Kinematical spin-fluctuation pairing in cuprates

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We propose a microscopic theory of superconductivity for systems with strong electron correlations such as cuprates in the framework of the extended Hubbard model where the inter-site Coulomb repulsion and electron-phonon interaction are taken into account. The Dyson equation for the normal and pair Green functions for the Hubbard operators (HOs) is derived. Due to the unconventional commutation relations for the HOs, a specific kinematical interaction of electrons with spin and charge fluctuations with a large coupling constant of a specific kinematical interaction of electrons with spin emerges that results in the $d$-wave pairing with high-$T_c$. Superconductivity can be suppressed only for a large inter-site Coulomb repulsion $V \gtrsim W$. Isotope effect on $T_c$ caused by electron-phonon interaction is weak at optimal doping and increases at low doping. The kinematical interaction is absent in the spin-fermion models and is lost in the slave-boson (-fermion) models treated in the mean-field approximation.

INTRODUCTION

To explain unconventional properties of cuprates one should take into account that cuprates are the Mott-Hubbard (more accurately, charge-transfer) doped insulators which cannot be described within the conventional band theory (for a review see, e.g., [1]). Under doping, a two-subband strongly-correlated metal emerges where the Fermi-liquid model fails to describe electronic excitations. The projected-type (Hubbard) operators referring to the two subbands must be introduced. A new energy scale of the order of the kinetic energy of electrons $W$ arises in the intraband hopping induced by the kinematical interaction for the HOs which is much larger than the antiferromagnetic exchange interaction $J$ induced by the interband hopping proposed by Anderson [2]. As shown in recent experiments [3, 4], short-range antiferromagnetic (AF) dynamical spin fluctuations survive in superconducting state even in the overdoped compounds. This justifies the spin-fluctuation mechanism of superconductivity proposed earlier within spin-fermion models (see, e.g., Refs. [3, 5]). We consider the spin-fluctuation mechanism of pairing induced by the kinematical interaction where the coupling constant is given by hopping parameters.

KINEMATICAL INTERACTION IN THE HUBBARD MODEL

To describe electronic systems with strong correlations the Hubbard model is commonly used [6]. We consider the extended Hubbard model on a square lattice

$$H = \sum_{i \neq j, \sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \frac{U}{2} \sum_i N_{i\sigma} N_{i\bar{\sigma}} + H_{c, ep}, \quad (1)$$

where $a_{i\sigma}^\dagger$ and $a_{i\sigma}$ are the Fermi creation and annihilation operators for electrons with spin $\sigma$ (\(\sigma = \pm 1\)) on the lattice site $i$, and $N_i = \sum_\sigma N_{i\sigma} = \sum_\sigma a_{i\sigma}^\dagger a_{i\sigma}$ is the number operator. $t_{ij}$ is the electron hopping parameters (the nearest-neighbor hopping parameter $t = 0.4$ eV is used as the energy unit). The on-site Coulomb interaction (CI) is $U$. The intersite CI $V_{ij}$ and electron-phonon interaction (EPI) $g_{ij}$ are defined by the Hamiltonian:

$$H_{c, ep} = \frac{1}{2} \sum_{i \neq j} V_{ij} N_i N_j + \sum_{i, j} g_{ij} N_i u_j, \quad (2)$$

where $u_j$ are atomic displacements in particular phonon modes. In the strong correlation limit, $U \gg t$, the projected electron operators referring to the single and double occupied subbands, the HOs, should be introduced [10]:

$$a_{i\sigma} = a_{i\sigma}^\dagger (1 - N_{i\bar{\sigma}}) + a_{i\sigma}^\dagger N_{i\bar{\sigma}} \equiv X_i^{\sigma 0} + X_i^{2\sigma}.$$

In terms of the HOs the model (1) reads

$$H = \varepsilon_1 \sum_i X_i^{\sigma \sigma} + \varepsilon_2 \sum_i X_i^{22} + \sum_{i \neq j, \sigma} t_{ij} \{X_i^{\sigma 0} X_j^{\sigma 0} + X_i^{2\sigma} X_j^{2\sigma} + \sigma (X_i^{2\sigma} X_j^{\sigma 2} + H.c.)\} + H_{c, ep}, \quad (3)$$

where $\varepsilon_1 = -\mu$ is the single-particle energy, $\varepsilon_2 = U - 2 \mu$ is the two-particle energy, and $\mu$ is the chemical potential. The HO $X_i^{\alpha \beta} = \langle i | \alpha \rangle \langle i | \beta \rangle$ describes transition from the state $| i, \beta \rangle$ to the state $| i, \alpha \rangle$ on the lattice site $i$ where $(\alpha, \beta)$ refer to four possible states: an empty state $(\alpha, \beta = 0)$, a singly occupied state $(\alpha, \beta = \sigma)$, and a doubly occupied state $(\alpha, \beta = 2)$. The number operator and the spin operators in terms of the HOs are defined as

$$N_i = \sum_\sigma X_i^{\sigma \sigma} + 2 X_i^{22}, \quad (4)$$

$$S_i^z = X_i^{\sigma \bar{\sigma}}, \quad S_i^z = \langle \sigma / 2 | [X_i^{\sigma \sigma} - X_i^{\bar{\sigma} \bar{\sigma}}] \rangle. \quad (5)$$
The HOs obey the completeness relation $X_i^{00} + \sum_\alpha X_i^{\alpha\alpha} + X_i^{22} = 1$, which rigorously preserves the constraint that at any lattice site $i$ only one quantum state $\alpha$ can be occupied. From the multiplication rule for the HOs $X_i^{\alpha\beta} X_i^{\gamma\delta} = \delta_{\beta\gamma} X_i^{\alpha\delta}$ follows their commutation relations

$$[X_i^{\alpha\beta}, X_j^{\gamma\delta}]_{\pm} = \delta_{ij} \left( \delta_{\beta\gamma} X_i^{\alpha\delta} \mp \delta_{\alpha\delta} X_i^{\gamma\beta} \right),$$

with the upper sign for the Fermi-type operators (such as $X_i^{\alpha\beta}$) and the lower sign for the Bose-type operators (such as the number $\downarrow$ or spin $\uparrow$ operators).

The unconventional commutation relations $\downarrow$ for HOs result in the so-called *kinematical* interaction introduced by Dyson in a general theory of spin-wave interactions [11]. To demonstrate the role of the kinematical interaction in the model [3] let us consider an equation of motion for the HO $X_i^{\alpha\beta}$:

$$i \frac{d}{dt} X_i^{\alpha\beta} = [X_i^{\alpha\beta}, H] = (U - \mu) X_i^{\alpha\beta} + [X_i^{\alpha\beta}, H_{c,\text{ep}}] + \sum_{i', \sigma'} t_{i\sigma'} \left( B_{i\sigma\sigma'}^{22} X_i^{\sigma'\sigma} - \sigma B_{i\sigma\sigma'}^{21} X_i^{\alpha\sigma'} \right) + \sum_{i, \sigma} t_{i\sigma} X_i^{\alpha\sigma} + \sigma X_i^{\alpha\sigma},$$

(7)

where the Bose-type operators are introduced

$$B_{i\sigma\sigma'}^{22} = (X_i^{\sigma\sigma'} + X_i^{\sigma\sigma}) \delta_{\sigma\sigma'} + X_i^{\sigma\sigma} \delta_{\sigma\sigma'},$$

$$B_{i\sigma\sigma'}^{21} = (N_i/2 + \sigma S_i^z) \delta_{\sigma\sigma'} + S_i^z \delta_{\sigma\sigma'},$$

(8)

We see that the hopping amplitudes depend on number and spin operators caused by the kinematical interaction. In phenomenological spin-fermion models a dynamical coupling of electrons with spin fluctuations is specified by fitting parameters (see, e.g., [3, 8]), while in Eq. 7 the interaction is determined by the hopping energy $t_{ij}$ fixed by the electronic dispersion.

**GENERAL FORMULATION**

We consider superconducting pairing in the Hubbard model [3] in the hole doping region. In this case the chemical potential $\mu$ is situated in the two-hole upper Hubbard subband and is determined by the equation for the average number of holes, $n = 1 + \delta = (N_i) \geq 1$.

To study the electronic spectrum and superconductivity in the model we introduce the two-time anticommutator Green function (GF) [12] expressed in terms of the four-component Nambu operators, $\hat{X}_{i\sigma}$ and $\hat{X}_i^{\dagger \sigma} = (X_i^{2\sigma} X_i^{\sigma\sigma} X_i^{\sigma2} X_i^{\sigma\sigma})$ for two subbands:

$$G_{ij\sigma}(t - t') = \langle \langle \hat{X}_{i\sigma}(t) | \hat{X}_{j\sigma}^{\dagger}(t') \rangle \rangle.$$

(10)

To calculate the GF we use the equation of motion method by differentiating the GF with respect to time $t$ and $t'$. Using the projection operator method [13] we derive the Dyson equation for the GF:

$$G_{\sigma}(k, \omega) = [\omega \tau_0 - E_\sigma(k) - Q \Sigma_{\sigma}(k, \omega)]^{-1} Q,$$

(11)

where $\tau_0$ is the $4 \times 4$ unit matrix and $Q = \langle \langle \{\hat{X}_{i\sigma}, \hat{X}_{i\sigma}^{\dagger}\} \rangle \rangle$. The electron excitation spectrum in the generalized mean-field approximation (GMFA) is determined by the time-independent matrix of correlation functions:

$$E_\sigma(k) = \frac{1}{N} \sum_\lambda e^{i\mathbf{k} \cdot \mathbf{r}_\lambda} \langle \langle \{\hat{X}_{i\sigma}, H\}, \hat{X}_{i\sigma}^{\dagger} \rangle \rangle Q^{-1}.$$

(12)

The self-energy operator is given by the multiparticle GF,

$$Q \Sigma_{\sigma}(k, \omega) = \langle \langle \hat{Z}_{k\sigma}^{(ir)} \hat{Z}_{k\sigma}^{(ir)} \rangle \rangle_{\omega} Q^{-1},$$

(13)

The irreducible operators $\hat{Z}_{k\sigma}^{(ir)} = \langle \hat{X}_{i\sigma}, H \rangle - \sum \hat{E}_{i\sigma} \hat{X}_{i\sigma}$ is determined by the equation $\langle \langle \{\hat{Z}_{k\sigma}^{(ir)}, \hat{X}_{i\sigma}^{\dagger} \} \rangle \rangle_\omega = 0$.

To calculate the self-energy matrix [13] we use the self-consistent Born approximation (SCBA) for the corresponding time-dependent multiparticle correlation functions. Assuming an independent propagation of Fermi-type excitations $X_i^{\sigma\sigma}$ and Bose-type excitations $B_{i\sigma\sigma'}$ on different lattice sites we write the time-dependent multiparticle correlation functions as a product of fermionic and bosonic correlation functions:

$$\langle \langle X_{m\sigma'}^{2\sigma'} B_{j\sigma\sigma'}(t) X_{i\sigma}(t) \rangle \rangle_{\omega \neq \omega_j, i \neq j}$$

$$= \langle \langle X_{m\sigma'}^{2\sigma'}(t) \rangle \rangle \langle \langle B_{j\sigma\sigma'}(t) \rangle \rangle_{\omega \neq \omega_j, i \neq j}$$

(14)

The time-dependent single-particle correlation functions are calculated self-consistently using the corresponding GFs. This approximation results in a self-consistent system of equations for the self-energy [13] and the GF [11].

The GFs for two subbands $1(2)$ in the normal state in the imaginary frequency representation can be written as

$$\{G_{1(2)}(k, \omega_n)\}^{-1} = i \omega_n - \varepsilon_{1(2)}(k) - \Sigma(k, \omega_n),$$

(15)

where $\varepsilon_{1(2)}(k)$ are the quasiparticle energy [12] in GMFA. The self-energy for the two subbands can be approximated by the same function:

$$\Sigma(k, \omega_n) = -\frac{T}{N} \sum_m \sum_\alpha \lambda^{(+)}(\mathbf{q}, \mathbf{k}, \mathbf{q} - \mathbf{k} \mid \omega_n - \omega_m)$$

$$\times \left( G_1(\mathbf{q}, \omega_n) + G_2(\mathbf{q}, \omega_m) \right)$$

$$\equiv i \omega_n \left[ 1 - Z_k(\omega_n) \right] + X_k(\omega_n).$$

(16)

In Fig. 1 we show the doping dependence of $Z(\mathbf{q}) = Z_0(0)$ which weakly depends on $\delta$ in the underdoped case for $\delta \lesssim 0.15$ but sharply decreases in the overdoped region.
GAP EQUATION AND $T_c$

Using the equation for the anomalous (pair) GF we derive equation for the superconducting gap function \([14]\). In the linear approximation, for the gap in the two-hole subband $\varphi_k(\omega) = \sigma \varphi_{2,\sigma}(k, \omega)$ we obtain the equation

$$\varphi(k, \omega_n) = \frac{T_e}{N} \sum_{q,m} \frac{(1 - b(q))^2 \varphi(q, \omega_m)}{[\omega_m Z_q(\omega_m)]^2 + [\varepsilon_2(q) + X_q(\omega_m)]^2}$$

$$\times \{ J(k - q) - V(k - q) + \lambda(\omega)(q, k - q | \omega_n - \omega_m) \}, \quad (17)$$

where $b(q)$ takes into account the hybridization effects of the two Hubbard subbands. $J(q)$ and $V(q)$ are the exchange interaction and the inertsite CI. The frequency-dependent interaction is given by the function

$$\lambda^{(\pm)}(q, k | \nu_n) = \mp t(q)^2 \chi_{sf}(k, \nu_n)$$

$$\mp [V(k)^2 \chi_{cf}(k, \nu_n) + |g(q)|^2 \chi_{ph}(k, \nu_n)], \quad (18)$$

where $t(q)$ is the Fourier component of the hopping parameter $t_{ij}$. The spectral density of spin ($sf$), charge ($cf$) fluctuations and phonons ($ph$) are given in terms of the dynamical susceptibility by the relations \([12]\):

$$\chi_{sf}(q, \omega) = -\langle S_q S_{-q} \rangle / \omega, \quad \chi_{cf}(q, \omega) = -\langle \delta N_q \delta N_{-q} \rangle / \omega,$$

and $\chi_{ph}(q, \omega) = -\langle u_q u_{-q} \rangle / \omega$.

For comparison of various contributions to the pairing we consider the gap equation close to the Fermi energy, $\varphi(k) = \varphi(k, \omega = 0)$. In this case instead of the dynamical susceptibility the static susceptibility $\chi(q) = \text{Re} \chi(q, \omega = 0)$ appears in the gap equation:

$$\varphi(k) = \frac{T_e}{N} \sum_q \frac{(1 - b(q))^2 \varphi(q)}{[Z(q)]^2 2\varepsilon(q) \tanh \frac{\varepsilon(q)}{2T_e}}$$

$$\times \{ J(q - k) - V(q - k) + |V(q - k)|^2 \chi_{cf}(q - k)$$

$$+ |g(q - k)|^2 \chi_{ph}(k - q, \theta(\omega_0 - \varepsilon(q)))$$

$$- |t(q)|^2 \chi_{sf}(k - q, \theta(\omega_s - \varepsilon(q))) \}, \quad (19)$$

where $\varepsilon(q) = \varepsilon_2(q)/Z(q)$ is the renormalized energy. Here $\omega_0 = 0.1t$ and $\omega_s = J = 0.4t$ are the cutoff energies for phonon and spin-fluctuation excitations. Note, that in cuprates $J(q) \lesssim V(q)$ and therefore the AF exchange interaction $J(q)$ cannot provide superconducting pairing proposed by Anderson \([2]\).

To solve Eq. \(19\) we should introduce models for static susceptibilities. The spin susceptibility is determined by the function

$$\chi_{sf}(k) = \frac{\chi_0}{1 + \varepsilon^2 (1 + \gamma(k))}, \quad (20)$$

where $\gamma(k) = (1/2)(\cos k_x + \cos k_y)$ and $\xi$ is the AF correlation length. The strength of the spin-fluctuation interaction is given by the susceptibility at the AF wave vector $Q = (\pi, \pi)$, $\chi_Q = \chi_{sf}(Q)$, which is fixed by the normalization condition $\langle S_Q^2 \rangle = (3/4)(1 - \delta)$:

$$\chi_Q = \frac{3(1 - \delta)}{2 \omega_s} \left\{ \frac{1}{N} \sum_q \frac{1}{\varepsilon_2(q)} \right\}^{-1} \quad (21)$$

For the EPI we adopt a model with strong forward scattering proposed in Ref. \([13]\). The static interaction in the model is determined by:

$$g_{ep}(k) = |g(k)|^2 \chi_{ph}(k) = g_{ep} \frac{\xi_{ch}^2}{1 + \xi_{ch}^2 k^{-2}}, \quad (22)$$

where the doping dependent parameter $\xi_{ch} = 1/(2\delta)$ determines the radius of a “correlation hole”.

To estimate various contributions in the gap equation \([19]\) we consider the $d$-wave model gap, $\varphi(k) = (\Delta/2)(\cos k_x - \cos k_y)$. At first we consider solution of the gap equation \([19]\) for $T_c$ in the weak coupling approximation (WCA), $Z(q) = 1$. As shown in Fig. 2, the largest contribution comes from the spin-fluctuation pairing induced by the kinematical interaction which is given by the averaged over the Fermi surface constant $g_{sf} = \langle |t(q)|^2 \chi_{sf}(k - q) \rangle_{FS} \approx 4t \approx 2$ eV. Charge fluctuations and EPI contributions appear to be small since only the angular momentum $l = 2$ of these interactions give contributions to the $d$-wave pairing \([14]\).
In the strong coupling approximation (SCA) in Eq. (17) values of $T_c$ are reduced by an order of magnitude as shown in Fig. 3 in comparison with the WCA in Fig. 2 due to large values of renormalization parameter $Z(q)$ in Fig. 1. $T_c$ dependence on the nearest neighbor intersite CI $V$ in Fig. 3 reveals that the d-wave pairing does not exceed the kinematical interaction of the order of the kinetic energy, $V \lesssim 4t$.

To study the isotope effect on $T_c$ within the gap equation (19) we consider the mass-dependent phonon frequency $\omega_0 = \omega_0(0) \sqrt{M_0/(M_0 + \Delta M)} = \omega_0(0)(1 - \beta)$. We neglect the polaronic effect for the d-wave electron-phonon coupling constant $g_{ep}$ (for discussion see Ref. [19]). The result of numerical solution of the gap equation (19) for the oxygen isotope exponent (β = 1/16) $\alpha = -d \log T_c/d \log M$ is shown in Fig. 4 for two values of EPI $g_{ep} = 5t$ and $g_{ep} = 2.5t$ in Eq. (22). In accordance with an analytical estimation, $\alpha = (1/2)g_{ep}/(g_{ep} + g_{sf})$, $\alpha$ increases for larger values of $g_{ep}$. The doping dependence of the exponent agrees with experiments (see, e.g., [18]): it is quite small, $\alpha = 0.09 - 0.18$, close to the optimal doping while drastically increases in the underdoped case at $\delta < 0.1$, $\alpha = 0.38 - 0.68$ for $g_{ep} = 2.5t - 5t$, respectively. Similar results were obtained in Ref. [19] within the $t$-$J$ model with EPI.

To summarize, we have shown that in the limit of strong correlations a new coupling parameter, of the order of the kinetic energy of electrons, appears in the two-subband regime for the Hubbard model and brings about d-wave superconductivity with high-$T_c$. This kinematical interaction is lost in the spin-fermion models and the slave-boson (fermion) models treated in MFA.

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