ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА
2010. Т. 41. ВЫП. 7

THEORY OF HIGH-TEMPERATURE SUPERCONDUCTIVITY IN CUPRATES

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A microscopic theory of electronic spectrum and superconducting pairing in the high-temperature cuprate superconductors is presented. The theory is based on consideration of strong electron correlations within the Bogoliubov polar model. The Dyson equation is derived by using the equation of motion method for the thermodynamic Green functions in terms of the Hubbard operators. The self-energy is evaluated in the noncrossing approximation for electron scattering on spin and charge fluctuations induced by kinematic interaction. The theory demonstrates that a strong Coulomb repulsion results in the anomalous electronic spectrum and unconventional (d-wave) superconducting pairing with high T_c mediated by the antiferromagnetic exchange and spin fluctuations.

PACS: 74.20.-z

INTRODUCTION

Despite intensive studies of high-temperature superconductivity (HTSC) in the cuprates for more than twenty years after its discovery by Bednorz and Müller [1], a commonly accepted mechanism of HTSC is still lacking. One of the promising mechanisms of HTSC is based on a model of strongly correlated electrons originally proposed by Anderson [2]. In the model, interaction of charge carriers with antiferromagnetic (AF) spin fluctuations induced by strong correlations is believed to be responsible for the anomalous normal state properties of the cuprates and can be the origin of the superconducting pairing. Another approach is based on consideration of spin-fluctuation pairing within phenomenological spin-fermion models (for a review see [3]).

In the present paper, a consistent microscopic theory for the electronic spectrum and superconductivity for the Bogoliubov polar model [4] is formulated. A preliminary version of the theory was proposed by Bogoliubov et al. [5] at the early times of HTSC studies. The theory is based on the solution of the Dyson equation derived for the thermodynamic Green functions (GFs) in terms of the Hubbard operators (HOs) with a self-energy evaluated in the noncrossing approximation (NCA). Below we outline the main equations of the theory. The results of numerical studies presented at the Bogoliubov Conference can be found in [6, 7].

1. MODEL AND DYSON EQUATION

We consider a simplified version of the Bogoliubov polar model [4] where only the largest term in the Coulomb interaction on one lattice site is taken into account. This model is known as the Hubbard model [8]. By considering superconductivity in cuprates only one CuO_2 plane can be taken into account which is described by an effective Hubbard model on a square lattice

$$H = \varepsilon_1 \sum_{i,\sigma} X_i^{\sigma\sigma} + \varepsilon_2 \sum_i X_i^{22} + \sum_{i\neq j,\sigma} \{ t_{ij}^{11} X_i^{\sigma 0} X_j^{0\sigma} + \\ + t_{ij}^{22} X_i^{2\sigma} X_j^{\sigma 2} + \sigma t_{ij}^{12} (X_i^{2\bar\sigma} X_j^{0\sigma} + \text{h.c.}) \}, \quad (1)$$

where $X_i^{nm} = |in\rangle\langle im|$ are the HOs for the four states for holes $n, m = |0\rangle$, $|\sigma\rangle$, $|2\rangle = |\uparrow\downarrow\rangle$, $\sigma = \pm 1 \equiv (\uparrow, \downarrow)$, $\bar\sigma = -\sigma$. Here $\varepsilon_1 = \varepsilon_d - \mu$ is the energy of the d-type one-hole state in the lower Hubbard band (LHB) and $\varepsilon_2 = 2\varepsilon_1 + U_{\text{eff}}$ is the energy of the two-hole p-d singlet state in the upper Hubbard band (UHB) for holes. The effective Coulomb energy in Eq. (1) is the charge-transfer energy $U_{\text{eff}} = \Delta_{pd} = \epsilon_p - \epsilon_d$. The parameters $t_{ij}^{\alpha\beta}$ are the hopping integrals where the superscripts 2 and 1 refer to the UHB and the LHB, respectively. The chemical potential μ depends on the average *hole* occupation number

$$n = \langle N_i \rangle, \quad N_i = \sum_\sigma X_i^{\sigma\sigma} + 2X_i^{22}. \quad (2)$$

We emphasize here that the Hubbard model (1) does not involve a dynamical coupling of electrons (holes) with fluctuations of spins or charges. This occurs due to the *kinematic* interaction caused by the unconventional commutation relations for the HOs: $[X_i^{\alpha\beta}, X_j^{\gamma\delta}]_\pm = \delta_{ij}(\delta_{\beta\gamma} X_i^{\alpha\delta} \pm \delta_{\delta\alpha} X_i^{\gamma\beta})$. For example, the equation of motion for the HO $X_i^{\sigma 2}$ has the form

$$\frac{i\,d X_i^{\sigma 2}}{dt} = [X_i^{\sigma 2}, H] = (\varepsilon_1 + U_{\text{eff}}) X_i^{\sigma 2} + \sum_{l\neq i,\sigma'} \big(t_{il}^{22} B_{i\sigma\sigma'}^{22} X_l^{\sigma' 2} - \\ - \sigma t_{il}^{21} B_{i\sigma\sigma'}^{21} X_l^{0\bar\sigma'} \big) - \sum_{l\neq i} X_i^{02} \left(t_{il}^{11} X_l^{\sigma 0} + \sigma t_{il}^{21} X_l^{2\bar\sigma} \right), \quad (3)$$

$$B_{i\sigma\sigma'}^{22} = (X_i^{22} + X_i^{\sigma\sigma})\delta_{\sigma'\sigma} + X_i^{\sigma\bar\sigma}\,\delta_{\sigma'\bar\sigma} = \left(\frac{N_i}{2} + S_i^z \right) \delta_{\sigma'\sigma} + S_i^\sigma \delta_{\sigma'\bar\sigma}, \\ B_{i\sigma\sigma'}^{21} = \left(\frac{N_i}{2} + S_i^z \right) \delta_{\sigma'\sigma} - S_i^\sigma\,\delta_{\sigma'\bar\sigma}. \quad (4)$$

Here $B_{i\sigma\sigma'}^{\alpha\beta}$ are Bose-like operators related to the particle number operator N_i in (2) and spin operators $S_i^\alpha = X_i^{\sigma\bar\sigma}$, $S_i^z = (1/2) \sum_\sigma \sigma X_i^{\sigma\sigma}$.

To consider the superconducting pairing in the model (1), we define the thermodynamic anticommutator GF [9] as the 4×4 matrix

$$\mathsf{G}_{ij\sigma}(\omega) = \langle\langle \hat{X}_{i\sigma} \mid \hat{X}^{\dagger}_{j\sigma} \rangle\rangle_{\omega} = \begin{pmatrix} \hat{G}_{ij\sigma}(\omega) & \hat{F}_{ij\sigma}(\omega) \\ \hat{F}^{\dagger}_{ij\sigma}(\omega) & -\hat{G}_{ji\bar{\sigma}}(-\omega) \end{pmatrix}, \tag{5}$$

in terms of the four-component Nambu operator $\hat{X}_{i\sigma}$ and its conjugate operator $\hat{X}^{\dagger}_{i\sigma} = (X_i^{2\sigma}\, X_i^{\bar{\sigma}0}\, X_i^{\bar{\sigma}2}\, X_i^{0\sigma})$. Here the normal $\hat{G}_{ij\sigma}$ and anomalous $\hat{F}_{ij\sigma}$ components of the GF (5) are 2×2 matrices which are coupled by the symmetry relations for the anticommutator retarded GFs [9].

By applying the equation of motion method for the GF (5), we can derive the Dyson equation which in the $(\mathbf{q}, \omega)$ representation reads [6, 10]:

$$\mathsf{G}_{\sigma}(\mathbf{q}, \omega) = (\omega\tilde{\tau}_0 - \mathsf{E}_{\sigma}(\mathbf{q}) - \Sigma_{\sigma}(\mathbf{q}, \omega))^{-1}\, \mathsf{Q}, \tag{6}$$

where $\tilde{\tau}_0$ is the unity matrix and $\mathsf{Q} = \langle\{\hat{X}_{i\sigma}, \hat{X}^{\dagger}_{i\sigma}\}\rangle = \langle \hat{X}_{i\sigma}\hat{X}^{\dagger}_{i\sigma} + \hat{X}^{\dagger}_{i\sigma}\hat{X}_{i\sigma}\rangle$. The energy $\mathsf{E}_{\sigma}(\mathbf{q})$ determines the zero-order GF $\mathsf{G}^0_{\sigma}(\mathbf{q}, \omega)$ and is found from the orthogonality condition: $\langle\{[\hat{X}_{i\sigma}, H] - \sum_l \mathsf{E}_{il\sigma}\hat{X}_{l\sigma},\, \hat{X}^{\dagger}_{j\sigma}\}\rangle = 0$. This results in the equation for the frequency matrix

$$\mathsf{E}_{ij\sigma} = \langle\{[\hat{X}_{i\sigma}, H], \hat{X}^{\dagger}_{j\sigma}\}\rangle\, \mathsf{Q}^{-1} = \begin{pmatrix} \hat{\varepsilon}_{ij\sigma} & \hat{\Delta}_{ij\sigma} \\ \hat{\Delta}^{*}_{ji\sigma} & -\hat{\varepsilon}_{ji\bar{\sigma}} \end{pmatrix}. \tag{7}$$

The self-energy operator $\Sigma_{\sigma}(\mathbf{q}, \omega)$ in (6) is defined by the *proper* part of the scattering matrix $\mathsf{T} = \Sigma + \Sigma\, \mathsf{G}^0\, \mathsf{T}$ and is given by the equation [6, 10]

$$\Sigma_{\sigma}(\mathbf{q}, \omega) = \langle\langle \hat{Z}^{(ir)}_{\mathbf{q}\sigma} \mid \hat{Z}^{(ir)\dagger}_{\mathbf{q}\sigma} \rangle\rangle^{(\mathrm{prop})}_{\omega}\, \mathsf{Q}^{-1}, \tag{8}$$

where the *irreducible* $\hat{Z}$-operator is given by the equation: $\hat{Z}^{(ir)}_{i\sigma} = [\hat{X}_{i\sigma}, H] - \sum_l \mathsf{E}_{il\sigma}\hat{X}_{l\sigma}$. Dyson equations (6)–(8) give an exact representation for the GF (6). To obtain a closed system of equations, the multiparticle GF in self-energy operator (8) should be calculated. This GF describes processes of inelastic scattering of electrons (holes) on charge and spin fluctuations due to kinematic interaction as demonstrated by Eq. (3).

2. SYSTEM OF SELF-CONSISTENT EQUATIONS

Using the commutation relations for the HOs, we evaluate the frequency matrix (7). For the normal component $\hat{\varepsilon}_{ij\sigma}$ in the $\mathbf{k}$ space we obtain [7]

$$\begin{aligned} \varepsilon_{1,2}(\mathbf{k}) &= \frac{1}{2}[\omega_2(\mathbf{k}) + \omega_1(\mathbf{k})] \mp \frac{1}{2}\Lambda(\mathbf{k}), \\ \Lambda(\mathbf{k}) &= \{[\omega_2(\mathbf{k}) - \omega_1(\mathbf{k})]^2 + 4W(\mathbf{k})^2\}^{1/2}, \end{aligned} \tag{9}$$

where $\omega_1(\mathbf{k}) = 4t\alpha_1\gamma(\mathbf{k}) + 4t'\beta_1\gamma'(\mathbf{k}) - \mu$, $\omega_2(\mathbf{k}) = 4t\alpha_2\gamma(\mathbf{k}) + 4t'\beta_2\gamma'(\mathbf{k}) + U_{\rm eff} - \mu$, and $W(\mathbf{k}) = 4t\alpha_{12}\gamma(\mathbf{k}) + 4t'\beta_{12}\gamma'(\mathbf{k})$. Here t and t' are the hopping parameters for the nearest neighbors (n.n.) and the next n.n. (n.n.n), respectively, with $\gamma(\mathbf{k}) = (1/2)(\cos k_x + \cos k_y)$, $\gamma'(\mathbf{k}) = \cos k_x \cos k_y$. Because of the kinematic interaction, the spectrum is renormalized: $\alpha_{1(2)} = Q_{1(2)}[1+C_1/Q^2_{1(2)}]$, $\beta_{1(2)} = Q_{1(2)}[1 + C_2/Q^2_{1(2)}]$, $\alpha_{12} = \sqrt{Q_1Q_2}[1 - C_1/Q_1Q_2]$, $\beta_{12} = \sqrt{Q_1Q_2}[1 - C_2/Q_1Q_2]$. Here, beyond the Hubbard-I approximation given by the factors $Q_1 = (1 - n/2)$ and $Q_2 = n/2$, the renormalization caused by spin correlation functions for the n.n. $C_1 = \langle \mathbf{S}_i\mathbf{S}_{i\pm a_x/a_y}\rangle$ and the n.n.n. $C_2 = \langle \mathbf{S}_i\mathbf{S}_{i\pm a_x\pm a_y}\rangle$, respectively, are taken into account. They considerably suppress the hopping parameters for the n.n.: $\alpha_{1(2)} \ll 1$ since due to the AF correlations $C_1 < 0$ with $|C_1| = 0.1 - 0.2$.

The superconducting pairing in the Hubbard model occurs already in the mean-field approximation (MFA) which is given by the anomalous component $\hat{\Delta}_{ij\sigma}$ of the matrix (7). For the diagonal components we have [6]

$$\Delta^{22}_{ij\sigma} = -\frac{\sigma t^{12}_{ij}\langle X^{02}_i N_j\rangle}{Q_2}, \quad \Delta^{11}_{ij\sigma} = \frac{\sigma t^{12}_{ij}\langle N_j X^{02}_i\rangle}{Q_1}. \tag{10}$$

We see that the pairing occurs at a single site ($X^{02}_i = X^{0\downarrow}_i X^{\downarrow 2}_i = a_{i\downarrow}\, a_{i\uparrow}$) but in different Hubbard subbands. The anomalous averages $\langle X^{02}_i N_j\rangle$ can be calculated directly by using the equation for the pair commutator GF $L_{ij}(t-t') = \langle\langle X^{02}_i(t) \mid N_j(t')\rangle\rangle$ without *any decoupling* approximations [6]. Below we consider the hole-doped case, $n = 1 + \delta > 1$ with the Fermi level in the UHB. In this case we obtain in the two-site approximation

$$\langle X^{02}_i N_j\rangle = -\sigma \left(\frac{4t^{12}_{ij}}{U_{\rm eff}}\right) \langle X^{\sigma 2}_i X^{\bar{\sigma}2}_j\rangle, \quad \Delta^{22}_{ij\sigma} = \frac{J_{ij}\langle X^{\sigma 2}_i X^{\bar{\sigma}2}_j\rangle}{Q_2}, \tag{11}$$

where the exchange interaction $J_{ij} = 4(t^{12}_{ij})^2/U_{\rm eff}$. This equation is equivalent to the gap equation in the t-J model where the pairing is mediated by the exchange interaction (see, e.g., [11] and references therein).

The self-energy (8) is calculated in the NCA which assumes an independent propagation of the Fermi-like excitations $X_j = X^{0\sigma}_j\, (X^{\bar{\sigma}2}_j)$ and Bose-like excitations B_i (4) in the many-particle correlation functions that gives

$$\langle B_i(t)X_j(t)B_l(t')X_m(t')\rangle \simeq \langle X_j(t)X_m(t')\rangle\langle B_i(t)B_l(t')\rangle|_{(i\neq j,\, l\neq m)}. \tag{12}$$

Using the spectral representation for these correlation functions, a self-consistent system of equations for the normal component of the GF can be derived [7]

$$\begin{aligned} G^{22}_N(\mathbf{k},\omega) &= [1 - b(\mathbf{k})]G_2(\mathbf{k},\omega) + b(\mathbf{k})G_1(\mathbf{k},\omega), \\ G_{1(2)}(\mathbf{k},\omega) &= [\omega - \varepsilon_{1(2)}(\mathbf{k}) - \Sigma(\mathbf{k},\omega)]^{-1}, \end{aligned} \tag{13}$$

where the hybridization parameter $b(\mathbf{k}) = [\varepsilon_2(\mathbf{k}) - \omega_2(\mathbf{k})]/[\varepsilon_2(\mathbf{k}) - \varepsilon_1(\mathbf{k})]$. The self-energy for the GF (13) can be approximated by the equation

$$\Sigma(\mathbf{k},\omega) = \sum_{\mathbf{q}} \int\limits_{-\infty}^{+\infty} dz\, K^{(+)}(\omega, z|\mathbf{q}, \mathbf{k}-\mathbf{q}) \Big(-\frac{1}{\pi}\,\mathrm{Im}\,[G_1(\mathbf{q},z) + G_2(\mathbf{q},z)]\Big). \quad (14)$$

The gap equation for the UHB can be written as

$$\varphi_{2,\sigma}(\mathbf{k},\omega) = \sum_{\mathbf{q}} \int\limits_{-\infty}^{+\infty} dz \left[\frac{J_{\mathbf{k}-\mathbf{q}}}{2} \tanh\frac{z}{2T} + K^{(-)}(\omega, z|\mathbf{q}, \mathbf{k}-\mathbf{q})\right] \Phi_{\sigma}^{22}(\mathbf{q}, z), \quad (15)$$

where $J_{\mathbf{k}} = 4J\gamma(\mathbf{k})$ and $\Phi_{\sigma}^{22}(\mathbf{k},\omega) = (-1/\pi)\,\mathrm{Im}\,F_{\sigma}^{22}(\mathbf{k},\omega)$ is the spectral density of the anomalous GF. In the linear approximation in respect to the gap function it reads: $F_{\sigma}^{22}(\mathbf{k},\omega) = -G_N^{22}(\mathbf{k},-\omega)\varphi_{2,\sigma}(\mathbf{k},\omega)G_N^{22}(\mathbf{k},\omega)$. The kernel of the integral equations (14), (15) is given by the expression

$$K^{(\pm)}(\omega, z|\mathbf{q}, \mathbf{k}-\mathbf{q}) = |t(\mathbf{q})|^2 \int\limits_{-\infty}^{+\infty} d\Omega \frac{\tanh\dfrac{z}{2T} + \coth\dfrac{\Omega}{2T}}{2(\omega - z - \Omega)}\, \chi_{\mathrm{sc}}^{\prime\prime(\pm)}(\mathbf{k}-\mathbf{q}, \Omega), \quad (16)$$

where the interaction is determined by $t(\mathbf{q}) = 4t\gamma(\mathbf{q}) + 4t'\gamma'(\mathbf{q})$ and the dynamic spin and charge susceptibility $\chi_{\mathrm{sc}}^{\prime\prime(\pm)}(\mathbf{q},\omega) = (-1/\pi)\,\mathrm{Im}\,[\langle\langle \mathbf{S}_{\mathbf{q}} | \mathbf{S}_{-\mathbf{q}} \rangle\rangle_{\omega} \pm (1/4)\langle\langle N_{\mathbf{q}} | N_{-\mathbf{q}} \rangle\rangle_{\omega}]$ in terms of the GFs for spin $\mathbf{S}_{\mathbf{q}}$ and number $N_{\mathbf{q}}$ operators.

3. DISCUSSION

To elucidate the mechanism of HTSC in the present theory, we consider a weak-coupling approximation for the gap function (15):

$$\varphi_{2,\sigma}(\mathbf{k}) = \sum_{\mathbf{q}} [J_{\mathbf{k}-\mathbf{q}} - \lambda(\mathbf{q}, \mathbf{k}-\mathbf{q})] \frac{\varphi_{2,\sigma}(\mathbf{q})}{2E_2(\mathbf{q})} \tanh\frac{E_2(\mathbf{q})}{2T}, \quad (17)$$

where $\lambda(\mathbf{q}, \mathbf{k}-\mathbf{q}) = |t(\mathbf{q})|^2 \chi_s(\mathbf{k}-\mathbf{q}, 0)$ and $E_2(\mathbf{q}) = [\varepsilon_2(\mathbf{q})^2 + |\varphi_{2,\sigma}(\mathbf{q})|^2]^{1/2}$. We emphasize that there are essentially *two channels* of superconducting pairing. The first one is mediated by the AF exchange interaction J which lowers the electronic kinetic energy due to intersubband hopping in a lattice with short-range AF order. The retardation effects in this pairing are negligible which results in the coupling of all the charge carriers in the conduction subband W and in a T_{c} determined by the Fermi energy μ: $T_{\mathrm{c}}^{\mathrm{ex}} \simeq \sqrt{\mu(W-\mu)}\,\exp(-1/V_{\mathrm{ex}})$, where $V_{\mathrm{ex}} \simeq JN_d(\mu)$ and $N_d(\mu)$ is the density of electronic states for the d-wave pairing. This pairing mechanism has been originally proposed by Anderson [2] in his resonant-valence-bond (RVB) theory and is absent in conventional metals. The second channel is the spin-fluctuation pairing due to hopping in one Hubbard subband which is usually considered in spin-fermion models. By taking into account both channels, we obtain for T_c the estimation: $T_c = \omega_s \exp(-1/\widetilde{V}_{sf})$, $\widetilde{V}_{sf} = V_{sf} + V_{ex}/[1 - V_{ex} \ln(\mu/\omega_s)]$, where $V_{sf} \simeq \lambda_s N(\mu)$, $\lambda_s \sim t^2/\omega_s$ is the coupling constant, and $\omega_s \sim J$ is the characteristic energy for spin-fluctuations. Even for a weak coupling, $V_{ex} \simeq V_{sf} \simeq 0.2$ a high $T_c = 100-200$ K follows from this estimation due to the enhancement of the coupling constant $\widetilde{V}_{sf}$ for $(\mu/\omega_s) \gg 1$. It should be stressed that in our microscopic theory the coupling function in the gap equation (15) (or (17)) is given by the same parameters (t, t', J) of the Hubbard model (1) contrary to spin-fermion models where this interaction is a fitting parameter.

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