«ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА»
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UNCONVENTIONAL SUPERCONDUCTORS

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The problem of electronic spectrum and superconductivity in strongly correlated electronic liquids is discussed. A microscopical theory within the framework of the t-J model is considered. Constraint of no double occupancy for electron hopping results in the kinematical interaction that induces strong electron-electron coupling by spin and charge fluctuations. Rigorous treatment of the constraints is achieved by applying the Hubbard operator technique within the Green's function method of Bogoliubov.

1. INTRODUCTION

In developing a theory of superconductivity it is necessary to solve two problems which are of foremost importance and which are definitely interrelated: namely, what is the nature of the normal state for the electrons in the metal and what is the mechanism of the formation of the superconducting phase? While in conventional superconductors the picture of the Fermi liquid with a properly determined spectrum of quasiparticles (QP) near the Fermi surface is well established, in recently discovered unconventional metals, as heavy-fermion compounds and copper oxides we have many experimental evidences for anomalous behavior of low-energy electronic excitation spectra. These materials can be called marginal electronic liquids where strong electron correlations play an important role and the conventional Fermi-liquid description in terms of single-particle excitations may be violated. Therefore, the Bardeen–Cooper–Schrieffer (BCS) theory of pairing which works perfectly well for the system of weakly bounded QP in conventional metals, can be questioned for the system of electrons with strong Coulomb correlations.

In the present report we discuss the problem of high-temperature superconductivity in copper oxides. In spite of an unprecedented scientific activity we are still far from the solution of the problem and there is no consensus on theoretical explanation of unusual normal and superconducting behavior of high temperature superconductors (for a review of experiment and theory see, for example, Ref. 1). Experimental studies of high-temperature superconductors have provided strong support for a major role of strong electron correlations in copper-oxide materials as it first has been proposed by P.W. Anderson [2,3].

The simplest model allowing for the electron correlations is the one-band Hubbard model [4]:

$$H = -\sum_{ij\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where t_{ij} is an effective transfer integral and U is the Coulomb one-site energy. In the strong coupling limit, $U \gg |t_{ij}|$, we can reduce the Hubbard model (1) (or a more realistic for copper oxides p-d model [5]) to the t-J model [6]:

$$H_{t-J} = -\sum_{i,j\sigma} t_{ij} \tilde{c}^+_{i\sigma} \tilde{c}_{j\sigma} + J \sum_{\langle ij \rangle} (\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} n_i n_j). \tag{2}$$

Here the electron operators $\tilde{c}^+_{i\sigma} = c^+_{i\sigma}(1 - n_{i-\sigma})$ act in the space without double occupancy. $n_i = \sum_\sigma \tilde{c}^+_{i\sigma} \tilde{c}_{i\sigma}$ is the number operator for electrons. The second term describes spin-1/2 Heisenberg antiferromagnet (AF) with exchange energy J for the nearest neighbors which is equal to $J = 4t^2/U$ for the Hubbard model (1) or can be considered as independent parameter in the case of the p-d model. In the model two main features of a doped hole motion in copper-oxides are properly taken into account: constraints on no double occupancy for holes on lattice sites due to strong electron correlations and interaction of holes with AF spin fluctuations that brings about strong renormalization of the QP spectrum. Exclusion of doubly occupied states in electronic hopping and strong coupling of charge carriers with spin fluctuations make it difficult to apply mean field type approximations or perturbation theory.

To deal with the strong coupling limit for the Hubbard model and the t-J model a number of numerical methods for finite clusters has been developed (for reviews see [7], [8]). These studies show strong antiferromagnetic correlations which lead to the formation of the $d_{x^2-y^2}$ pairing correlations. However, the finite cluster calculations due to known limitations (finite size effects, few filling fractions, etc.) can give only restricted information. For instance, as it was shown recently by applying the constrained-path Monte Carlo method [9] to the two-dimensional Hubbard model, small lattice sizes and weak interactions show $d_{x^2-y^2}$ pairing correlations while with increasing lattice size or interaction they vanish. So to prove superconducting pairing in the strong coupling limit an analytical treatment is highly demanded.

The main problem in studies of the t-J model is the so-called kinematical interaction imposed by the projected character of electron operators acting in the subspace of singly occupied lattice sites. To take into account the constraints of no double occupancy different types of slave-boson (-fermion) technique were proposed (see [10–13] and references therein). In the mean field approximation (MFA) the local constraints are approximated by a global one, that reduces the

problem to free fermions and bosons in the mean field [10]. To treat the constraints in a systematic way, in [11, 12] a large-N expansion, with N being a number of states (orbitals) at a lattice cite, was used. In that approach the local constraints are relaxed and a weak coupling approximation is possible. By using the $1/N$ expansion, the d-wave superconducting instability induced by the exchange interaction was obtained in the t-J model close to half filling [12].

Another method is based on the Baym-Kadanoff variational technique for Green's functions in terms of the Hubbard operators [14]. The method was used in [15, 16], also in the limit of large N, to consider superconducting pairing in the t-J model. It was shown that in the lowest order of $1/N$ there is a strong compensation of different contributions to the pairing interaction and for $J = 0$ the superconducting T_c is extremely small. For a finite J the d-wave superconducting instability mediated by exchange and charge fluctuations was obtained below $T_c \simeq 0.01t$. However, in the large-N expansion the kinematical interaction is suppressed and this approach, being rigorous in the limit $N \to \infty$, is difficult to extrapolate to real spin systems with $N = 2$.

A formally rigorous method to treat the unconventional commutation relations for the projected electron operators is based on the diagram technique for the Hubbard operators [17] since in this method the local constraints are rigorously implemented by the Hubbard operator algebra. A superconducting pairing due to the kinematical interaction in the Hubbard model in the limit of strong electron correlations ($U \to \infty$) was first obtained by Zaitsev and Ivanov [18] who studied the lowest order diagrams for a two-particle vertex equation. Their approximation, being equivalent to the MFA for a superconducting order parameter, gives only the s-wave pairing. Close results were obtained for the Hubbard model in [19,20] by applying the Bogoliubov equation of motion method for the thermodynamical Green's functions. However, as was shown later [21, 22], the s-wave pairing in the limit of strong correlations violates an exact requirement of no single-site pairs and should be rejected. In [21, 22] the BCS mean field theory for the t-J model was developed within the formally exact projection technique [23] for Green's functions in terms of the Hubbard operators. It was proved that the d-wave superconducting pairing mediated by the exchange interaction is thermodynamically stable and has high $T_c \simeq 0.1\ t$ for $J \simeq 0.4\ t$.

On the basis of the diagram technique, detailed studies of spin fluctuations and superconducting pairing in the t-J model were performed by Izyumov et al. [24]. Summation of the first order diagrams for the self-energy reproduced the results of the MFA in [21, 22]. In the second order diagrams only the exchange interaction J was taken into account while the corresponding contributions due to the kinematical interaction t_{ij} were disregarded. Estimations done in the weak coupling limit for the Dyson equation revealed quite a low superconducting T_c.

In the limit of small hole concentrations, one can consider a one-hole motion on the antiferromagnetic background within the spin-polaron representation for

the t-J model [25,26]. A number of studies of this model (see, e.g., [27,28] and references therein) predicts that a doped hole dressed by antiferromagnetic spin fluctuations can propagate coherently as a spin-polaron QP even for a finite hole doping [28]. It was suggested that the same spin fluctuations could mediate a superconducting pairing of the spin-polaron QP. This problem was treated in the framework of the weak coupling BCS formalism for a phenomenological model of QP with numerically evaluated spectrum [29, 30]. A self-consistent numerical solution of the Dyson equations for spin-polarons and magnons in the t-J model has been given in [31]. A strong renormalization of the hole spectrum due to spin-fluctuations and the d- wave pairing of spin-polaron QP with maximum $T_c \simeq 0.01t$ were obtained.

However, numerical studies [32] of the 2D t-J model at moderate doping have questioned the single spin-polaron QP picture for the paramagnetic regime. To elucidate the problem, in the recent paper [33] we propose a theory of electron spectrum and superconducting pairing for the t-J model in paramagnetic state by applying the projection technique [23] for the Green's function method of Bogoliubov [34]. Below we present the main results of this approach.

2. APPLICATION OF BOGOLIUBOV GREEN'S FUNCTION

By using the Hubbard operator (HO) representation for $\tilde{a}^+_{i\sigma} = X^{\sigma 0}_i$ and $\tilde{a}_{j\sigma} = X^{0\sigma}_j$ we write the Hamiltonian of the t-J model (2) in the form:

$$H_{t-J} = -\sum_{i\neq j,\sigma} t_{ij} X^{\sigma 0}_i X^{0\sigma}_j - \mu \sum_{i\sigma} X^{\sigma\sigma}_i + \frac{1}{4}\sum_{i\neq j,\sigma} J_{ij}\left(X^{\sigma\bar{\sigma}}_i X^{\bar{\sigma}\sigma}_j - X^{\sigma\sigma}_i X^{\bar{\sigma}\bar{\sigma}}_j\right), \tag{3}$$

where $\bar{\sigma} = -\sigma$. We introduced also the chemical potential μ which can be calculated from the equation for the average number of electrons $n = \sum_\sigma \langle X^{\sigma\sigma}_i\rangle = \sum_\sigma \langle X^{\sigma 0}_i X^{0\sigma}_i\rangle$.

To discuss the superconducting pairing within the model (3) we consider the thermodynamical GF introduced by Bogoliubov and Tyablikov [34]

$$\hat{G}_{ij,\sigma}(t-t') = \langle\langle \Psi_{i\sigma}(t) | \Psi^+_{j\sigma}(t')\rangle\rangle \tag{4}$$

in terms of the Nambu operators:

$$\Psi_{i\sigma} = \begin{pmatrix} X^{0\sigma}_i \\ X^{\bar{\sigma}0}_i \end{pmatrix}, \qquad \Psi^+_{i\sigma} = \begin{pmatrix} X^{\sigma 0}_i & X^{0\bar{\sigma}}_i \end{pmatrix}. \tag{5}$$

By differentiating the GF (4) over time t we get for the Fourier component the following equation

$$\omega \hat{G}_{ij\sigma}(\omega) = \delta_{ij}\hat{Q}_\sigma + \langle\langle [\Psi_{i\sigma}, H] \mid \Psi_{j\sigma}\rangle\rangle_\omega, \tag{6}$$

where $\hat{Q_\sigma} = \begin{pmatrix} Q_\sigma & 0 \\ 0 & Q_{\bar{\sigma}} \end{pmatrix}$ with $Q_\sigma = \langle X_i^{00} + X_i^{\sigma\sigma} \rangle$. By using the completeness relation for the HO

$$X_i^{00} + \sum_\sigma X_i^{\sigma\sigma} = 1, \tag{7}$$

which rigorously preserves the constraint of no double occupancy we can write for the correlation function in a spin-singlet state $Q_\sigma = 1 - \langle X_i^{\bar{\sigma}\bar{\sigma}} \rangle = 1 - n/2 = Q$. To calculate the many-particle GF in the left-hand side of Eq. (6) we use the equation of motion for the HO:

$$\left(i\frac{d}{dt} + \mu \right) X_i^{0\sigma} = -\sum_l t_{il} B_{i\sigma\sigma'} X_l^{0\sigma'} + \frac{1}{2} \sum_l J_{il} (B_{l\sigma\sigma'} - \delta_{\sigma\sigma'}) X_i^{0\sigma'}, \tag{8}$$

where we have introduced the operator

$$B_{i\sigma\sigma'} = (X_i^{00} + X_i^{\sigma\sigma})\delta_{\sigma'\sigma} + X_i^{\bar{\sigma}\sigma}\delta_{\sigma'\bar{\sigma}} = (1 - \frac{1}{2}N_i + \sigma S_i^z)\delta_{\sigma'\sigma} + S_i^{\bar{\sigma}}\delta_{\sigma'\bar{\sigma}}. \tag{9}$$

The Bose-like operator (9) describes electron scattering on spin and charge fluctuations caused by the nonfermionic commutation relations for the HO (the first term in (8) – the kinematical interaction) and by the exchange spin-spin interaction (the second term in (8)).

By projecting out the linear part of the equation of motion (8) we introduce the zero-order GF in the generalized mean field approximation (MFA)

$$\hat{G}^0_{ij\sigma}(\omega) = Q\{\omega\hat{\tau}_0\delta_{ij} - \hat{E}_{ij\sigma}\}^{-1}, \tag{10}$$

with the frequency matrix $\hat{E}_{ij\sigma}$

$$\hat{E}_{ij\sigma} = \langle \{ [\Psi_{i\sigma}, H], \Psi^+_{j\sigma} \} \rangle \; Q^{-1} \; . \tag{11}$$

The nonlinear part of equation of motion (8) gives the irreducible GF in Eq. (6) which is essentially many-particle GF. By writing down an equation of motion for them with respect to the second time t' for the right-hand side operator $\Psi^+_{j\sigma}(t')$ and performing the same projection procedure we can obtain the Dyson equation for the GF (4) in the form (see [33]):

$$\hat{G}_{ij\sigma}(\omega) = \hat{G}^0_{ij\sigma}(\omega) + \sum_{kl} \hat{G}^0_{ik\sigma}(\omega) \; \hat{\Sigma}_{kl\sigma}(\omega) \; \hat{G}_{lj\sigma}(\omega), \tag{12}$$

where the self-energy operator $\hat{\Sigma}_{kj\sigma}(\omega)$ is defined by the equation

$$\hat{\Sigma}_{ij\sigma}(\omega) = Q^{-1} \langle\langle \hat{Z}^{(irr)}_{i\sigma} \mid \hat{Z}^{(irr)^+}_{j\sigma} \rangle\rangle^{(irr)}_\omega \; Q^{-1} \; , \tag{13}$$

with $\hat{Z}^{(irr)}_{i\sigma} = [\Psi_{i\sigma}, H] - \sum_l \hat{E}_{il\sigma}\Psi_{l\sigma}$, $\langle\{\hat{Z}^{(irr)}_{i\sigma}, \Psi^+_{j\sigma}\}\rangle = 0$. The self-energy operator (13) is given by the irreducible part, (irr), of the scattering matrix that has no parts connected by the single zero-order GF (10).

To calculate the self-energy operator (13) we employ the noncrossing approximation (or the self-consistent Born approximation) which is given by the two-time decoupling of the corresponding many-particle correlation functions [33]:

$$\langle X^{\sigma' 0}_{j'} B^+_{j\sigma\sigma'} X^{0\sigma'}_{i'}(t) B_{i\sigma\sigma'}(t)\rangle|_{j\neq j', i\neq i'} \simeq \langle X^{\sigma' 0}_{j'} X^{0\sigma'}_{i'}(t)\rangle\langle B^+_{j\sigma\sigma'} B_{i\sigma\sigma'}(t)\rangle \ . \quad (14)$$

Using the spectral representation for the GF, we obtain in the noncrossing approximation the following expression for the normal (diagonal) and anomalous (nondiagonal) components of the self-energy, $\tilde{\Sigma}_{\alpha\beta}(k,\omega) = Q\hat{\Sigma}_{\alpha\beta}(k,\omega)$, in the $\mathbf{k}$-space:

$$\tilde{\Sigma}^{\sigma}_{11(12)}(k,\omega) = \frac{1}{N}\sum_q \int\!\!\!\int_{-\infty}^{+\infty} dz d\Omega N(\omega, z, \Omega)\lambda_{11(12)}(q, k-q \mid \Omega) A^{\sigma}_{11(12)}(q,z), \quad (15)$$

where $N(\omega, z, \Omega) = [\tanh(z/2T) + \coth(\Omega/2T)]/2(\omega - z - \Omega)$. Here we introduce for the GF $\tilde{G}_{\alpha\beta}(k,\omega) = (1/Q)\hat{G}_{\alpha\beta}(k,\omega)$ the spectral density:

$$A^{\sigma}_{11(12)}(q,z) = -\frac{1}{\pi}\mathrm{Im}\ \tilde{G}^{\sigma}_{11(12)}(q, z + i\delta). \quad (16)$$

The electron-electron interaction functions caused by spin-charge fluctuations are given by

$$\lambda_{11(12)}(q, k-q \mid \Omega) = g^2(q, k-q)[-\frac{1}{\pi}\mathrm{Im}\ D^{+(-)}(k-q, \Omega + i\delta)], \quad (17)$$

where $g(q, k-q) = t(q) - \frac{1}{2}J(k-q)$. The spectral density for the spin-charge fluctuations is defined by the boson-like commutator GF

$$D^{\pm}(q,\Omega) = \langle\langle \mathbf{S}_q \mid \mathbf{S}_{-q}\rangle\rangle_{\Omega} \pm \frac{1}{4}\langle\langle n_q \mid n^+_q\rangle\rangle_{\Omega}, \quad (18)$$

for the spin $\mathbf{S}_q$ and number density n_q operators.

The resulting Dyson equation (12) can be written in the form

$$\tilde{G}^{\sigma}(k,\omega) = \{\omega\hat{\tau}_0 - (E^{\sigma}_k - \mu + \delta\mu)\hat{\tau}_3 - \Delta^{\sigma}_k\hat{\tau}_1 - \tilde{\Sigma}(k,\omega)\}^{-1}, \quad (19)$$

where $\hat{\tau}_0$, $\hat{\tau}_1$, $\hat{\tau}_3$ are the Pauli matrices. The energy of the quasiparticles E^{σ}_k, the renormalization of the chemical potential $\delta\mu$, and the gap function Δ^{σ}_k in the MFA are given by $\mathbf{k}$-representation of Eq.(11).

The equation for the anomalous self-energy in Eq. (15) in comparison with the diagram technique [24] has an additional contribution proportional to $t^2(q)$ due to the kinematical interaction in (17) which enhances the d-wave pairing.

By using the imaginary frequency technique a numerical study of the linearized system of the Dyson equations (19),(15) was performed in [33]. The electron spectral density Eq.(16) shows QP excitations at the FS crossing and a dispersive incoherent band. For small hole concentration the QP dispersion is small while the intensity of the incoherent band is quite large. With doping the QP band width strongly increases and the incoherent band is suppressed. The results for single-electron spectral functions are in general agreement with the studies within exact-diagonalization technique [32]. The occupation numbers $N(\mathbf{k})$ have the characteristic behavior for strongly correlated systems. Being large throughout the BZ, due to the incoherent contribution, they show only a small drop at the FS. The volume of the FS at small doping is proportional to the hole concentration δ that does not obey the Luttinger theorem. The superconducting pairing due to the exchange and the kinematic interactions (in the second order) has the d-wave symmetry and high $T_c \simeq 0.04t \simeq 200$ K. The calculations confirm the results of the d-wave superconducting pairing obtained within the spin-polaron $t-J$ model [31].

The advantage of the proposed microscopical theory of the d-wave spin-fluctuation superconducting pairing, in comparison with phenomenological approaches based on the Fermi liquid models close to AFM instability, is that we rigorously take into account local constraints of no double occupancy due to strong correlations that result in electron–spin-fluctuation interaction. Therefore in our approach we used only two basic parameters for the model, the hopping energy, t_{ij}, and the (super)exchange energy, J, which are characteristic of strongly correlated systems and no artificial parameters for electron scattering on antiferromagnetic spin-fluctuation were introduced as in phenomenological theories [35].

Generalization of the calculations for the asymmetric (p-d) Hubbard model [36] is presented in [37]. A possibility of $s+d$ mixing of the order parameter (the gap function) in orthorhombic phase is discussed in [38].

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