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SUPERCONDUCTIVITY

Spatial Structure of Superconducting Correlations of $d_{x^2-y^2}$ Symmetry in High-Temperature Superconductors

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Abstract—The spatial structure of the correlation function of the order parameter of the $d_{x^2-y^2}$ symmetry has been investigated within the *t*–*J* model in the generalized mean field approximation taking into account the "no-double occupancy" constraint due to strong electron correlations. A slow decay of the correlation function to the thirtieth coordination sphere has been found. The limitation by pairing of only the nearest neighbors makes it possible to take into account less than 17% of the superconducting correlations.

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1. INTRODUCTION

In all numerical methods of investigation of the magnetic mechanism of superconductivity, for example, in the quantum Monte Carlo (QMC) method, or in the method of exact diagonalization of the Hamiltonian, a finite size of the cluster under consideration restricts the size of the Cooper pair $B_{ij} = \langle c_{i\downarrow}^{+} c_{j\uparrow}^{+} \rangle$ by a distance r_{ij} with a very small number of coordination spheres [1–5]. As a rule, pair correlation functions are very small, which causes the contradictory conclusions of the authors of different works on the possibility of the $d_{x^2-y^2}$ superconductivity in the limit of strong electron correlations (SEC) in the scope of the Hubbard or *t*–*J* models (see discussion in [5]). In this situation, the question arises: what is the degree of trustworthiness of the results obtained for small clusters? What is the size of the Cooper pair, and can we limit ourselves by taking into account the pairing of the nearest neighbors only?

In this paper, we answer this question in the scope of the variant of the mean field theory constructed taking into account the SEC. Various approaches to the description of the magnetic mechanism of superconductivity are known [6–11]. We follow the approach [12], where the local prohibition of two-electron states due to the SEC is taken into account. The advantage of this approach is the formulation of the *t*–*J* model and superconductivity theory in the representation of the Hubbard *X*-operators instead of conventional single-electron operators of creation/annihilation of electrons. The algebra of *X*-operators allows us to exactly take into account the "no-double occupancy" constraint at all stages of calculations. The superconductivity theory [12] was recently generalized taking into account the electron–phonon interaction (EPI) along with the magnetic one [13].

2. CORRELATION FUNCTION OF COOPER PAIRS IN THE *t*–*J* MODEL

In high-temperature superconductors of the $La_{2-x}Sr_xCuO_4$ type, the hole with spin σ in the site $\mathbf{R}_i$ is described by the Hubbard operator $X_i^{2,\bar{\sigma}} = |2\rangle\langle -\sigma|$. It is the excitation between d^9p^6 spin doublet with one hole $|-\sigma\rangle$, ($\sigma = \pm 1/2$) and two-hole Zhang–Rice singlet $d^9p^6 + d^8p^6|2\rangle$. The two-electron $d^{10}p^6$ states (zero of holes) are forbidden due to the SEC and excluded from the Hilbert space so that the condition of the completeness of the local basis set $\{|+1/2\rangle, |-1/2\rangle, |2\rangle\}$ has the form

$$\sum_{\sigma} |\sigma\rangle\langle\sigma| + |2\rangle\langle 2| = 1.$$

Under these conditions, the superconducting pairing of the Hubbard fermions is described by an anomalous average

$$B_{\mathbf{q}} = \langle X_{\mathbf{q}}^{\sigma,2} X_{-\mathbf{q}}^{-\sigma,2} \rangle. \quad (1)$$

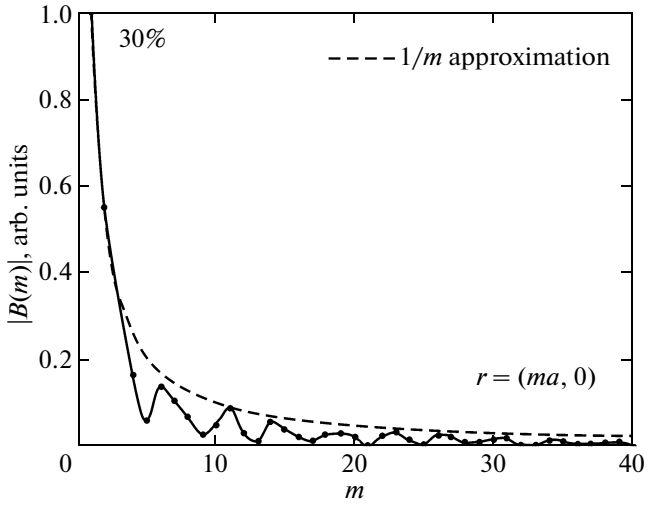

Fig. 1. Amplitude of the correlation function along the x axis at optimal doping.

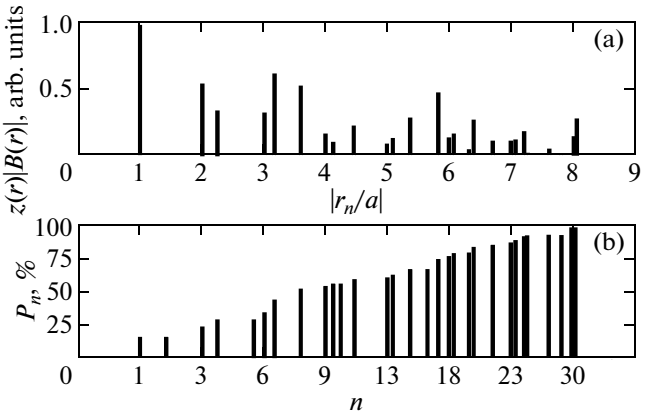

Fig. 2. (a) Correlation function and (b) percentage of correlations taken into account for the nth coordination sphere. $n \le 30$.

In the case of the $d_{x^2-y^2}$ symmetry, the gap $\Delta_{\mathbf{k}}$ is determined as follows:

$$\Delta_{\mathbf{k}} = \frac{1-x}{1+x}\frac{1}{N}\sum_{\mathbf{q}}(J_{\mathbf{k}+\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}})B_{\mathbf{q}}, \qquad (2)$$

where x is the concentration of doping with complete number of holes $n_h = 1 + x$ per formula unit of $La_{2-x}Sr_xCuO_4$ and $J_{\mathbf{k}}$ is the exchange interaction Fourier transform $J = 2t^2/U$. The gap depends on the wave vector as $\Delta_{\mathbf{k}} = \Delta_0\varphi_{\mathbf{k}}$, and $\varphi_{\mathbf{k}} = 0.5(\cos k_x a - \cos k_y a)$. Correlation function (1) is

$$B_{\mathbf{q}} = \frac{\Delta_{\mathbf{q}}F_{0\sigma}}{2E_{\mathbf{q}}}\tanh\frac{E_{\mathbf{q}}}{2k_BT}, \qquad (3)$$

where $F_{0\sigma} = (1+x)/2 = \langle X^{\sigma\sigma}\rangle + \langle X^{22}\rangle$ is the spectral weight of the hole determined by the occupation numbers of the initial and final states, $E_{\mathbf{q}} = (\xi_{\mathbf{q}}^2 + \Delta_{\mathbf{q}}^2)^{1/2}$, and $\xi_{\mathbf{q}}$ is the electron dispersion in the normal phase. At $T = 0$, the equation for the gap takes the form

$$A = \frac{1}{N}\sum_{\mathbf{q}}\lambda_J\frac{4\varphi_{\mathbf{q}}^2}{E_{\mathbf{q}}}, \quad \lambda_J = \frac{1-x}{2}J. \qquad (4)$$

The addition of the EPI with a constant λ_{ph} to the t–J model retains the form of the equation for the gap but with a renormalized coupling constant [13]: $\lambda_J \longrightarrow \lambda_{tot}$, where

$$\lambda_{tot} = \lambda_J + \lambda_{ph}\theta(\omega_D - |\xi_{\mathbf{q}}|).$$

As usual in the BCS theory, here, the Heaviside θ-function cuts pairing out of a narrow region of the order of the Debye frequency ω_D wide near the Fermi level. A final expression for a pair correlation function takes the form

$$B(\mathbf{r}) = \frac{1}{N}\sum_{\mathbf{q}}\frac{\Delta_0\varphi_{\mathbf{q}}F_{0\sigma}}{2E_{\mathbf{q}}}e^{i\mathbf{q}\cdot\mathbf{r}}. \qquad (5)$$

We calculated this function with the parameters of the t–J model calculated from the first principles by the LDA + GTB method for $La_{2-x}Sr_xCuO_4$ [14] and the EPI parameter found from the equalization of the calculated and experimental values of the isotope-effect by oxygen in $La_{2-x}Sr_xCuO_4$ [13].

The amplitude of the correlation function (5) along the x axis, from $\mathbf{r}$ ($m = 0$) to $\mathbf{r}$ ($m = 40$), is presented in Fig. 1. The dashed line shows approximation $1/m$, which can be obtained analytically from Eq. (5) taking into account the main contribution in the right side from the vicinity of the Fermi level, where $E_{\mathbf{q}} = \Delta_{\mathbf{q}}$. The value $|B(1, 0)|$ is of about 30% of the sum

$$\sum_{m=1}^{40}|B(m, 0)|,$$

which shows that we lose very many if we restrict ourselves by the consideration of nearest neighbors only. For a two-dimensional square lattice, we analyzed not only function $|B(r)|$ but also the product of this function by coordination number z_n for the nth coordination sphere. The function $z(r_n)|B(r_n)|$ is constructed in Fig. 2a. The contribution of the first coordination sphere is of about 17% of the summary one. In order to evaluate the part of correlations taken into account in the confinement by the mth coordination sphere, we calculated the quantity

$$P_m = \sum_{n=1}^{m} z(r_n)|B(r_n)| \Big/ \sum_{n=1}^{30} z(r_n)|B(r_n)|, \qquad (6)$$

which is shown in Fig. 2b.

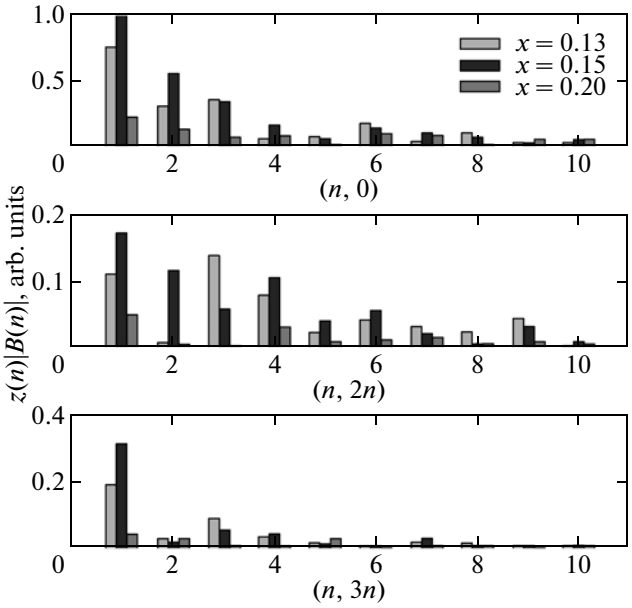

Fig. 3. Correlation functions with $r_n = (n, 0)$, $(n, 2n)$, and $(n, 3n)$ for doping concentrations $x = 0.13$, 0.15, and 0.20.

The correlation function depends on the degree of doping x. The presented results were obtained at $x = 0.15$ near the optimal doping. In Fig. 3, we present the dependences of the correlation function along three spatial directions $r_n = (n, 0)$, $(n, 2n)$, and $(n, 3n)$ for lightly doped $x = 0.13$, almost optimally doped $x = 0.15$, and heavily doped $x = 0.20$ compositions. It is evident from Fig. 3 that the concentration dependence is nonmonotonic, and in some directions, the correlation for the lightly doped composition is stronger than that for the optimal doping.

3. CONCLUSIONS

According to our calculations, the superconducting correlations are spatially distributed and slowly decrease with a distance. We restricted ourselves by $|\mathbf{r} \le 8a \approx 30|$ Å, which corresponds to 30 coordination spheres on a square lattice. The calculation to $n = 40$ showed that the longer range correlations are close to zero. The size of the Cooper pair calculated by us is close to the experimental value of the correlation length $\xi \approx 30$ Å in high-temperature superconductors.

Our results show that the numerical calculations for small clusters always strongly underestimate the energy gain of the superconducting phase compared with the normal phase.

This work had appeared as a response to the rhetorical question of D. Scalapino during discussion of contradictory QMC results for the superconductivity theory in cuprates.

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