[b_{R_i,+,l} b_{R_j,+,l}^\dagger b_{R_{i,m},+,l}^\dagger b_{R_{j,m},+,l}^\dagger].
$$

After some algebra we have for the commutator on the right-hand side above

$$
[\bar{b}_{l,+,l}^\dagger \bar{b}_{l,+,l} \bar{b}_{l,+,l} \bar{b}_{m,+,l}] = \delta_{l,l}(1 - \bar{n}_{l,+,l}) \bar{b}_{l,+,l} \bar{b}_{m,+,l} - \delta_{l,l} \delta_{m,l}(1 - \delta_{l,l}) \bar{b}_{l,+,l} \bar{b}_{l,+,l} \\
\quad + \delta_{m,l}(1 - \bar{n}_{l,+,l}) \bar{b}_{l,+,l} \bar{b}_{m,+,l} - \delta_{m,l} \delta_{l,l}(1 - \delta_{l,l}) \bar{b}_{l,+,l} \bar{b}_{m,+,l} \\
\quad - \delta_{m,l} \delta_{l,l}(1 - \delta_{l,l})(1 - \bar{n}_{l,+,l}) \bar{b}_{l,+,l} \bar{b}_{l,+,l} \\
\quad + \delta_{m,l} \delta_{l,l} \bar{b}_{l,+,l} \bar{b}_{m,+,l} + \delta_{m,l} \delta_{l,l} \bar{b}_{l,+,l} \bar{b}_{m,+,l} - \delta_{m,l} \delta_{l,l} \bar{b}_{l,+,l} \bar{b}_{m,+,l} \\
\quad - \delta_{m,l} \delta_{l,l} \bar{b}_{l,+,l} \bar{b}_{m,+,l} + \delta_{m,l} \delta_{l,l}(1 - \delta_{l,l}) \bar{b}_{l,+,l} \bar{b}_{l,+,l}.
$$

To the above we apply the local mean-field approximation for the number operators of holes, i.e.,

$$
\bar{n}_{l,+,l} \rightarrow \langle \bar{n}_{l,+,l} \rangle = \frac{n_{h}}{2}.
$$

Further, since the system is nonmagnetic, we can neglect terms which make spins flip.
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together with terms ending up with $O(1/N)$ to the main terms when Fourier transformed. Thus we obtain

$$[\tau^{(+)}(k), \tau^{(-)}(k')] = 2\delta_{kk'}\left(1 - \frac{n_h}{2}\right)\tau^{(z)}(k), \quad (A\cdot 2)$$

where

$$\tau^{(z)}(k) = \frac{1}{2} (\bar{n}_r(k) + \bar{n}_l(-k) - 1) \quad \text{with} \quad \bar{n}_\sigma(k) = \bar{b}_{k,\sigma}^\dagger \bar{b}_{k,\sigma}. \quad (A\cdot 3)$$

In a similar manner we calculate commutators of $\tau^{(z)}$ with $\tau^{(\pm)}$ to get

$$[\tau^{(\pm)}(k), \tau^{(z)}(k')] = \pm \delta_{kk'}\left(1 - \frac{n_h}{2}\right)\tau^{(\pm)}(k). \quad (A\cdot 4)$$

Therefore if we define the pseudo-spin operators, $\bar{\tau}$, by

$$\bar{\tau}^{(z)}(k) = \frac{1}{2} \left(1 - \frac{n_h}{2}\right) (\bar{n}_r(k) + \bar{n}_l(-k) - 1) = \frac{1}{\left(1 - \frac{n_h}{2}\right)} \tau^{(z)}(k) \quad (A\cdot 5)$$

and

$$\bar{\tau}^{(\pm)}(k) = \frac{1}{\left(1 - \frac{n_h}{2}\right)} \left[ \bar{b}_{k,\uparrow}^\dagger \bar{b}_{k,\downarrow}^\dagger \right] = \frac{1}{\left(1 - \frac{n_h}{2}\right)} \tau^{(\pm)}(k), \quad (A\cdot 6)$$

then we can show from (A\cdot 2, 4) that the pseudo-spin operators satisfy the $SU(2)$ commutation relations (2\cdot 16a, b).

Appendix B

We shall provide the matrix elements appeared in Eq. (3\cdot 7). By inserting the effective interaction (2\cdot 13d) and the gap function (3\cdot 4) into the gap equation (3\cdot 2) we can obtain them as follows:

$$P(T) = 1 + 4\left(1 - \frac{n_h}{2}\right)^2 T_1(3A(T) - B(T) - C(T)),$$

$$Q(T) = 4\left(1 - \frac{n_h}{2}\right)^2 T_1(3B(T) - D(T) - E(T)),$$

$$R(T) = 4\left(1 - \frac{n_h}{2}\right)^2 T_1(3C(T) - E(T) - F(T)),$$

$$S(T) = -\left(1 - \frac{n_h}{2}\right)^2 \{ V_1 B(T) + 4 \bar{T}_1 (2C(T) + B(T)) + 4 T_1 A(T) \},$$

$$T(T) = 1 - \left(1 - \frac{n_h}{2}\right)^2 \{ V_1 D(T) + 4 \bar{T}_1 (2E(T) + D(T)) + 4 T_1 B(T) \},$$

$$U(T) = -\left(1 - \frac{n_h}{2}\right)^2 \{ V_1 E(T) + 4 \bar{T}_1 (2F(T) + E(T)) + 4 T_1 C(T) \},$$
\[ V(T) = -\left(1 - \frac{n_N}{2}\right)^2 \{2V_1C(T) + 8\tilde{T}_iB(T) + 4T_iA(T)\}, \]
\[ W(T) = -\left(1 - \frac{n_N}{2}\right)^2 \{2V_1E(T) + 8\tilde{T}_iD(T) + 4T_iB(T)\}, \]
\[ Z(T) = 1 - \left(1 - \frac{n_N}{2}\right)^2 \{2V_1F(T) + 8\tilde{T}_iE(T) + 4T_iC(T)\}, \]

where
\[ A(T) = 1, \]
\[ B(T) = \cos k_xa + \cos k_ya, \]
\[ C(T) = \cos k_xa \cos k_ya, \]
\[ D(T) = (\cos k_xa + \cos k_ya)^2, \]
\[ E(T) = \cos k_xa \cos k_ya (\cos k_xa + \cos k_ya), \]
\[ F(T) = \cos^2 k_x \cos^2 k_y. \]

In the above \( \cdots \cdots \) denotes
\[ \cdots \cdots = -\frac{1}{N_{k \in C}} \sum (\cdots \cdots) \frac{\tanh \frac{1}{2} \beta E(k)}{2E(k)}. \]

References