Backward Scattering and Coexistent State in Two-Dimensional Electron System

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The results of the mean field studies on the effects of the backward scattering with large momentum transfer in a two-dimensional electron system are extended to the case with various types of the Fermi surface and coupling constants. It is found that the coexistent state of $d$-wave superconductivity, antiferromagnetism and $\pi$-triplet pair can be stabilized quite generally near half filling.

KEYWORDS: two-dimensional system, saddle-point singularity, backward scattering, $d$-wave superconductivity, antiferromagnetism, $\pi$-triplet pair

§1. Introduction

In recent years the electronic states in two-dimensional systems in the copper oxide high-$T_c$ superconductors have been studied intensively. Especially in the normal state near the optimal doping, a very flat dispersion of quasiparticle excitations around ($\pi,0$) and (0,$\pi$), i.e., the extended saddle-point singularity, has been revealed in the angle resolved photoemission spectroscopy (ARPES) experiments. This flatness of dispersion is more prominent than that obtained in the single-particle band calculations such as local-density approximation (LDA). This behavior has been attributed to the many-body correlation effects based on the results of quantum Monte Carlo (QMC) simulations and propagator-renormalized fluctuation-exchange (FLEX) approximation or to the dimple of the CuO$_2$ planes from the recent LDA calculations. It is the well-known fact that saddle points in the electronic structure result in the van Hove singularities (vHs) in the electronic density of states (DOS). Especially for two-dimensional case, they produce logarithmic divergence in the DOS. Therefore, their existence near the Fermi level has important physical consequences.

In the hole-doped case, such as YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) or Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO), the Fermi level lies near ($\pi,0$) and (0,$\pi$). This might be responsible for unconventional physical properties, such as the normal-state resistivity with $T$-linear temperature dependence or the superconducting gap of the $d_{x^2-y^2}$ symmetry. On the other hand, in the underdoped region, a pseudogap

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of the $d_{x^2-y^2}$ symmetry, which is consistent with the superconducting gap symmetry, has been observed around $(\pi, 0)$ and $(0, \pi)$ above the superconducting critical temperature.\[^{11,12,13}\] It has been indicated that there is strong coupling between quasiparticle excitations near the flat band and collective excitations centered near $(\pi, \pi)$.\[^{14}\]

In the electron-doped case, such as Nd$_{2-x}$Ce$_x$CuO$_{4+\delta}$ (NCCO), however, the Fermi level lies far above $(\pi, 0)$ and $(0, \pi)$, and instead gets close to $(\pm \pi/2, \pm \pi/2)$.\[^{2,15,16}\] The Fermi surface agrees very well with LDA results.\[^{17}\] This might be related to conventional (or Fermi-liquid type) physical properties, such as normal-state resistivity with $T$-square temperature dependence\[^{18}\] or the superconducting gap which is nodeless on the Fermi surface (or BCS-like gap function).\[^{19}\]

Theoretically, various shapes of the Fermi surface can be reproduced by introducing not only nearest-neighbor hopping $t$ but also next-nearest-neighbor hopping $t'$. Studies looking for the instabilities have been carried out with a special emphasis on $(\pi, 0)$ and $(0, \pi)$ in the 2D Hubbard model, by use of the renormalization group method\[^{20,21}\] and QMC.\[^{22}\] These studies have shown that $d$-wave superconductivity prevails over antiferromagnetism by the effect of $t'$. In our preceding letter\[^{23}\] we have studied possible ordered states with a special emphasis on the effects of the backward scattering processes with large momentum transfer between two electrons near $(\pi, 0)$ and $(0, \pi)$ by introducing $g_1$ and $g_3$ processes, which correspond to ’exchange’ and ’Umklapp’ processes, respectively. The mean field phase diagram for a special case, $g_1 = g_3$, and for the YBCO type Fermi surface, was determined. In this paper, results of more detailed studies for general cases with various shapes of the Fermi surface and for several choices of $g_1$ and $g_3$ will be presented. In §2, we introduce the model Hamiltonian and three types of order parameters, i.e., $d$-wave Cooper pair, Néel order and $\pi$-triplet pair. In §3, we determine the phase diagram in the plane of temperature, $T$, and the hole (or electron) doping rate, $\delta$ (or $x$). §4 is devoted to conclusion and discussion.

We take unit of $\hbar = k_B = 1$.

§2. Model

We consider a two-dimensional square lattice with the kinetic energy given by,

\[
H_0 = - \sum_{<ij>\sigma} t_{ij} \{ c_{i\sigma}^\dagger c_{j\sigma} + (\text{h.c.}) \} - \mu \sum_i c_{i\sigma}^\dagger c_{i\sigma},
\]

\[
= \sum_{\rho\sigma} \xi_{\rho\sigma} c_{\rho\sigma}^\dagger c_{\rho\sigma},
\]

(2.1)

where $t_{ij}$ is the transfer integral, $c_{i\sigma}(c_{i\sigma}^\dagger)$ is the annihilation (creation) operator for the electron on the i-th site with spin $\sigma$, and $\mu$ is the chemical potential. The energy dispersion $\xi_p = \epsilon_p - \mu$ is given by

\[
\epsilon_p = -2t(\cos p_x + \cos p_y) - 4t' \cos p_x \cos p_y
\]

\[
- 2t''(\cos 2p_x + \cos 2p_y),
\]

(2.2)
including $t$ (nearest neighbor), $t'$ (next nearest neighbor) and $t''$ (third neighbor), as shown in Fig. 1. We take $t$ as the energy unit, i.e., $t = 1$ and the lattice constant is also taken as unity. The energy band $\epsilon_p$ has saddle points at $(\pm \pi, 0)$ and $(0, \pm \pi)$. The number of independent saddle points in the 1st Brillouin zone is equal to 2.

Fig. 1. The transfer integrals on a 2D square lattice; $t$ (nearest neighbor), $t'$ (next nearest neighbor) and $t''$ (third neighbor).

The 1st Brillouin zone is usually taken as shown in Fig. 2 (a). In this case, however, the saddle points lie on the zone boundaries. In order to treat the scattering processes between two electrons around the saddle points unambiguously, it is convenient to choose the 1st Brillouin zone inside which the saddle points lie, as shown in Fig. 2 (b). It consists of the region A and B including $Q_A \equiv (\pi, 0)$ and $Q_B \equiv (0, \pi)$, respectively. We note that $w_p \equiv \text{sgn}(\cos p_y - \cos p_x) = +1(-1)$ for $p \in A(B)$, which determines the symmetry of the superconducting order parameter, as we shall see later.

Now we introduce effective interaction between two electrons in the region A and B, just as in the g-ology in one-dimensional electron system. Here we treat only the backward scattering with large momentum transfer, shown in Fig. 3, i.e., $g_1$ and $g_3$, in analogy with normal and Umklapp processes in our previous work for one-dimensional electron system.\[24]\ We take only interactions between two electrons with antiparallel spins into account, as in the Hubbard model, i.e., $g_1 \equiv g_{1\perp}$ and $g_3 \equiv g_{3\perp}$. We treat the above Hamiltonian in the mean field approximation. We are interested in the repulsive case,

\[0 \leq g_1 \leq g_3. \tag{2.3}\]

We consider three types of the scattering channels:

(1) Cooper-pair channel
This channel consists of the scattering processes as shown in Fig. 4 (a), where a pair of two electrons with total momentum $2Q_A$ is scattered to that with total momentum $2Q_B$ and vice versa. This is included only in $g_3$ processes. We note that this channel is represented in the original 1st Brillouin zone as shown in Fig. 4 (b), where there exist only normal processes between two electrons with total momentum equal to zero. Therefore, we naturally introduce the order parameters of the Cooper-pair,

$$\begin{align*}
\Delta_A &= \sum'_{k} \langle c_{Q_A-k\downarrow} c_{Q_A+k\uparrow} \rangle, \\
\Delta_B &= \sum'_{k} \langle c_{Q_B-k\downarrow} c_{Q_B+k\uparrow} \rangle,
\end{align*}$$

\begin{equation}
(2.4)
\end{equation}

It is to be noted that $Q_A \pm k$ and $Q_B \pm k$ always lie in the region A and B, respectively, for $k$ satisfying $|k_x| + |k_y| < \pi$ shown in Fig. 5. This is the reason for the choice of the Brillouin zone as shown in Fig. 2 (b).
For $g_3 > 0$, the order parameters, $\Delta_A$ and $\Delta_B$, can be non-zero only in the case,

$$\Delta_1 \equiv g_3 \Delta_A = -g_3 \Delta_B,$$

i.e., the superconducting gap has $d_{x^2-y^2}$ symmetry:

$$\Delta_{x^2-y^2} \equiv \sum_p w_p < c_{-p \downarrow} c_{p \uparrow}> ,$$

$$= \Delta_A - \Delta_B,$$

$$= \frac{2}{g_3} \Delta_1.$$
We note that this superconducting gap function is nodeless in spite of $d_{x^2-y^2}$ symmetry, i.e., only its sign changes across the boundary between the region A and B and its magnitude is constant all over the 1st Brillouin zone, which means that it changes discontinuously along the region boundary. This can be more clearly seen from the fact that we can rewrite (2.5) as $\Delta(p) = g_3\Delta_1 w_p = g_3\Delta_1 \text{sgn}(\cos p_y - \cos p_x)$. It is due to our choice of the 1st Brillouin zone as Fig. 2 (b) and introduction of the 'Umklapp' scattering $g_3$ with momentum dependence ignored.

This channel is the same as 'pair-tunneling' of two electrons located around $Q_A$ and $Q_B$, which favors $d_{x^2-y^2}$ pairing, in the 2D Hubbard model. These interaction processes are not present as important factors in the recent model by Assaad et al., who have introduced the additional interaction expressed as the square of the single-particle nearest-neighbor hopping.

(2) density-wave channel

This channel, consisting of the scattering processes with momentum transfer equal to $Q \equiv (\pi, \pi)$, as shown in Fig. 6 (a), is included in both $g_1$ and $g_3$ processes. In the original 1st Brillouin zone, this is represented as shown in Fig. 6 (b), where there exist both normal and Umklapp processes.

We introduce staggered carrier density of each spin,

\[
\begin{align*}
\Delta_{\uparrow} &= \sum'_k <c_{Q_B+k\uparrow}^\dagger c_{Q_A+k\uparrow}>, \\
\Delta_{\downarrow} &= \sum'_k <c_{Q_B-k\downarrow}^\dagger c_{Q_A-k\downarrow}>.
\end{align*}
\]

For (2.3), they can be non-zero only in the case,

\[
\Delta_{\uparrow} = -\Delta_{\downarrow}^* \equiv \text{real},
\]

\[
\Delta_2 \equiv g_s \Delta_{\uparrow} = -g_s \Delta_{\downarrow},
\]

Fig. 6. The density-wave channel (a) in our Brillouin zone and (b) in the original Brillouin zone.
where $g_s \equiv g_1 + g_3$. This is the commensurate spin-density-wave (C-SDW) or antiferromagnetic (AF) state. The staggered magnetization (Néel order) $M$ is given by

$$M \equiv \frac{1}{N} \sum_i (-1)^i < S_i^z >,$$

$$= \frac{1}{2} \sum_p < c_{p+Q \uparrow}^\dagger c_{p \downarrow}^\uparrow - c_{p+Q \downarrow}^\dagger c_{p \uparrow}^\downarrow >,$$

$$= \text{Re}(\Delta_\uparrow - \Delta_\downarrow),$$

$$= \frac{2}{g_s} \Delta_2.$$

In this paper, we consider the commensurate case only. The validity of this assumption will be discussed in §4.

(3) π-pair channel

This channel, consisting of the scattering processes between two electrons with total momentum equal to $Q$, as shown in Fig. 7 (a), is included only in $g_1$ processes. In the original 1st Brillouin zone, this is represented as shown in Fig. 7 (b), where there exist both normal and Umklapp processes (only the latter case is shown in the figure). We introduce the order parameters of π-pair,

$$\begin{align*}
\Delta_+ &= \sum'_{k} < c_{Q_A-k\downarrow} c_{Q_B+k\uparrow} >, \\
\Delta_- &= \sum'_{k} < c_{Q_B-k\downarrow} c_{Q_A+k\uparrow} >.
\end{align*}$$

(2.10)

For $g_1 > 0$, they can be non-zero only in the case

$$\Delta_3 \equiv g_1 \Delta_+ = -g_1 \Delta_-,$$

(2.11)
There are four quasiparticle energy bands, 
\[ \pi_{\text{triplet}} \equiv \sum_{p\sigma} w_p < c_{-p+Q \sigma} c_{p\sigma} > , \]  
\[ = -2(\Delta_+ - \Delta_-) , \]  
\[ = -\frac{4}{g_1} \Delta_3 . \]  

It is necessary to decouple the Hamiltonian by use of this order parameter because if dSC and AF coexist \( \pi \)-triplet pair always results. This important fact has been indicated by Psaltakis et al. in slightly different context. This \( \pi \)-triplet pair was not taken into account in the calculation based on the slave-boson mean field approximation in the 2D \( t-J \) model, where only dSC and AF are simultaneously taken into account.

By use of the above three order parameters, we obtain the mean field Hamiltonian as follows:

\[ H^{MF} = \sum_k \psi_k^\dagger M_k \psi_k + E_c , \]  
\[ \psi_k^\dagger = (c_{Q_A+k\uparrow}, c_{Q_A-k\downarrow}, c_{Q_B+k\uparrow}, c_{Q_B-k\downarrow}) , \]  
\[ M_k = \begin{pmatrix} a_k & -\Delta_1 & -\Delta_2 & \Delta_3 \\ -\Delta_1^* & -a_k & -\Delta_3^* & -\Delta_2 \\ -\Delta_2 & -\Delta_3 & b_k & \Delta_1 \\ \Delta_3^* & -\Delta_2 & \Delta_1^* & -b_k \end{pmatrix} \]  
\[ a_k \equiv \xi_{Q_A\pm k}, b_k \equiv \xi_{Q_B\pm k} , \]  
\[ E_c = 2 \left( \frac{1}{g_3} |\Delta_1|^2 + \frac{\Delta_2^2}{g_s} + \frac{|\Delta_3|^2}{g_1} \right) - \mu \]  

There are four quasiparticle energy bands, \( \pm E_+(k) \) and \( \pm E_-(k) \),

\[ E_{\pm}(k) = \sqrt{\frac{a_k^2 + b_k^2}{2} + |\Delta_1|^2 + (\Delta_2)^2 + |\Delta_3|^2 \pm A(k)} , \]  
\[ A(k) \equiv \sqrt{ (a_k - b_k)^2 \left( \frac{a_k + b_k}{2} \right)^2 + |\Delta_3|^2 + [(a_k + b_k)(\Delta_2) - 2Re(\Delta_1^*\Delta_3)]^2} , \]

where we note that \( a_k \leftrightarrow b_k, A(k) \leftrightarrow A(k) \) and \( E_{\pm}(k) \leftrightarrow E_{\pm}(k) \) as we exchange \( k_x \) and \( k_y \).

The self-consistent equations are given by

\[ \Delta_1 = \frac{g_3}{4} \sum_k \sum_{\alpha=\pm} \frac{1}{E_\alpha(k)} \tanh \frac{E_\alpha(k)}{2T} \left\{ \Delta_1 + \alpha \frac{2\Delta_3}{A(k)} [Re(\Delta_1^*\Delta_3) - a_k\Delta_2] \right\} , \]  
\[ \Delta_2 = \frac{g_4}{4} \sum_k \sum_{\alpha=\pm} \frac{1}{E_\alpha(k)} \tanh \frac{E_\alpha(k)}{2T} \left\{ \Delta_2 \left[ 1 - \alpha \frac{(a_k - b_k)^2}{2A(k)} \right] - \alpha \frac{2a_k}{A(k)} [Re(\Delta_1^*\Delta_3) - a_k\Delta_2] \right\} , \]  
\[ \Delta_3 = \frac{g_1}{4} \sum_k \sum_{\alpha=\pm} \frac{1}{E_\alpha(k)} \tanh \frac{E_\alpha(k)}{2T} \left\{ \Delta_3 \left[ 1 + \alpha \frac{(a_k - b_k)^2}{2A(k)} \right] + \alpha \frac{2\Delta_1}{A(k)} [Re(\Delta_1^*\Delta_3) - a_k\Delta_2] \right\} , \]  
\[ n = 1 - \sum_k \sum_{\alpha=\pm} \frac{1}{E_\alpha(k)} \tanh \frac{E_\alpha(k)}{2T} \left\{ a_k \left[ 1 + \alpha \frac{(a_k - b_k)^2}{2A(k)} \right] - \alpha \frac{2\Delta_2}{A(k)} [Re(\Delta_1^*\Delta_3) - a_k\Delta_2] \right\} , \]
where \( n \) is the electron filling, which is related to the hole doping \( \delta \) and the electron doping \( x \) by \( \delta = 1 - n \) and \( x = n - 1 \), respectively. These equations satisfy \( \frac{\partial F}{\partial \Delta_1} = \frac{\partial F}{\partial \Delta_2} = \frac{\partial F}{\partial \Delta_3} = 0 \), where \( F \) is the free energy per one lattice site in the canonical ensemble given by

\[
F = -2T \sum_k \left\{ \log \left[ 2 \cosh \frac{E_+(k)}{2T} \right] + \log \left[ 2 \cosh \frac{E_-(k)}{2T} \right] \right\} + E_c + \mu n. \tag{2.16}
\]

The electronic density of states \( \rho(\epsilon) \) is given by

\[
\rho(\epsilon) = \sum_k' \sum_{\alpha, \alpha'} \delta(\epsilon - \alpha' E_\alpha(k)) \\
\times \left\{ 1 + \frac{\alpha'}{E_\alpha(k)} \left( a_k \left[ 1 + \alpha \frac{(a_k - b_k)^2}{2A(k)} \right] \right) \right.
\left. - \frac{2\Delta_2}{A(k)} [\text{Re}(\Delta_1^* \Delta_3) - a_k \Delta_2] \right\}, \tag{2.17}
\]

which is related with \( n \) by \( n = \int_{-\infty}^{\infty} d\epsilon \rho(\epsilon) f(\epsilon, T) \), where \( f(\epsilon, T) = (e^{\epsilon/T} + 1)^{-1} \) is the Fermi distribution function.

### §3. Results

The self-consistent equations (2.15) are solved numerically and the phase diagram has been determined in the plane of temperature \( T \) and the doping rate \( \delta \) or \( x \). It is easily understood from (2.15) that [1] if two of the three order parameters coexist, another one always results and [2] for \( g_1/t = 0 \), \( \pi \)-triplet pair cannot exist \( (\Delta_3 \equiv 0) \), i.e., there exists no coexistent state and dSC prevails over AF. We note that it is energetically favorable to take both \( \Delta_1 \) and \( \Delta_3 \) to be real for the coexistent state. We choose \( t' \) and \( t'' \) so that the bare band width \( W \) is equal to \( 8t \) and reproduce various shapes of the Fermi surface. We fix the value \( g_3/t = 5.0 \).

In the numerical calculation of the DOS (2.17), we approximate \( \delta \)-function by

\[
\delta(\epsilon) = -\lim_{\eta \to 0^+} \frac{\partial}{\partial \eta} f(\epsilon, \eta) = \lim_{\eta \to 0^+} \{4\eta \cosh^2 \frac{\epsilon}{2\eta}\}^{-1}, \tag{3.1}
\]

with a finite value \( \eta/t \equiv 0.01 \).

First we include \( t \) only \( (t'/t = t''/t = 0) \). In this case, there is perfect nesting property \( \epsilon_p = -\epsilon_{p+Q} \) or \( b_k = -a_k - 2\mu \). Since the quasiparticle dispersion depends on \( k \) only through \( a_k \), it is convenient in the numerical calculation to rewrite (2.15), (2.16) and (2.17) by use of the following identity for any function \( g \) of \( a_k \),

\[
\sum_k' g(a_k) = \frac{1}{2} \int d\epsilon \rho_0(\epsilon) g(\epsilon - \mu). \tag{3.2}
\]

\( \rho_0(\epsilon) \) is the bare DOS given by

\[
\rho_0(\epsilon) = \sum_p \delta(\epsilon - \xi_p),
\]
\[ = \frac{1}{2\pi^2 t} K \left( \sqrt{1 - \left( \frac{\varepsilon}{4t} \right)^2} \right) \theta(4t - |\varepsilon|), \]  

(3.3)

where \( K \) is the complete elliptic integral of the 1st kind \( K(k) \equiv \int_0^1 \frac{dx}{\sqrt{(1-x^2)(1-k^2x^2)}} \) and \( \theta \) is the step function.

We show the bare Fermi surface in Fig. 8 for a few values of the hole doping \( \delta \) (it is sufficient to consider the hole-doped case due to the particle-hole symmetry). The saddle points lie on the Fermi surface in the half-filled case.

Fig. 8. The Fermi surface in the case without \( t' \) and \( t'' \) for a few values of the hole doping \( \delta \).

We show the phase diagram in Fig. 9 for two different choices of the coupling constants, \( g_1 = g_3 \) and \( g_1 = g_3/2 \). In the half-filled case, as the temperature is lowered, AF gets stabilized, and since there is no free carriers in the presence of the SDW gap, dSC cannot arise even in \( T = 0 \). On the other hand, near half filling, there are free carriers even in the AF state, and dSC also can be stabilized in the low temperature region. This result is similar to the spin-bag picture.\(^{29}\) It is important that the coexistence of AF and dSC always results in \( \pi \)-triplet pair. Such a close relationship between dSC and AF has been indicated by SO(5) theory.\(^{30}\) For smaller \( g_1 \), AF region and therefore the coexistent region are reduced.

We note that for \( g_1 = 0 \) and \( \delta = 0 \), due to the perfect nesting property, \( \Delta_1 \) and \( \Delta_2 \) are determined by the same equation, i.e., AF and dSC are degenerate.

In Fig. 10 we show the DOS in the coexistent state near the optimal doping which gives the highest onset temperature of dSC. There exists energy gap in the DOS at the Fermi level.

Next we consider the hole-doped case with the YBCO type Fermi surface. We choose \( t'/t = -1/5 \) and \( t''/t = 1/7 \). The Fermi surface is shown in Fig. 11 for a few values of the hole doping \( \delta \). In this
Fig. 9. The phase diagram in the case without $t'$ and $t''$ for $g_3/t = 5.0$ and $g_1/t = 5.0, 2.5$.

Fig. 10. The electronic DOS in the case without $t'$ and $t''$ in the coexistent state for $g_3/t = g_1/t = 5.0$ and $T = 0$ near the optimal doping $\delta = 0.21$. The Fermi level lies at $\epsilon = 0$.

case, the saddle points lie on the Fermi surface near $\delta = 0.44$.

We show the phase diagram in Fig. 12 for two different choices of the coupling constant, $g_1 = g_3$ and $g_1 = g_3/2$. For $\delta = 0$, only AF can be stabilized, and near half filling there exists coexistent state of dSC, AF and $\pi$-triplet pair. For $g_1 = g_3$, compared with the perfect nesting case, the effect of nesting near $\delta = 0$ is suppressed and the onset temperature of AF is lower. On the other hand, near $\delta \sim 0.4$, the saddle points lying near the Fermi surface lead to the enhancement of the order parameters of both dSC and AF.
Fig. 11. The Fermi surface for the YBCO case for a few values of the hole doping $\delta$.

Fig. 12. The phase diagram for the YBCO case for $g_3/t = 5.0$ and $g_1/t = 5.0, 2.5$.

In Fig. 13 we show the DOS in the coexistent state near the optimal doping. The DOS has an energy gap at the Fermi level.

Finally we consider the electron-doped case with the NCCO type Fermi surface. We choose $t'/t = -1/3$ and $t''/t = 1/10$. The Fermi surface is shown in Fig. 14 for a few values of the electron doping $x$. In this case, the saddle points lie on the Fermi surface near $x = 0.28$.

We show the phase diagram in Fig. 15 for two different choices of the coupling constant, $g_1 = g_3$ and $g_1 = g_3/2$. In this case the saddle points are not located near the Fermi surface and there is a suppression of the onset temperature of AF and dSC compared with the above two cases.
Fig. 13. The electronic DOS for the YBCO case in the coexistent state for $g_3/t = g_1/t = 5.0$ and $T = 0$ near the optimal doping $\delta = 0.30$. The Fermi level lies at $\epsilon = 0$.

Fig. 14. The Fermi surface for the NCCO case for a few values of the electron doping $x$.

In Fig. 16 we show the DOS in the coexisting state near the optimal doping. The energy gap lies at the Fermi level in the DOS.

§4. Conclusion

We have studied possible ordered states of interacting electrons on a square lattice with a special emphasis on the backward scattering, $g_1$ and $g_3$, i.e., ‘exchange’ and ‘Umklapp’ processes, respectively, between two electrons around $(\pi,0)$ and $(0,\pi)$ for various shapes of the Fermi surface.

We focus on the case that $g_3$, which is related with the superconducting state with $d_{x^2-y^2}$ type of the gap, is about half of the bare band width, $W/t = 8.0$, i.e., $g_3/t = 5.0$. For $g_1 = 0$, $d$-wave
superconducting state (dSC) competes with and prevails over antiferromagnetism (AF) even in the half-filled case. For $0 < g_1 \leq g_3$ with $g_1/g_3$ not so small, only AF can be stabilized in the half-filled case and coexist with dSC near half filling. Especially in the coexistent state, $\pi$-triplet pair always results and the DOS has an energy gap at the Fermi level, independent of the hole or electron doping rate. The above conclusion is qualitatively independent of the shapes of the Fermi surface.

As we have indicated in §2, we have assumed C-SDW throughout this paper. In general, however, away from half filling, the incommensurate SDW (IC-SDW) should be expected with $Q \neq (\pi, \pi)$. 

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**Fig. 15.** The phase diagram for the NCCO case for $g_3/t = 5.0$ and $g_1/t = 5.0, 2.5$.

**Fig. 16.** The electronic DOS for the NCCO case in the coexistent state for $g_3/t = g_1/t = 5.0$ and $T = 0$ near the optimal doping $x = 0.22$. The Fermi level lies at $\epsilon = 0$. 
Therefore, it is not clear whether this coexistent state can be stabilized or not when we include IC-SDW. In fact, the instability towards incommensurate IC-SDW depends strongly on momentum-dependence of both the zero-frequency susceptibility, $\chi_0(q)$, and effective interaction. We note, however, the following facts: [1] There exists the region where $\chi_0(q)$ shows maximum at $q = (\pi, \pi)$ near half filling at low temperature, in the present choices of the Fermi surface. [2] $g_1$ and $g_3$ can be considered to have maximum at $q = (\pi, \pi)$ ($q$ stands for the momentum transfer of one electron), although the $q$-dependence of $g_1$ and $g_3$, which is not explicitly indicated in this paper, is irrelevant under the assumption of C-SDW of interest. These facts result in RPA susceptibility showing maximum at $q = (\pi, \pi)$ leading to C-SDW at least near half filling at low temperature where the coexistent state is possible.

With respect to the superconducting gap symmetry, in the case that $(\pm \pi/2, \pm \pi/2)$ lies near the Fermi surface, not only $d_{x^2-y^2}$ component but also other ones can mix. Recent QMC calculations show that not only $d_{x^2-y^2}$ but also $d_{xy}$ pairing correlation are enhanced in the 2D Hubbard model, and new ordered state with a mixing of extended s-wave component with total momentum $(\pi,0)$ and $(0,\pi)$ and the usual $d_{x^2-y^2}$ component has been discovered in the 2D $t$-$J$ model, in the mean field and Gutzwiller approximations. Their results are closely related to the fact that the original $d_{x^2-y^2}$-wave superconducting gap has nodes around $(\pm \pi/2, \pm \pi/2)$, i.e., the fact that Umklapp scattering between two quasiparticles on the Fermi surface around these points is possible may lead to form the full gap all over the Fermi surface. Our $d_{x^2-y^2}$-wave superconducting gap, however, has no node, i.e., changes discontinuously along the boundary between the region A and B, as already discussed in §2. Therefore, in our model, we cannot discuss the mixing of another component in the superconducting gap function in addition to the $d_{x^2-y^2}$-wave component. This is the future problem.

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