Underlying Pairing States of High $T_c$ Superconductivity

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In this work, I present a microscopic theory I proposed recently to describe high-$T_c$ superconductivity in cuprates. I show that coherent pairing states consisting of extended singlet Cooper pairs and triplet $\pi$ pairs can manifest the co-existence of the Mott insulating antiferromagnetic order and the $d$-wave superconducting order. From this configuration of coherent pairing states, I can describe both the single electron properties and the low energy collective excitations in high $T_c$ superconductivity in the same framework. The quasiparticle can be derived directly with respect to the coherent pairing states. While, the low-lying quantum fluctuations associated with spin-wave and charge excitation can be investigated from the path integral of the coherent pairing states.

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I. Introduction

Discovery of high-$T_c$ superconductivity in copper-oxides reveals very attractive, but also extremely complicated, new phenomena in strongly correlated electron systems [1]. One of the most striking phenomena is that cuprates undergo a transition from the Mott insulating antiferromagnetic (AF) order to the $d$-wave superconducting (dSC) order under copings. Theorists have tried various different mechanisms, such as the theory of resonating valence bond (RVB) states of singlet pairs introduced by Anderson a decade ago [2] and the SO(5) unified theory of AF and dSC order parameters proposed by S. C. Zhang recently [3], to explain this metal-insulator transition. However, a microscopic description of this AF to dSC transition has not yet been completed.

In this work, I report a microscopic theory I proposed recently to describe high-$T_c$ superconductivity in cuprates [4]. In this theory, I show that coherent pairing states consisting of extended singlet Cooper pairs and triplet $\pi$ pairs can manifest the co-existence of the Mott insulating antiferromagnetic order and the $d$-wave superconducting order. At half-filling, this configuration describes an insulating AF ordering arisen from the mixing of singlet and triplet pairs. Upon doping with holes the $d$-wave pairing gap appears, and above a certain level cuprates become superconducting. In this AF to dSC transition, the nature of no-double-occupied-sites and the presence of triplet $\pi$ pairs play an very important role.

Based on the square lattice structure of layered copper-oxides, the cuprate ground state $|\Psi\rangle$ may be obtained by projecting out all states of no double occupied sites from the following
generalized pairing state $|\Psi\rangle$:

$$
|\Psi\rangle = \prod_{k} \exp \left \{ \eta_{1}(k) c_{k}^{\dagger} c_{k+Q}^{\dagger} + \eta_{2}(k) c_{k+Q}^{\dagger} c_{k}^{\dagger} + \eta_{3}(k) c_{k}^{\dagger} c_{k+Q}^{\dagger} c_{k+Q} c_{k} + \eta_{4}(k) c_{k}^{\dagger} c_{k+Q}^{\dagger} c_{k+Q} c_{k} + \eta_{5}(k) c_{k}^{\dagger} c_{k+Q}^{\dagger} c_{k+Q} c_{k} + \eta_{6}(k) c_{k}^{\dagger} c_{k+Q}^{\dagger} c_{k+Q} c_{k} - H.c. \right \} |0\rangle,
$$

where the production of $k$ over the momentum space is restricted in the reduced (half) first Brillouin zone, and the complex parameters $\eta_{i}(k)$ are generally link-dependent pairing wave functions. The parity symmetry in the $x$-$y$ plane requires $\eta_{i}(k) = \eta_{i}(-k)$. In the generalized coherent state theory [5], $|\Phi\rangle$ is a product (over $k$) of the local SO(8)/U(4) coherent pairing states [6]. In fact, Eq. (1) is also a multi-pair generalization of the standard Su(2) BCS pairing state or RVB states (after projection). Explicitly, we may rewrite $\eta_{1}(k) = \eta_{s}(k) + \eta_{d}(k)$, $\eta_{2}(k) = \eta_{s}(k) - \eta_{d}(k)$, $\eta_{3}(k) = \eta_{s}(k) + \eta_{d}(k)$, $\eta_{4}(k) = \eta_{s}(k) - \eta_{d}(k)$, and $\eta_{5}(k) = \eta_{s}(k)$. Then, Eq. (1) consists of all electron pairs concerned in the study of superconductivity. These are the ordinary s-wave Cooper pairs, the extended (i.e. valence bond) singlet pairs [including the extended s-wave, d-wave and $s + \alpha d$ pairs], the quasispin $\eta$ pairs, the singlet $p$-wave $\pi$ pairs, and finally the triplet $\pi$ pairs.

However, not all these pairs must be equally important in high $T_{c}$ superconductivity. Indeed, it is no need to include the ordinary s-wave pairs and the quasispin $\eta$ pairs for the AF phase at half-filling. This is because the ordinary s-wave pairs and the quasispin $\eta$ pairs describe the conventional s-wave SC order parameter and the CDW order parameter in the negative-$U$ Hubbard model. The “Shiba” particle-hole transformation on bipartite lattices $c_{j}^{\dagger} \rightarrow c_{j}^{\dagger}$, $c_{j}^{\dagger} \rightarrow c_{j}^{\dagger}$ or $(-1)^{i}c_{j}^{\dagger}$ for $i \in A$ or $B$ sublattice, maps these order parameters in the negative-$U$ Hubbard model into the staggered AF magnetic order parameters in the positive-$U$ Hubbard model at half filling. This leads to $\eta_{1}(k) = -\eta_{2}(k)$ and $\eta_{3}(k) = \eta_{4}(k)$. In addition, the cuprate ground states must also be imposed by the constraint of no-double-occupied-sites due to the strong repulsive Coloumb interaction of the on-site electrons. Instead of using Gutzwiller projector $P_{G}$ to remove double occupied sites from $|\Psi\rangle$, it is equivalent to require that $|\Psi\rangle$ must satisfy the constraint $\langle \Phi | \sum_{i} (n_{i} n_{i}) | \Phi \rangle = 0$, where summation to $i$ over the lattice sites. In the mean-field approximation of (1), it is reduced to the global constraint:

$$
\frac{n_{s}^{2}}{4N^{2}} - m_{s}^{2} + |\Delta_{s}|^{2} + |\Delta_{\eta}|^{2} = 0,
$$

where $n_{s}$ is the total electron number, $m_{s}$ denotes the magnitude of the long-range AF order parameter, and $\Delta_{s}$ and $\Delta_{\eta}$ are averaged order parameters of the ordinary s-wave Cooper pairs and the quasispin $\eta$ pairs which vanish ($\Delta_{s} = \Delta_{\eta} = 0$) under the conditions $\eta_{1}(k) = -\eta_{2}(k)$ and $\eta_{3}(k) = \eta_{4}(k)$. Therefore, $m_{s}^{2} = \frac{n_{s}^{2}}{4N^{2}}$. At half-filling, it gives $m_{s} = 0.5$ which is the same result as in Néel states. The constraint of no-double-occupied-sites also indicates that the ordinary s-wave pairs and the quasispin $\eta$ pairs cannot be formed even after hole doping!

One of the importances of taking the cuprate ground states as the coherent pairing states (1) is that it naturally introduces a quasiparticle picture with respect to the states, $\alpha_{k\sigma} |0\rangle = 0 \rightarrow \gamma_{k\sigma} |\Phi\rangle = 0$, by the generalized Bogoliubov transformation,

$$
\left[ \begin{array}{c} \beta_{k} \\ \beta_{k}^{\dagger} \end{array} \right] = \left[ \begin{array}{cc} W_{k} & -Z_{k}^{\dagger} \\ Z_{k} & W_{k}^{\dagger} \end{array} \right] \left[ \begin{array}{c} \alpha_{k} \\ \alpha_{k}^{\dagger} \end{array} \right],
$$

(3)
to the Nambu basis: \( \alpha_k^\dagger = \{ \nu, \alpha_k, \alpha_k + Q, \alpha_k + Q^\dagger \} \), and \( \beta_k^\dagger = \{ \gamma_k, \gamma_k, \gamma_k + Q, \gamma_k + Q^\dagger \} \). Here, \( W_k^2 + Z_k Z_{-k} = 1 \) and \( Z_k = \eta \sin \sqrt{\eta^2 \eta} / \sqrt{\eta^2 \eta} \) with

\[
\eta(k) = \frac{1}{Z} \begin{bmatrix}
0 & \eta_1(k) & \eta_2(k) & \eta_3(k) \\
-\eta_1(k) & 0 & \eta_4(k) & \eta_5(k) \\
-\eta_2(k) & -\eta_4(k) & 0 & \eta_6(k) \\
-\eta_3(k) & -\eta_5(k) & -\eta_6(k) & 0 \\
\end{bmatrix}.
\] (4)

With this quasiparticle picture, one can study various quasiparticle properties in high \( T_c \) superconductivity, including the single hole spectrum near the half-filling, the \( d \)-wave like gap in optimal dopings and the \( d \)-wave like spin-gap in underdopings, and also the evolution of different fermi surfaces recently observed in different cuprate components.

On the other hand, the over-completeness of coherent pairing states also span a basic state space for the description of the collective excitations observed in cuprate superconductivity, such as the 41 meV resonance. The partition function can be expressed in terms of path integral of the coherent pairing states:

\[
Z(\beta) = \int [d\mu(Z(\tau))] \exp \left\{ -\int_0^\beta d\tau \mathcal{L}[Z(\tau), \dot{Z}(\tau)] \right\},
\] (5)

where

\[
\mathcal{L}[Z(\tau), \dot{Z}(\tau)] = \langle \Phi(\tau) | i \frac{d}{d\tau} | \Phi(\tau) \rangle - \langle \Phi(\tau) | H | \Phi(\tau) \rangle
\] (6)

is an effective Lagrangian defined on the space of the pairing wave-functions, and the \( H \) is the Hamiltonian of strong correlated electron system, such as the Hubbard model or \( t-J \) model Hamiltonian. This effective Lagrangian contains two terms. The second term is just a matrix element of Hamiltonian operator in the coherent pairing states. Minimization of this matrix element with respect to the pairing wave-functions leads to a generalized BCS or RVB theory of the extended singlet pairs mixed with triplet pairs [4]. The first term is a generalized Berry phase in pairing states, which will induce a non-abelian topological gauge field to describe quantum fluctuations in collective excitations.

Here I only focus on the application of the above general theory to the cuprate ground states. Totally spin singlet of cuprate ground states requires \( \eta_1(k) = -\eta_0(k) \). Combining with the non-existence of the ordinary \( s \)-wave pairs and quasispin \( \eta \) pairs by \( \eta_1(k) = -\eta_2(k), \eta_3(k) = \eta_4(k) \), the generalized Bogoliubov transformations are restricted by \( z_{1k} = -z_{2k}, z_{3k} = z_{4k}, z_{5k} = -z_{6k} \), and \( z_{jk} \) is a matrix element of \( Z_k \) with the same form as (4). These restrictions on the pairing wave functions are also necessary for the manifestation of the \( d \)-wave pairing symmetry of valence bonds because it implies \( \eta_j(k + Q) = -\eta_j(k) \). Furthermore, because of the spin rotational symmetry, without loss of the generality we can define \( z_{3k} = z_{6k}, z_{3k} = z_{4k} \cos 2\theta_k \) and \( z_{5k} = z_{\pi k} \sin 2\theta_k \). The AF and dSC gap order parameters in the coherent pairing states are given by

\[
m_s = \frac{2}{N} \sum_{k} \sum_{\nu}^0 \left( z_{\nu k} z_{\nu k}^* + z_{\nu k}^* z_{\nu k} \right), \quad \Delta_d = \frac{1}{N} \sum_{k} d(k) \left( z_{\nu k}^+ w_{k}^+ + z_{\nu k} w_k^* \right)
\] (7)

where \( z_{\nu k} \equiv z_{\nu k} \pm z_{\nu k} \), and \( w_k^* = \sqrt{1 - |z_k^*|^2} \). Obviously, without the triplet pairs (i.e., \( z_{\pi k} = 0 \), the AF order vanishes and the dSC order parameter is reduced to the RVB-type state.
FIG. 1. Gap order parameters via dopings at zero temperature. The (top) solid line is for $t'/J = 0$, and the middle and bottom lines are for $t'/J = 0.2$ and $0.3$, respectively.

To be explicit, we may determine the ground state from the $t - J$ model. When all electrons in ground states are paired, the $t$-term vanishes by the pairing symmetry $z_{1k} = -z_{2k}$ for any doing. The next order hoping ($t^3$-term) has a non-zero expectation value in $|\Phi\rangle$. The ground states can be determined by minimizing the $t^3 - J$ Hamiltonian, which leads to the gap equation at zero-temperature,

$$\Delta_k = \frac{1}{N} \sum_k V_{kk} \frac{\Delta_{k0}}{2E_{k0}}$$

where $\Delta_k \equiv \Delta_d d(k) + \Delta_{es} \gamma(k)$, $V_{kk} = J[d(k)d(k^0) + \gamma(k)\gamma(k^0)]$ and $E_k = \{J^2 \Delta_k^2 + |\varepsilon(k) - \mu - 2(1 - \delta)J|^2\}^{1/2}$ with $\varepsilon(k) = -4t^3 \cos k_x \cos k_y$. The fixed electron number gives $-\frac{2}{N} \sum_k \frac{\varepsilon(k)}{\mu} 2[1, \delta] = 1 - 2\delta$, and $\mu$ is the chemical potential. The numerical solutions of (8) show that the $d$-wave gap order parameter appears after dopings (but $\delta < 0.5$) with maximum peak $\Delta_d \approx 0.07 \sim 0.10$ at $\delta \approx 0.15 \sim 0.20$ (the typical optimal doping region) for $t^3/J = 0.30 \sim 0.20$. This is in good agreement with the experimental observations of $d$-wave superconducting states in cuprates. It is also striking that the extended $s$-wave superconducting states only emerge in overdoped region of $\delta > 0.5$. The separation of the $d$-wave states in optimal dopings from the extended $s$-wave states in overdopings is controlled by the $t^0$-term. Here $t^0$ must be positive. For a negative $t^0$, the ordering of $\Delta_d$ and $\Delta_{es}$ in terms of $\delta$ will be exchanged, which has been excluded by experiments. If we let $t^0 = 0$, then $\Delta_d = \Delta_{es}$ which has the maximum value at doping $\delta = 0.5$. This may correspond to the symmetry limit of Zhang's SO(5) theory, although generally the pairing wave functions determined here do not form a rigorous global SO(5) group structure. The results are plotted in Fig. 1.

Further applications to the description of dynamical and thermal properties of quasiparticles and collective excitations measured in cuprate superconductors are in progress.

References