s+d pairing in orthorhombic phase of copper-oxides

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A microscopical theory of electronic spectrum and superconductivity is formulated within the two-dimensional anisotropic $t$–$J$ model with $t_x \neq t_y$ and $J_x \neq J_y$. Renormalization of electronic spectrum and superconductivity mediated by spin-fluctuations are investigated within the Eliashberg equation in the weak coupling approximation. The gap function has $d+s$ symmetry with the extended $s$-wave component being proportional to the asymmetry $t_y-t_x$. Some experimental consequences of the obtained results are discussed.

Recently the $d$-wave symmetry of superconducting pairing in cuprates was unambiguously confirmed by observation of half-integer magnetic flux quantum \cite{1}. In a tetragonal phase of copper oxides the s-wave component must be strongly suppressed due to on-site Coulomb correlations. For the 2D $t$-$J$ model it follows from the constraint of no double occupancy on a single site given by the identity \cite{2}:

$$\langle \hat{a}_{i,\sigma} \hat{a}_{i,-\sigma} \rangle = \frac{1}{N} \sum_{k_x,k_y} \langle \hat{a}_{k,\sigma} \hat{a}_{-k,-\sigma} \rangle = 0, \quad (1)$$

for the projected electron operators $\hat{a}_{i,\sigma} = a_{i,\sigma}(1-n_{i,-\sigma})$. The anomalous correlation function $\langle \hat{a}_{k,\sigma} \hat{a}_{-k,-\sigma} \rangle$ is proportional to the gap function, $\Delta(k_x,k_y)$, multiplied by a positive function symmetric in respect to the $D_{4h}$ point group which defines the symmetry of the Fermi surface (FS). Therefore to satisfy the condition (1) the gap function should have a lower symmetry, e.g. $B_{1g}$, ”$d$-wave” symmetry (see, e.g. \cite{3}): $\Delta_d(k_x,k_y) = -\Delta_d(k_y,k_x)$.

In the orthorhombic phase the FS has a lower symmetry, e.g., $D_{2h}$, and the condition (1) can be fulfilled for a gap function of the same symmetry (within the $E_{1g}$ irreducible representation) which can be written in a general form ("$d+s$"):

$$\Delta(k_x,k_y) = \Delta_d(k_x,k_y) + \epsilon \Delta_s(k_x,k_y). \quad (2)$$

where $\Delta_s(k_x,k_y) = \Delta_s(k_y,k_x)$ is the ”extended $s$-wave” component.

In the present paper we calculate superconducting $T_c$ for the 2D $t$-$t'$-$J$ model within the theory developed by us in \cite{4}, both in tetragonal and orthorhombic phases. The orthorhombic ($D_{2h}$) distortion is taken into account by introducing the asymmetric hopping parameters $t_{ij}$ and the exchange interaction $J_{ij}$ for the nearest neighbors (n.n.) in the form: $t_{x/y} = t(1 + \alpha)$, $J_{x/y} = J(1 + \beta)$ where the asymmetry parameters are supposed to be small quantities: $\alpha \sim \beta \sim 0.1$.

The Dyson equations for the matrix Green function (GF) in the Nambu notation was obtained by the equation of motion method for the Hubbard operators as described in \cite{4}. For estimation of the role of orthorhombic deformation we consider here only the weak-coupling approximation. However, to take into account strong electronic correlations in the $t$-$J$ model due to restricted hopping in the singly occupied subband we write the single-electron spectral density in the form: $A(k,\omega) \simeq Z_k \delta(\omega + \mu - E_k) + A_{inc}(\omega)$. The quasiparticle weight $Z_k$ and the incoherent part $A_{inc}(\omega)$ are coupled by the sum rule for the spectral density: $\int_{-\infty}^{+\infty} d\omega A(k,\omega) = 1 - n/2$. To fix the value of $Z_k$ we assume that the FS for quasiparticles with spectrum $E_k$ obeys the Luttinger theorem: the average number of electrons is equal to the number of states in $k$-space below the chemical potential $\mu$: $n = (1/N) \sum_{k,\sigma} \{ \exp[\mu - E_k - \mu]/T \} + 1^{-1}$.

From these conditions we have estimations: $Z \simeq (1-n)/(1-n/2)$ and $A_{inc}(\omega) \simeq (n/2)^2/(1-n/2)(W - \Gamma)$ where we have suggested that the coherent band lies in the range...
\[ \Delta_k = \frac{1}{N} \sum_q K(q,k - q) \frac{Z^2_q \Delta_q}{2 \Omega_q} \tanh \frac{\Omega_q}{2T} \] 

where \( \Omega_q = \left[ (E_q - \mu)^2 + \Delta^2_q \right]^{1/2} \) and \( E_q \approx -t_{eff}[\gamma(q) + \eta(q)] - t'_{eff}\gamma'(k) \) with renormalized due to strong correlations hopping parameters and \( \gamma(q) = (1/2)(\cos q_x + \cos q_y) \), \( \eta(q) = (1/2)(\cos q_x - \cos q_y) \), \( \gamma'(q) = \cos q_x \cos q_y \) [4].

\[ K(q,k - q) = \{ 2g(q,k - q) - \lambda(q,k - q) \} \] 

with the vertex \( g(q,k - q) = \xi(k - q)/2 \) and \( \lambda(q,k - q) = 2t^2(q,k - q)\chi(k - q) \). The first term in the vertex, \( t(q) \), is due to the kinematical interaction caused by constraints and the second one, \( J(q) \), is the exchange coupling. They have different \( q \)-dependence and are effective at different doping. The spin-fluctuation coupling in \( \lambda(q,k - q) \) is defined by the static spin susceptibility \( \chi(k - q) \) for which we used the model \( \chi(q) = \chi_0 / [1 + \xi^2(1 + \gamma(q))] \) where the antiferromagnetic (AFM) correlation length \( \xi \) is a fitting parameter while \( \chi_0 \) is normalized by the condition: \( 1/N \sum_i \langle \sigma^x_i \rangle = (3/4)n \).

We performed numerical solution of Eq. \( (3) \) for the gap in the form \( \Delta_{q'}(k_x, k_y) = \Delta_{q}(k) \) and \( \Delta_{q}(k_x, k_y) = \Delta_{\gamma}(k) \). By taking into account the constraint of no double occupancy, Eq. \( (1) \), we estimate the weight \( \epsilon \) of the \( s \)-component. The critical temperature \( T_c(\delta) \) (in units of \( t \)) is shown on Fig.\( 1 \) in the tetragonal, \( \alpha = 0.0 \), (bold line) and orthorhombic, \( \alpha = 0.1 \), (dashed line) phases for \( J = 0.4t \), \( \xi = 2 \), \( t' = 0.0 \). Suppression of \( T_c \) in the orthorhombic phase is due to a deformation of the FS resulting in a less favourable electron pairing by the AFM spin fluctuations. Increasing of AFM interaction due to larger \( J \) or/and \( \xi \) strongly enhances \( T_c \) though does not change the shape of the curve. Its maximum at \( \delta \approx 0.35 \) is due to an interplay between the shape of the FS (defined by the quasiparticle spectrum \( E_q \)) and the coherent spectral weight \( Z^2 \) in Eq. \( (3) \).}

\[ \Delta \leq \omega \leq \Gamma \] while the incoherent band lies below the coherent band in the range \(-W \leq \omega \leq -\Gamma \). By taking into account the renormalization of the coherent part of the spectral weight by \( Z \) we write the equation for the gap in the weak coupling approximation in the form:

\[ \Delta_k = \frac{1}{N} \sum_q K(q,k - q) \frac{Z^2_q \Delta_q}{2 \Omega_q} \tanh \frac{\Omega_q}{2T}, \] 

where \( \Omega_q = \left[ (E_q - \mu)^2 + \Delta^2_q \right]^{1/2} \) and \( E_q \approx -t_{eff}[\gamma(q) + \eta(q)] - t'_{eff}\gamma'(k) \) with renormalized due to strong correlations hopping parameters and \( \gamma(q) = (1/2)(\cos q_x + \cos q_y) \), \( \eta(q) = (1/2)(\cos q_x - \cos q_y) \), \( \gamma'(q) = \cos q_x \cos q_y \) [4].

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