Antiferromagnetic exchange and spin-fluctuation pairing in cuprate superconductors

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A microscopic theory of superconductivity is formulated within an effective p-d Hubbard model for a CuO$_2$ plane. By applying the Mori-type projection technique, the Dyson equation is derived for the Green functions in terms of Hubbard operators. The antiferromagnetic exchange caused by interband hopping results in pairing of all carriers in the conduction subband and high $T_c$ proportional to the Fermi energy. Kinematic interaction in intraband hopping is responsible for the conventional spin-fluctuation pairing. Numerical solution of the gap equation proves the d-wave gap symmetry and defines $T_c$ doping dependence. Oxygen isotope shift and pressure dependence of $T_c$ are also discussed.

I. INTRODUCTION

A unique property of cuprates is the huge antiferromagnetic (AFM) superexchange interaction $J \simeq 1500$ K which causes a long-range AFM order in the undoped regime, while in the metallic state results in strong AFM dynamical spin fluctuations. These are responsible for anomalous normal state properties of cuprates and for superconducting pairing as originally proposed by P.W. Anderson$^1$. In a number of studies of the reduced one-band t-J model (see, e.g.$^{2,3}$ and references therein) it was shown that the AFM exchange interaction results in d-wave pairing with high $T_c$. However, to assess the origin of the AFM pairing mechanism one has to consider the original two-band p-d model for CuO$_2$ plane without reducing it to an effective t-J model with instantaneous exchange interaction in one subband by projecting out the intersubband hopping. In fact, this transformation is used in derivation of the BCS model with an instantaneous electron interaction by projecting out electron-phonon coupling in the original electron-ion model.

In this paper a microscopic theory of superconductivity within the effective p-d Hubbard model is presented. By applying a projection technique for the matrix Green function in terms of Hubbard operators the Dyson equation is derived$^4$. It is found that the mean-field solution results in d-wave superconducting pairing mediated by the exchange interaction due to interband hopping, similar to the t-J model. The self-energy caused by the kinematic interaction in the intraband hopping is calculated in the non-crossing approximation. It defines the conventional spin-fluctuation pairing. Numerical solution of the gap equation gives the doping dependence of superconducting $T_c$ and wave-vector dependence of the gap which are in agreement with experiments$^4$. $T_c$ increase under pressure and oxygen isotope effect in cuprates are also discussed$^3$.

II. DYSON EQUATION

Starting from the original two-band p-d model for CuO$_2$ plane we can reduce it to an effective two-band Hubbard model by applying the cell-cluster perturbation theory (see, e.g.$^5$):

$$
H = E_1 \sum_{i,\sigma} X_i^{1\sigma} + E_2 \sum_i X_i^{22} + \sum_{i,j,\sigma,\bar{\sigma}} \{t_{ij}^{11} X_i^{1\sigma} X_j^{0\bar{\sigma}} + t_{ij}^{22} X_i^{2\sigma} X_j^{2\bar{\sigma}} + 2 \sigma t_{ij}^{12} (X_i^{2\sigma} X_j^{0\bar{\sigma}} + H.c.) \},
$$

where $X_i^{nm} = |in\rangle \langle im|$ are Hubbard operators for four states $n, m = |\sigma\rangle, |\bar{\sigma}\rangle = |\uparrow\downarrow\rangle$, $\sigma = \pm 1/2$, $\bar{\sigma} = -\sigma$. $E_1 = \epsilon_d - \mu$ and $E_2 = 2E_1 + \Delta$ are energy levels of the lower Hubbard subband (one-hole Cu d-like states) and the upper Hubbard subband (two-hole p-d singlet states), respectively. $\mu$ is the chemical potential, $\Delta = \epsilon_p - \epsilon_d \sim 3$ eV is the charge transfer energy and $t \sim \Delta/2$ is the p-d hybridization parameter. The hopping integrals $|t_{ij}^{12}| \ll |\Delta|$, e.g. $t_{ij}^{22} = t_{nn} \simeq 0.14t \sim 0.2$ eV, which means that the Hubbard model (1) corresponds to a strong correlation limit. We treat it within the Hubbard operator technique to preserve rigorously a constraint of no double occupancy of any quantum state $|in\rangle$ which follows from the completeness relation: $X_i^{00} + X_i^{1\sigma} + X_i^{0\bar{\sigma}} + X_i^{22} = 1$.

To discuss the superconducting pairing we introduce the four-component Nambu operators $\tilde{X}_{i\sigma}$ and $\tilde{X}^\dagger_{i\sigma}$ and define the $4 \times 4$ matrix Green function (GF)$^6$:

$$
\tilde{G}_{ij\sigma}(t-t') = \langle \langle \tilde{X}_{i\sigma}(t) | \tilde{X}_{j\sigma}(t') \rangle \rangle,
$$

$$
\tilde{G}_{ij\sigma}(\omega) = \begin{pmatrix}
\tilde{F}_{ij\sigma}(\omega) & \tilde{G}_{ij\sigma}(\omega) \\
\tilde{G}_{ji\bar{\sigma}}(\omega) & -\tilde{G}_{ji\bar{\sigma}}(-\omega)
\end{pmatrix},
$$

where $\tilde{X}_{i\sigma} = (X_i^{2\sigma} X_i^{0\bar{\sigma}} X_i^{2\bar{\sigma}} X_i^{0\sigma})$. $\tilde{G}_{ij\sigma}$ and $\tilde{F}_{ij\sigma}$ are the two-subband normal and anomalous matrix components, respectively. By applying the projection technique for the equation of motion method for GF (2) we derive the Dyson equation in the $(q, \omega)$-representation$^7$: 

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\[
\left( \tilde{G}_\sigma(q, \omega) \right)^{-1} = \left( \tilde{G}^0_\sigma(q, \omega) \right)^{-1} - \tilde{\Sigma}_\sigma(q, \omega),
\]

where \( \tilde{\chi} = \langle \{ \tilde{X}_{i\sigma}, \tilde{X}_{\bar{j}\bar{\sigma}}^\dagger \} \rangle \). The zero-order GF within the generalized mean-field approximation (MFA) is defined by the frequency matrix which in the site representation reads

\[
\tilde{E}_{ij\sigma} = \tilde{A}_{ij\sigma} \tilde{\chi}^{-1}, \quad \tilde{A}_{ij\sigma} = \langle \{ [\tilde{X}_{i\sigma}, H], \tilde{X}_{\bar{j}\bar{\sigma}}^\dagger \} \rangle.
\] (4)

The self-energy operator in the Dyson equation (3) in the projection technique method is defined by a proper part (having no single zero-order GF) of the many-particle GF in the form

\[
\tilde{\Sigma}_\sigma(q, \omega) = \tilde{\chi}^{-1} \langle \{ \tilde{Z}^{(ir)}_\sigma | \tilde{Z}^{(ir)}_\sigma \rangle \rangle \chi^{-1}.
\] (5)

Here the irreducible \( Z \)-operator is given by the equation:

\[
Z^{(ir)}_\sigma = \{ [\tilde{X}_{i\sigma}, H], \tilde{X}_{\bar{j}\bar{\sigma}}^\dagger \} \text{ which follows from the orthogonality condition: } \langle \{ \tilde{Z}^{(ir)}_\sigma | \tilde{X}_{\bar{j}\bar{\sigma}}^\dagger \} \rangle = 0.
\]

The equations (3)-(5) provide an exact representation for the GF (2). Its calculation, however, requires the use of some approximation for the self-energy matrix (5) which describes finite lifetime effects (inelastic scattering of electrons on spin and charge fluctuations).

### III. MEAN-FIELD SOLUTION

In the MFA the electronic spectrum and superconducting pairing are described by the zero-order GF in Eq. (3) where the frequency matrix (4) reads:

\[
\tilde{A}_{ij\sigma} = \begin{pmatrix} \tilde{\omega}_{ij\sigma} & \tilde{\Delta}_{ij\sigma} \\ \tilde{\Delta}_{i\sigma}^* & -\tilde{\omega}_{j\bar{\sigma}} \end{pmatrix}.
\] (6)

Here \( \tilde{\omega}_{ij\sigma} \) and \( \tilde{\Delta}_{ij\sigma} \) are \( 2 \times 2 \) matrices for the normal and anomalous components, respectively. The normal component defines quasiparticle spectra of the model in the normal state which have been studied in detail in.\(^5\) The anomalous component defines the gap functions, e.g., for the singlet subband we have:

\[
\tilde{\Delta}_{ij\sigma} = -2\sigma \tilde{t}_{ij}^{12} \langle X_{ij\sigma}^{12} N_j \rangle, \quad (i \neq j)
\] (7)

where \( N_j = \sum_{\alpha} X_{i\alpha}^{\sigma\sigma} + 2 X_{ij}^{22} \) is the number operator. In terms of the Fermi operator: \( c_{i\sigma} = X_{i\sigma}^{1\sigma} + 2\sigma X_{ij}^{22} \) we can write the anomalous average as \( \langle c_{i\bar{\sigma}} c_{\bar{j} \bar{\sigma}} N_j \rangle = \langle X_{i\sigma}^{01} X_{i\bar{\sigma}}^{12} N_j \rangle = \langle X_{ij}^{02} N_j \rangle \) since other products of Hubbard operators vanish according to multiplication rules for them: \( X_{i\sigma}^{\alpha\beta} X_{i\bar{\sigma}}^{\gamma\delta} = \delta_{\alpha\gamma} \delta_{\beta\delta} X_{i\sigma}^{\beta\delta} \). Therefore, the anomalous correlation functions describe the pairing at one lattice site but in different subbands.

The same anomalous correlation functions were obtained in MFA for the original Hubbard model in Refs.\(^7\)-\(^9\). To calculate them in\(^7\),\(^9\) the Roth procedure was applied based on decoupling of operators on the same lattice site in the time-dependent correlation function: \( \langle c_{i\bar{\sigma}}(t) | c_{\bar{j} \bar{\sigma}}(t') N_j(t') \rangle \). However, the decoupling of Hubbard operators on one lattice site is not unique and therefore unreliable. The use of kinematic restrictions for the Hubbard operators\(^8\) instead of decoupling also did not produce a unique solution.

We calculated the correlation function \( \langle X_{i\sigma}^{02} N_j \rangle \) without any decoupling from the equation of motion of the corresponding commutator GF \( L_{ij}(t - t') = \langle X_{i\sigma}^{02}(t) | N_j(t') \rangle \). By neglecting exponentially small terms of the order of \( \exp(-\Delta/T) \) we obtain for the correlation function in the singlet subband \((i \neq j)^4:\)

\[
\langle X_{i\sigma}^{02} N_j \rangle = -(1/\Delta) \sum_{m \neq i, \sigma} 2\sigma \tilde{t}_{im}^{12} \langle X_{i\sigma}^{m\sigma} X_{i\bar{\sigma}}^{22} N_j \rangle
\]

\[
\simeq -(4\tilde{t}_{ij}^{12}/\Delta)2\sigma \langle X_{i\sigma}^{22} X_{j\bar{\sigma}}^{12} \rangle.
\] (8)

The approximate value is derived in the two-site approximation usually applied for the \( t-J \) model: \( X_{m\bar{j} \bar{\sigma}}^{22} = 2X_{ij}^{22} \). Therefore, the gap equation (7) in the case of hole doping reads

\[
\Delta_{ij\sigma}^{22} = -2\sigma \tilde{t}_{ij}^{12} \langle X_{ij\sigma}^{02} N_j \rangle = J_{ij} \langle X_{i\sigma}^{22} X_{j\bar{\sigma}}^{12} \rangle
\] (9)

where \( J_{ij} = (4\tilde{t}_{ij}^{12})/\Delta \). It is the conventional exchange interaction pairing in the \( t-J \) model. For electron doping analogous calculations for the anomalous correlation function \( \langle 2 - N_j X_{ij}^{02} \rangle \) gives for the gap function \( \Delta_{ij\sigma}^{11} = J_{ij} \langle X_{i\sigma}^{02} X_{j\bar{\sigma}}^{12} \rangle \).

We conclude that the anomalous contributions to the zero-order GF, Eq. (3), are described by conventional pairs of quasi-particles in one subband and there are no new composite operator excitations, the "cexons", proposed in\(^9\).

### IV. SELF-ENERGY

The self-energy matrix (5) can be written in the form

\[
\tilde{\Sigma}_{ij\sigma}(\omega) = \tilde{\chi}^{-1} \begin{pmatrix} \tilde{M}_{ij\sigma}(\omega) & \tilde{\Phi}_{ij\sigma}(\omega) \\ \tilde{\Phi}^{\dagger}_{j\bar{\sigma}}(\omega) & -\tilde{M}_{j\bar{\sigma}}(\omega) \end{pmatrix} \tilde{\chi}^{-1},
\] (10)

where the \( 2 \times 2 \) matrices \( \tilde{M} \) and \( \tilde{\Phi} \) denote the normal and anomalous contributions to the self-energy, respectively. We calculate them in the non-crossing, or the self-consistent Born approximation (SCBA). In SCBA, Fermi-like and Bose-like excitations in the many-particle GF in (10) are assumed to propagate independently which is given by the decoupling of the corresponding time-dependent correlation functions as follows:

\[
\langle B_\sigma(t) X_\sigma(t') \rangle \simeq \langle X_\sigma(t) X_\sigma(t') \rangle (1 \neq \sigma \neq 2) \nonumber
\]

\[
\simeq \langle X_\sigma(t) X_\sigma(t') \rangle (B_\sigma(t) B_\sigma(t')).
\] (11)
results in pairing of all charge carriers in the conduction subband:
\[ T_c \simeq \sqrt{\mu(W - \mu)} \exp(-1/\lambda_{ex}), \]
where \( \lambda_{ex} \simeq JN(\mu) \), \( N(\mu) \) is the density of electronic states. For spin-fluctuation pairing we obtain a conventional BCS-like formula for \( T_c \):
\[ T_c \simeq \omega_s \exp(-1/\lambda_{sf}), \]
where \( \lambda_{sf} \simeq \lambda_s N(\mu) \).
By taking into account both contributions, a result similar to (16) is obtained, with an effective coupling constant: \( \lambda^{(eff)}_{sf} = \lambda_{sf} + \lambda_{ex}/[1 - \lambda_{ex}\mu(\mu/\omega_s)] \). By taking for estimate \( \mu = W/2 \simeq 0.35 \text{ eV} \), \( \omega_s \simeq J \simeq 0.13 \text{ eV} \) and \( \lambda_{sf} \simeq \lambda_{ex} \simeq 0.2 \) we get \( \lambda^{(eff)}_{sf} \simeq 0.2 + 0.25 = 0.45 \) and \( T_c \simeq 160 \text{ K} \), while the spin-fluctuation pairing alone gives \( T_c^0 \simeq \omega_s \exp(-1/\lambda_{sf}) \simeq 10 \text{ K} \).

A direct numerical solution of the gap equation (13) in\textsuperscript{4} proved the d-wave symmetry of the gap and gave the maximum \( T_c \sim 0.12t_{nn} \) for \( \mu \sim W/2 \) at an optimal doping \( \delta_{opt} \simeq 0.12 \). The spin-fluctuation interaction produces much lower \( T_c \) since it couples the holes in a narrow energy shell, \( \omega_s \ll \mu \), near the FS. Moreover, it vanishes along the lines \( |k_x| + |k_y| = \pi \) where \( \gamma(k) = 0 \).

While in electron-phonon superconductors \( T_c \) decreases under pressure, in cuprates it increases. In particular, in mercury superconductors \( dT_c/da \simeq -1.35 \times 10^3 \text{ K/A}^{10} \) (\( a \) is the in-plane lattice constant) and \( d\ln T_c/d\ln a \sim -50 \). From Eq. (15) we get an estimate:
\[ \frac{d\ln T_c}{d\ln a} = \frac{d\ln T_c}{d\ln J} \frac{d\ln J}{d\ln a} \sim -\frac{14}{\lambda} \sim -45, \]
for \( \lambda_{ex} \simeq 0.3 \), which is quite close to the experimentally observed one. Here we take into account that \( J(a) \propto t_{pd}^4 \) and \( t_{pd}(a) \propto 1/(a)^{7/2} \).

To explain a small oxygen isotope effect in cuprates, \( \alpha_c = -d\ln T_c/\ln M \leq 0.1 \), we can use Eq. (15). By taking into account the experimentally observed isotope shift for the Néel temperature in La\textsubscript{2}CuO\textsubscript{4}\textsuperscript{11}, \( \alpha_N = -d\ln T_N/\ln M \simeq 0.05 \) with \( T_N \sim J \) we get
\[ \alpha_c = -d\ln T_c/\ln M = -d\ln T_c/d\ln M \sim 0.16, \]
for \( \lambda \simeq 0.3 \) which is close to experiments.

To conclude, the present investigation proves the existence of a singlet \( d_{x^2-y^2} \)-wave superconducting pairing for holes or electrons in the \( p-d \) Hubbard model. It is mediated by the exchange interaction and antiferromagnetic spin-fluctuation scattering induced by the kinematic interaction, characteristic to the Hubbard model. These mechanisms of superconducting pairing are absent in the fermionic models (for a discussion, see Anderson\textsuperscript{12}) and are specific for cuprates.
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