Effects of the Backward Scattering in Two-Dimensional Electron System

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Effects of the backward scattering with large momentum transfer are examined in two-dimensional electron system with a special emphasis on electrons around \((\pi, 0)\), \((0, \pi)\). The phase diagram is shown in the plane of temperature \(T\) and hole doping \(\delta\) in the mean field approximation and it is found that \(d\)-wave superconductivity, antiferromagnetism and \(\pi\)-triplet pair can coexist near half filling.

KEYWORDS: two-dimensional system, very flat band, backward scattering, \(d\)-wave superconductivity, antiferromagnetism, \(\pi\)-triplet pair

In recent years the electronic states in two-dimensional systems in the hole-doped copper oxide high-\(T_c\) superconductors have been studied intensively. Especially, the anomalies in the normal state around \((\pi, 0)\) and \((0, \pi)\) have been elucidated in the angle resolved photoemission spectroscopy (ARPES) experiments. Near optimal hole doping, a very flat dispersion of quasiparticle excitations near the Fermi level around \((\pi, 0)\) and \((0, \pi)\) has been reported in materials such as YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) (YBCO) or Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\) (BSCCO). This flatness of dispersion is more prominent than that obtained in the single-particle band calculations such as local-density approximation (LDA). This ‘extended’ saddle-point 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. On the other hand, in the underdoped region, a pseudogap of the \(d_{x^2-y^2}\) symmetry has been observed around \((\pi, 0)\) and \((0, \pi)\) above the superconducting critical temperature. It has been indicated that there is strong coupling between quasiparticle excitations near the flat band and collective excitations centered near \((\pi, \pi)\).

Theoretically, such experimental features that the Fermi level approaches \((\pi, 0)\) and \((0, \pi)\) as hole doping rate is increased from half filling can be described by introducing not only nearest-neighbor hopping \(t\) but also next-nearest-neighbor hopping \(t'\). Actually studies looking for the instabilities...
with a special emphasis on \((\pi,0)\) and \((0,\pi)\) in the 2D Hubbard model have been carried out, by use of the renormalization group method\(^{12,13}\) and QMC.\(^{14}\) These studies have shown that \(d\)-wave superconductivity prevails over antiferromagnetism by the effect of \(t'\). In this letter, we consider the situation that the Fermi level approaches \((\pi,0)\) and \((0,\pi)\) as hole doping rate is increased from half filling. With a special emphasis on the effects of the backward scattering processes with large momentum transfer between two electrons near \((\pi,0)\) and \((0,\pi)\), we search for possible ordered states in the mean field approximation. It is found that three order parameters, \(d\)-wave Cooper pair, Neel order and \(\pi\)-triplet pair are stabilized, and the phase diagram in the plane of temperature, \(T\), and hole doping rate, \(\delta\), has been determined. We take unit of \(\hbar = k_B = 1\).

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

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

\[
= \sum_{\rho\sigma} \xi_{\rho} c_{\rho\sigma}^\dagger c_{\rho\sigma}, \tag{1}
\]

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 is given by

\[
\xi_{\rho} = -2t(\cos p_x + \cos p_y) - 4t' \cos p_x \cos p_y - 2t''(\cos 2p_x + \cos 2p_y) - \mu, \tag{2}
\]

including \(t\) (nearest neighbor), \(t'\) (next nearest neighbor) and \(t''\) (third neighbor), as shown in Fig. 1.

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We take \(t\) as the energy unit, i.e., \(t = 1\). The lattice constant is also taken as unity. We choose the values of \(t'\) and \(t''\) so that the Fermi surface of YBCO type is reproduced near half filling. In

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Fig. 1. Transfer integrals on a 2D square lattice; \(t\) (nearest neighbor), \(t'\) (next nearest neighbor) and \(t''\) (third neighbor).
this letter, we take the following choice as
\[ t' / t = -1/6, t'' / t = 1/5. \] (3)

In order to treat the scattering processes between two electrons around \((\pi,0)\) and \((0,\pi)\) unambiguously, we take the Brillouin zone as shown in Fig. 2, which consists of the region A and B including \((\pi,0)\) and \((0,\pi)\), respectively. We note that \(w_p \equiv \text{sgn}(\cos p_y - \cos p_x) = +1(-1)\) for \(p \in A(B)\). The Fermi surface in the half-filled case is also shown in Fig. 2.

Next we consider the interaction term. We can 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. \[ \] We take only interaction 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 under the assumption \(g_1 = g_3 \equiv g > 0\) for simplicity. By noting that there exist the scattering processes as shown in Fig. 4, we naturally introduce the following order parameters, i.e., Cooper-pair with total momentum equal to zero in the original 1st Brillouin zone which can be expressed as follows,
\[ \Delta_A = g \sum'_{k} < c_{Q_A - k\downarrow} c_{Q_A + k\uparrow} >, \quad \Delta_B = g \sum'_{k} < c_{Q_B - k\downarrow} c_{Q_B + k\uparrow} >, \] (4a)
and staggered carrier density of each spin,

\[ \Delta_\uparrow = g \sum_k' \langle c_{Q_B+k\uparrow}^\dagger c_{Q_A+k\uparrow} \rangle, \quad \Delta_\downarrow = g \sum_k' \langle c_{Q_B-k\downarrow}^\dagger c_{Q_A-k\downarrow} \rangle, \]

(4b)

and \( \pi \)-pair

\[ \Delta_+ = g \sum_k' \langle c_{Q_A-k\downarrow}^\dagger c_{Q_B+k\uparrow} \rangle, \quad \Delta_- = g \sum_k' \langle c_{Q_B-k\downarrow}^\dagger c_{Q_A+k\uparrow} \rangle, \]

(4c)

where \( Q_A = (\pi, 0) \) and \( Q_B = (0, \pi) \), respectively, and

\[ \sum_k' \equiv \sum_{|k_x|+|k_y|<\pi}. \]

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 \( |k_x|+|k_y|<\pi \). This is the reason for the choice of the Brillouin zone as shown in Fig. 2. We take

\[ \Delta_1 \equiv \Delta_A = -\Delta_B, \]
\[ \Delta_2 \equiv 2\Delta_\uparrow = -2\Delta_\downarrow^*, \]
\[ \Delta_3 \equiv \Delta_+ = -\Delta_-, \]

(5a, 5b, 5c)

so that each of the above three order parameters is possible independently of each other for \( g > 0 \). They stand for \( d \)-wave Cooper-pair, Neel order and \( \pi \)-triplet pair, respectively. We note that \( \Delta_2 \) is real for \( g_1 = g_3 \). Our \( g_3 \) processes included in the Cooper channel are the same as the ‘pair-tunneling’ of two electrons located around \((\pi,0)\) and \((0,\pi)\), 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.

We obtain the mean field Hamiltonian as follows:

\[ H^{MF} = \sum_k' \psi_k^\dagger M_k \psi_k + H_c, \]

(6a)
\[ \psi^\dagger_k = (c^\dagger_{Q_A+k} \uparrow, c_{Q_A-k} \downarrow, c^\dagger_{Q_B+k} \uparrow, c_{Q_B-k} \downarrow), \] (6b)
\[ M_k = \begin{pmatrix} a_k & -\Delta_1 & -\Delta_2 & \Delta_3 \\ -\Delta_1^* & -a_k & -\Delta_3^* & -\Delta_2 \\ -\Delta_2 & -\Delta_3 & b_k & \Delta_1 \\ \Delta_3^* & -\Delta_2^* & \Delta_1^* & -b_k \end{pmatrix}, \] (6c)
\[ a_k \equiv \xi_{Q_A \pm k}, b_k \equiv \xi_{Q_B \pm k}, \] (6d)
\[ H_c = \frac{1}{g} \left\{ 2(|\Delta_1|^2 + |\Delta_3|^2) + (\Delta_2)^2 \right\} - \mu. \] (6e)

There are four quasiparticle energy bands, \( \pm E_+(k) \) and \( \pm E_-(k) \),
\[ E_\pm(k) = \sqrt{\frac{a_k^2 + b_k^2}{2} + |\Delta_1|^2 + (\Delta_2)^2 + |\Delta_3|^2 \pm A(k)}, \] (7a)
\[ A(k) \equiv \sqrt{(a_k - b_k)^2 \left[ \left( \frac{a_k + b_k}{2} \right)^2 + |\Delta_3|^2 \right] + [(a_k + b_k)(\Delta_2) - 2\text{Re}(\Delta_1^* \Delta_3)]^2}. \] (7b)

The self-consistent equations are given by
\[ \Delta_1 = \frac{g}{4} \sum_k' \sum_{\alpha=\pm} \frac{1}{E_\alpha(k)} \tanh \frac{E_\alpha(k)}{2T} \left\{ \Delta_1 + \alpha \frac{2\Delta_3}{A(k)} \left[ \text{Re}(\Delta_1^* \Delta_3) - a_k \Delta_2 \right] \right\}, \] (8a)
\[ \Delta_2 = \frac{g}{2} \sum_k' \sum_{\alpha=\pm} \frac{1}{E_\alpha(k)} \tanh \frac{E_\alpha(k)}{2T} \left\{ \Delta_2 \left[ 1 + \alpha \left( \frac{a_k + b_k}{2A(k)} \right)^2 \right] - \alpha \frac{2\text{Re}(\Delta_1^* \Delta_3) a_k}{A(k)} \right\}, \] (8b)
\[ \Delta_3 = \frac{g}{4} \sum_k' \sum_{\alpha=\pm} \frac{1}{E_\alpha(k)} \tanh \frac{E_\alpha(k)}{2T} \left\{ \Delta_3 \left[ 1 + \alpha \left( \frac{a_k - b_k}{2A(k)} \right)^2 \right] + \alpha \frac{2\Delta_1}{A(k)} \left[ \text{Re}(\Delta_1^* \Delta_3) - a_k \Delta_2 \right] \right\}. \] (8c)
\[ n = 1 - \frac{1}{2} \sum_1^{\prime} \sum_{\alpha=\pm} \frac{1}{E_{\alpha}(k)} \tanh \frac{E_{\alpha}(k)}{2T} \left\{ (a_k + b_k) \left( 1 + \frac{2\alpha}{A(k)} \left[ \frac{(a_k - b_k)^2}{2} + \Delta_2^2 \right] \right) - \alpha \frac{4\Delta_2 \text{Re}(\Delta_1^* \Delta_3)}{A(k)} \right\} \]

where \( n \) is the electron filling, which is related to hole doping \( \delta \) by \( \delta = 1 - n \).

These equations are solved numerically, under the assumption that both \( \Delta_1 \) and \( \Delta_3 \) are real. The resultant phase diagram is shown in Fig. 5 in the plane of \( T \) and \( \delta \) for a choice of \( g/t = 5.0 \). In this case we find that \( d \)-wave superconductivity (dSC), antiferromagnetism (AF) and \( \pi \)-triplet pair can coexist near half filling. Such a close relationship between dSC and AF has been indicated by SO(5) theory. We note that if two of three order parameters coexist, another one always results. It is noted that the stability of antiferromagnetism near half filling is not due to the nesting but due to scattering processes involving both \( g_1 \) and \( g_3 \).

In summary, 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 the case of YBCO type Fermi surface. If we take \( g_1 = g_3 > 0 \), \( d \)-wave superconductivity (dSC), antiferromagnetism (AF) and \( \pi \)-triplet pair can coexist near half filling. On the other hand, the results of our preliminary calculations indicate that for \( g_1 \neq g_3 \) dSC can compete with AF and especially for \( g_1 = 0 \) dSC prevails over AF in the half-filled case. On the other hand, in the case of electron-doped materials such as \( \text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4+\delta \) (NCCO), the Fermi level lies far above \((\pi,0)\) and \((0,\pi)\), but gets close to \((\pm \pi/2, \pm \pi/2)\) for which 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. These results indicate that there exists a variety depending on the shape of the Fermi surface and scattering processes, which will be reported in detail elsewhere.

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[1] Z. -X. Shen and D. S. Dessau: Phys. Rep. 253 (1995) 1.
[2] Z. -X. Shen et al.: Science 267 (1995) 343.
[3] S. Massida, J. Yu and A. J. Freeman: Physica C 52 (1988) 251.
[4] H. Krakauer and W. E. Pickett: Phys. Rev. Lett. 60 (1988) 1665.
[5] N. Bulut, D. J. Scalapino and S. R. White: Phys. Rev. B 50 (1994) 7215.
[6] R. Putz, R. Preuss, A. Muramatsu and W. Hanke: Phys. Rev. B 53 (1995) 5133.
[7] O. K. Andersen, O. Jepsen, A. I. Liechtenstein and I. I. Mazin: Phys. Rev. B 49 (1994) 5145.
[8] A. G. Loeser, D. S. Dessau and Z. -X. Shen: Physica C 263 (1996) 208.
[9] A. G. Loeser et al.: Science 273 (1996) 325.
[10] H. Ding et al.: Nature (London) 382 (1996) 51.
[11] Z. -X. Shen and J. R. Schrieffer: Phys. Rev. Lett. 78 (1997) 1771.
[12] H. J. Schulz: Europhys. Lett. 4 (1987) 609
[13] J. V. Alvarez, J. Gonzalez, F. Guinea and M. A. H. Vozmediano: condmat/9705165.
[14] T. Husslein et al.: Phys. Rev. B 54 (1996) 16179.
[15] M. Murakami and H. Fukuyama: J. Phys. Soc. Jpn. 66 (1997) 2399.
[16] K. Kuroki and H. Aoki: preprint.
[17] F. F. Assaad, M. Imada and D. J. Scalapino: Phys. Rev. Lett. 77 (1996) 4592; condmat/9706173.
[18] S. C. Zhang: Science 275 (1997) 4126.
