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Mean-field study of possible electronic pairings in the CuO_2 plane of HTSO

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Abstract. The known three-band model of electrons in the CuO_2 plane of HTSO and the mean-field (MF) theory are used to classify the possible types of pairing and to find the contributions of all local interactions to the linearized MF Hamiltonian on the assumption of frozen lower bands. The on-centre interactions U_d and U_p on Cu $d_{x^2-y^2}$ and O p orbitals, the Coulomb (Q) and exchange (J) interactions of adjacent p and d orbitals and the terms K_d and K_p describing the correlated hopping are taken into account. The phase diagrams for transitions from normal state to each separate type of pairing (antiferromagnetic or superconducting) and solutions of self-consistent equations for the order parameters are studied numerically for various sets of parameters. The results show that, at certain doping after destruction of antiferromagnetic ordering, superconductivity might be expected at sufficiently large K_d and K_p . This requires the condition $\varepsilon_d - \varepsilon_p < 0$ for the renormalized energies of the Cu d and O p orbitals, i.e. the preferential occupation of the O site by holes. If $K_d = K_p$ and their values are equal to about the p-d transfer integral t , then only the s type of superconductivity is possible whereas, for $K_d = 0$, $K_p \approx 1.5t$, only the d type of superconductivity is revealed for the models considered.

1. Introduction

Since the discovery of high- T_c superconductivity [1] a great variety of different pairing mechanisms have been proposed, in particular those caused by local short-range attractive interaction [2]. However, the origin of the local attractive interaction has been unclear up to now.

The aim of this paper is to elucidate the question of whether the short-range electronic interactions constituting the chemical bond energies could give rise to an antiferromagnetic (AF) or superconducting (SC) pairing of electrons in the CuO_2 plane of HTSO? From this viewpoint, all local interactions of the electronic $d_{x^2-y^2}$, p_x and p_y orbitals of adjacent atoms in the CuO_2 plane are classified and analysed in terms of the mean-field (MF) theory for the upper band in the known three-band model [3–7] of the CuO_2 plane on the assumption of two frozen lower bands. The main parameters of model have been discussed in [8–12]. First the Hartree–Fock (HF) approximation is used to obtain the upper band parameters which vary with doping.

The MF theory with the band approach is used, unlike the MF studies [13–15] of electron pairing in the Mott–Hubbard approach. A comparative discussion of both approaches has been given in [16]. The present study takes into account a more detailed

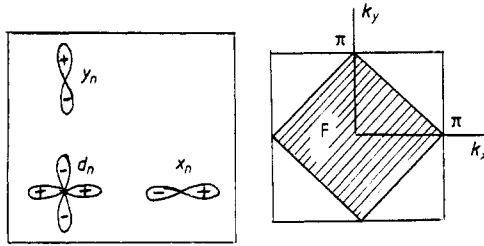


Figure 1.

picture of interactions in system (and not only on-site and inter-site parameters) and it is similar to that in [17]. Oles and Zaanen [17] have studied AF pairing by the MF theory and by the Gutzwiller *ansatz* method and have demonstrated only a restricted accuracy of the MF theory. Nevertheless the extension and the MF classification of all types of interaction in problems and a numerical study of models may be instructive in searching for new ideas.

Contrary to conventional opinion [2] the hopes for superconductivity may be connected with the correlated hopping interaction between all considered local interactions. Note that here we deal with the correlated hopping between the p and d orbitals instead of a similar effective hopping interaction between elementary sites. Moreover the existence of superconductivity depends crucially on $E_d = \varepsilon_d - \varepsilon_p$, i.e. on the difference between the renormalized energies of the p and d orbitals. If $E_d > 0$ the holes populate the Cu sites preferentially and the AF state spreads over a large range of doping and suppresses the SC state. When $E_d < 0$ the AF correlations of spins on Cu centres weaken and the AF state on O sites is unlikely because of frustration of oxygen sublattice. However, there is a large region of doping when superconductivity can exist for our models at $E_d < 0$ and sufficiently large K_d and K_p . It may be of s or d type depending on K_d/K_p .

2. The model Hamiltonian

The known model [3–7] for the bands is based on Cu $d_{x^2-y^2}$, O p_x and O p_y orbits which correspond to the electron creation operators $d_{n\sigma}^+$, $x_{n\sigma}^+$ and $y_{n\sigma}^+$. The Hamiltonian of the model is

$$H = H_0(t_0, \varepsilon_p^0, \varepsilon_d^0) + V_U + V_Q + V_J + V_K \quad (1)$$

where H_0 is the one-electron ‘zero’ Hamiltonian:

$$H_0 = +t_0 \sum_{\sigma} \sum_{(nm)} \zeta_{nm} (d_{n\sigma}^+ x_{m\sigma} - d_{n\sigma}^+ y_{m\sigma} + \text{HC}) + \sum_{n\sigma} \varepsilon_d d_{n\sigma}^+ d_{n\sigma} + \sum_{n\sigma} \varepsilon_p (x_{n\sigma}^+ x_{n\sigma} + y_{n\sigma}^+ y_{n\sigma}). \quad (2)$$

The summation of (m, n) is taken over nearest-neighbour Cu and O centres, i.e. $m - n$ is equal to zero or e_x or e_y , and $\zeta_{mn} = (-1)^{n-m}$ if the signs of the orbitals are chosen as in figure 1; t_0 , ε_d^0 and ε_p^0 are the ‘zero’ p–d transfer integral and orbital energies; V_U contains the one-centre Coulomb integrals U_d and U_p on atoms Cu and O; V_Q and V_J correspond to the Coulomb and exchange integrals Q and J for the nearest-neighbour p

and d orbitals, V_K describes the correlated hopping and provides dependence of actual p-d transfer integral on occupancy of these orbitals. V_J and V_k have the forms

$$V_J = -J \sum_{(mn)\sigma} \sum_{\sigma\sigma'} [(d_{n\sigma}^+ x_{m\sigma}^+ d_{n\sigma'} x_{m\sigma'}) + (\dots)_y] \quad (3a)$$

$$V_K = -K_d \sum_{(nm)\sigma} \xi_{nm} [(d_{n\sigma}^+ d_{n-\sigma}^+ x_{m-\sigma} d_{n\sigma} + \text{HC}) - (\dots)_y] \\ - K_p \sum_{(nm)\sigma} \xi_{nm} [(x_{n\sigma}^+ x_{n-\sigma}^+ d_{m-\sigma} x_{n\sigma} + \text{HC}) - (\dots)_y], \quad (3b)$$

Here $(\dots)_y$ denotes the same as the previous parentheses but for y operators. The signs of orbitals are chosen so that K_p , K_d and J are positive. The electronic representation (instead of the hole representation) is used here.

The ordinary HF approximation to (1) leads to the Hamiltonian which coincides with $H_0(t, \varepsilon_p, \varepsilon_d)$ but with the replacement of the parameters t_0 , ε_d^0 and ε_p^0 by the renormalized values

$$\varepsilon_d = \varepsilon_d^0 + U_d \rho_d + 4(2Q + J) \rho_d - 8K_d \rho_{pd} \\ \varepsilon_p = \varepsilon_p^0 + U_p \rho_p + 4(2Q + J) \rho_p - 4K_p \rho_{pd} \quad (4) \\ t = t_0 - (Q + 2J) \rho_{pd} - K_d \rho_d - K_p \rho_p$$

where $\rho_d = \langle d_{n\sigma}^+ d_{n\sigma} \rangle$, $\rho_p = \langle x_{n\sigma}^+ x_{n\sigma} \rangle$, $\rho_{pd} = \xi_{nm} \langle x_{m\sigma}^+ d_{n\sigma} \rangle$ are the average occupancies of the p and d orbitals and the bond order value for definite spin projection σ . The energies of the three bands (bonding, antibonding and dispersionless non-bonding bands) and the annihilation operators of the band states are

$$\varepsilon_{1(3)} = \bar{\varepsilon} - \mu \pm \sqrt{D^2 + W^2} \quad \varepsilon_2 = \varepsilon_p - \mu \quad (5)$$

$$a_{k\sigma}^\lambda = N^{-1/2} \sum_{n,\sigma} \exp(-ikn) (d_{n\sigma}, x_{n\sigma}, y_{n\sigma})_j A_{j\lambda} \quad j, \lambda = 1, 2, 3. \quad (6)$$

Here the upper band coefficients and parameters are

$$A_{j1} = (C, i \exp(-ik_x/2) S s_x, -i \exp(-ik_y/2) S s_y)_j \\ \bar{\varepsilon} = (\varepsilon_p + \varepsilon_d)/2 \quad D = (\varepsilon_p - \varepsilon_d)/2 \quad W = 2tw \\ s_x = \sin(k_x/2) \quad s_y = \sin(k_y/2) \quad w = \sqrt{s_x^2 + s_y^2} \\ C = \cos \theta \quad S = (\sin \theta)/w \quad \tan(2\theta) = -W/D. \quad (7)$$

If bands 2 and 3 are completely filled and only the upper band is partly occupied, then the self-consistent HF equations are

$$\rho_d = 1 - \frac{1}{N} \sum_k |A_{11}|^2 (1 - f_1) = \frac{1}{2} n(\mu) - 2\rho_p \\ \rho_{pd} = -\frac{1}{N} \sum_k [\text{Re}(A_{21}^* A_{11})] (1 - f_1) \quad (8) \\ n(\mu) = 6 - \frac{2}{N} \sum_k (1 - f_1) = N_h + 5$$

where n is a number of electrons on one site and N_h is the hole concentration associated

Table 1. Constants κ and functions φ in the operators Δ_μ^ν in equations (12) responsible for the SDW ($\mu = 1, 2, 3$) or CDW ($\mu = 0$) for three different types of symmetry ($\nu = 1-5$ or $\nu = 6-9$ or $\nu = 10, 11$). $\eta_\mu = 1$ for $\mu = 1, 2, 3$; $\eta_0 = -1$; $A_\mu = (Q/2 + \delta_{\mu 0}J)$; $F = \bar{C}S\bar{w}^2$; $\bar{F} = F(\bar{k})$; $\bar{S} = S(\bar{k})$; $\bar{C} = C(\bar{k})$; $\bar{w} = w(\bar{k})$; $f = s_x c_x$ (or $s_y c_y$ for $\nu = 6'-9'$). The rest of the notation is defined in equations (7).

ν	κ_μ^ν	φ_μ^ν	ν	κ_μ^ν	φ_μ^ν
1	$-\eta_\mu U_d$	$C\bar{C}$	6(6')	$-\eta_\mu U_p$	$iS\bar{S}f$
2	$-A_\mu$	$(F + \bar{F})$	7(7')	$-2A_\mu$	$i(C\bar{S} + S\bar{C})f$
3	$-A_\mu$	$i(F - \bar{F})$	8(8')	$-K_p/2$	$i(S\bar{C} + \bar{S}C + S\bar{S})f$
4	$-K_d/4$	$2C\bar{C} + F + \bar{F}$	9(9')	$K_p/2$	$i(S\bar{C} + \bar{S}C - S\bar{S})f$
5	$K_d/4$	$2C\bar{C} - F - \bar{F}$	10	$-A_\mu$	$(S\bar{C} - \bar{S}C)(s_x^2 - s_y^2)$
			11	$-A_\mu$	$i(S\bar{C} + C\bar{S})(s_x^2 - s_y^2)$

with doping; f_1 is the Fermi distribution function in the upper band. All HF calculations have been done at zero temperature.

In the representation of HF states (6) the Hamiltonian (1) includes interactions between states inside each band as well as those with and between states of different bands. The main approximation of the present study consists in retaining all interactions inside the upper band and neglecting those with and between states of lower bands which are assumed to be frozen. In such an approximation the interaction depends only on the creation operators $a_{k\sigma}^+$ of the upper band and takes the form

$$V = \frac{1}{2} \sum_{k_j \sigma_j} V(k_1 \sigma_1 \dots k_4 \sigma_4) a_{k_1 \sigma_1}^+ a_{k_2 \sigma_2}^+ a_{k_3 \sigma_3} a_{k_4 \sigma_4} \delta(k_1 + k_2 - k_3 - k_4) \tag{9}$$

where the matrix elements in (9) are calculated by the use of expansion (6).

Now the most general linearized Hamiltonian of the upper band contains three types of term with large phase volume, namely those with

$$(k_1 k_2 k_3 k_4) = \{(k, -\bar{k}', k', -\bar{k}), (k, -\bar{k}', -\bar{k}, k')\}$$

$$\text{or } (k, -k, -k', k') \text{ or } (k, \bar{k}, \bar{k}', k')$$

in addition to the usual HF terms. Here the vector \bar{k} is defined by

$$\bar{k} = e_x(\pi k_x / |k_x| - k_x) + e_y(\pi k_y / |k_y| - k_y). \tag{10}$$

Thus the obtained model interaction $V_{\text{mod}} = V_{\text{AF}} + V_{\text{SC}} + V_{\text{AA}}$ is

$$H_{\text{mod}} = H_0 + \sum \frac{\Delta_\mu^\nu \Delta_\mu^\nu}{\kappa_\mu^\nu} + \sum \frac{\Gamma_{SM}^{+\nu} \Gamma_{SM}^{+\nu}}{\gamma_S^\nu} + \sum \frac{Z_{SM}^{+\nu} Z_{SM}^{+\nu}}{\zeta_S^\nu} \tag{11}$$

$$\Delta_\mu^\nu = \kappa_\mu^\nu \sum' \varphi_\mu^\nu(k) t_\mu(k) \quad t_\mu(k) = \sum'' (\sigma_\mu)_{\sigma\sigma'} a_{\bar{k}\sigma}^+ a_{-k\sigma'} \tag{12}$$

$$\Gamma_{SM}^\nu = \gamma_{SM}^\nu \sum' g_S^\nu(k) r_{SM}^\nu(k) \quad r_{SM}^\nu(k) = \sum'' \sqrt{2} C_{\sigma\sigma'}^{SM} a_{-k\sigma'} a_{k\sigma} \tag{13}$$

$$Z_{SM} = \zeta_S^\nu \sum' \chi_S^\nu(k) z_{SM}(k) \quad z_{SM}(k) = \sum'' \sqrt{2} C_{\sigma\sigma'}^{SM} a_{\bar{k}\sigma}^+ a_{k\sigma}. \tag{14}$$

Here σ_μ , $\mu = 0, 1, 2, 3$, are the Pauli matrices; $C_{\sigma\sigma'}^{SM}$ are Clebsch–Gordon coefficients for spins $\frac{1}{2}$; the index ν enumerates all possible operators $\Delta, \Gamma, Z, \Sigma, \Sigma'$ and Σ'' are the

Table 2. Constants γ and functions g in the operators Γ_{SM}^ν in equation (13) corresponding to SC pairing: $\nu = 1-7$ or $\nu = 8-10$ for singlet pairing of s or d type; $\nu = 12, 12'$ for triplet pairing of p type. $f_d = s_x^2 - s_y^2$. The rest of the notation is the same as in table 1.

ν	$\frac{1}{2}\gamma_{s=0}^\nu$	$g_{s=0}^\nu$	ν	$\frac{1}{2}\gamma_{s=0}^\nu$	$g_{s=0}^\nu$	$\frac{1}{2}\gamma_{s=1}^\nu$	$g_{s=1}^\nu$
1	$U_d/2$	C^2	8	$U_p/4$	$S^2 f_d$		
2	$U_p/4$	$S^2 w^2$	9	$Q - J$	$CS f_d$		
3	$Q - J$	$CS w^2$	10	$-K_p/2$	$(S^2 + CS) f_d$		
4	$-K_d/2$	$2C^2 + CS w^2$	11	$K_p/2$	$(S^2 - CS) f_d$		
5	$K_d/2$	$2C^2 - CS w^2$					
6	$-K_p/2$	$(S^2 + CS) w^2$					
7	$K_p/2$	$(S^2 - CS) w^2$	12(12')			$2(Q + J)$	$CS s_x c_x$

sums over μ, ν, S, M or over k or over σ, σ' correspondingly. The constants κ and γ and weighting functions φ and g are given in tables 1 and 2. The similar values ζ and χ have been obtained. The reduction of H_{mod} to a separable form (11) follows from the properties of operators t, r, z discussed in appendix 1.

The first term in equation (10) (see table 1) refers to a possible spin-density wave (SDW) with polarization μ ($\mu = 1, 2, 3$) if the corresponding real order parameters (OPs) $\underline{\Delta}_\mu^\nu = \langle \Delta_\mu^\nu \rangle$ are non-zero. At $\mu = 0$ the real OP $\underline{\Delta}_0^\nu$ corresponds to a charge-density wave (CDW) with a double volume of the elementary site. Depending on the symmetry of function φ in (11) the OP $\underline{\Delta}$ means the alternation of the spin density ($\mu = 0$) or the charge density ($\mu = 0$) on copper ions ($\nu = 0$) or on oxygen ions ($\nu = 6, 6'$) or on the p-d bonds or corresponds to the state of the orbital antiferromagnet with charge (or spin) currents of some symmetry. Note that the relation $U_p < U_d$ and degeneracy of the SDW on oxygen connected with frustration of the oxygen sublattice make the AF ordering of spins on oxygen sites less probable than on Cu sites. The properties of the operators Δ_μ^ν and interpretation of the corresponding real OPs $\underline{\Delta}_\mu^\nu = (\Delta_\mu^\nu)^*$ are discussed in appendix 2.

The second term in (10) is responsible for the SC pairing in the singlet ($S = 0$) or triplet ($S = 1$) states if the corresponding OPs $\underline{\Gamma}_{SM}^\nu = \langle \Gamma_{SM}^\nu \rangle = 0$. The symmetry of the function $g(k)$ in (13) determines the s, p or d type of pairing. The third term in (10) refers to the alternating anomalous averages (AAS) $\langle a_{n\sigma}^+ a_{n\sigma'}^+ \rangle \sim (-1)^{n_x + n_y}$.

The results in tables 1 and 2 allow us to choose the possible types of pairing (which is expected to give a positive energy gain) and to elucidate the role of each type of interaction in the corresponding pairing. If only the Coulomb interactions V_U and V_Q are taken into account, then only AF pairing can be energetically favourable, but not CDW or SC pairing which have all positive constants κ or γ in this case. However, at sufficiently large values of the correlated hopping contributions ($\sim K_d, K_p$) or of exchange integral J the resultant effective constants κ, γ, ζ can also become negative. This refers to CDW on oxygen ions or on p-d bonds ($\mu = 0, \nu = 6-9$ or $\mu = 0, \nu = 10-11$ in table 1) or to the singlet SC pairing of s or d type ($\nu = 1-7$ or $\nu = 8-10$ in table 2). For instance, if $\varepsilon_p = \varepsilon_d$ and the upper band is half populated, then $D = 0, C = 1/\sqrt{2}, S = 1/\sqrt{2} w \sim 1/\sqrt{2}$ near the 2D Fermi surface and the resultant effective constants for SC s or SC d pairing are estimated as [18]

$$\begin{aligned} \gamma_s^{\text{eff}} &= U_d/8 + U_p/16 + (Q - J)/4 - K_d - K_p/2 \\ \gamma_d^{\text{eff}} &= U_p/16 + (Q - J)/4 - K_p/2 \end{aligned}$$

with $g_s^{\text{eff}} \approx 1$ and $g_d^{\text{eff}}(k) \approx s_x^2 - s_y^2$. If one uses the values (15) for D , t , U_d , U_p and Q estimated in [8] and sufficiently large values of the rest of the parameters $K_d \approx K_p \approx t$, $J = (0-1.8)t$, then $\gamma_s^{\text{eff}} = -(0.15-0.55)$ eV and $\gamma_d^{\text{eff}} = -(0.1-0.6)$ eV.

3. Linearized Hamiltonian and self-consistent equations for the order parameters

A Hamiltonian for the upper band $\varepsilon(k) = \varepsilon_1(k)$ in equation (6) together with the retained model interaction (11)

$$H = H_1 + V_{\text{mod}} \quad H_1 = \sum [\varepsilon(k) - \mu] a_{k\sigma}^+ a_{k\sigma} \quad (15)$$

can be transformed directly to the corresponding linearized Hamiltonian of general form:

$$H_L = H_1(\varepsilon_p, \varepsilon_d, t) + 2 \sum_{\nu\mu} \frac{\Delta_\mu^\nu \underline{\Delta}_\mu^\nu}{K_\mu^\nu} + \sum_{\nu SM} \frac{(\Gamma_{SM}^{\nu+} \underline{\Gamma}_{SM}^\nu + \text{HC})}{\gamma_S^\nu} + \sum_{\nu SM} \frac{(Z_{SM}^{\nu+} \underline{Z}_{SM}^\nu + \text{HC})}{\zeta_S^\nu} + C_L. \quad (16)$$

Here $\underline{\Delta}_\mu^\nu = \langle \Delta_\mu^\nu \rangle$ are the set of the real OPs corresponding to the averages of the Hermitian operators Δ , and $\underline{\Gamma}_{SM}^\nu = \langle \Gamma_{SM}^\nu \rangle$ and $\underline{Z}_{SM}^\nu = \langle Z_{SM}^\nu \rangle$ are generally complex OPs. The constant C_L in (16) is

$$C_L = - \sum_{\nu\mu} \frac{\Delta_\mu^{\nu 2}}{K_\mu^\nu} - \sum_{\nu SM} \frac{|\underline{\Gamma}_{SM}^\nu|^2}{\gamma_S^\nu} - \sum_{\nu SM} \frac{|\underline{Z}_{SM}^\nu|^2}{\zeta_S^\nu}. \quad (17)$$

Use the standard method to find the spectrum $E_\lambda(k)$ and the structure of quasi-particles for the Hamiltonian H_L and close self-consistent equations for OPs. The creation and annihilation operators $\beta_\lambda^+(k)$, $\beta_\lambda(k)$ of quasiparticles obey the equations

$$[\beta_\lambda, H_L] = -E_\lambda \beta_\lambda \quad (18)$$

and are constructed as a linear combination of operators $a_{k\sigma}^+$, $a_{k\sigma}$. The number of terms in the expansion depends on number of operators Δ , Γ , Z in H_L . In general, if all OPs in H_L are non-zero, the commutation of H_L with $a_{k\uparrow}^+$, for example, generates eight operators which may serve as a basis set for the expansion of $\beta_\lambda(k)$, $\lambda = 1-8$. Then the number of independent vectors k is reduced by a factor of 4 when the spin doubling of the original operators $a_{k\sigma}$ is taken into account.

For simplicity we consider the situation with one type of SDW polarization $\mu = 3$ and with one projection $M = 0$ of anomalous OP in (16). Then $\beta_\lambda(k)$ is expanded on the basis of four operators $\{a_{k\uparrow}, a_{-\bar{k}\uparrow}, a_{-k\downarrow}^+, a_{\bar{k}\downarrow}^+\}$ which for uniformity will be called the new operators $b_j(k)$:

$$\beta_\lambda(k) = \sum b_j(k) U_{j\lambda}(k) \quad \beta_\lambda^+(k) = \sum (U^+)_{\lambda j} b_j^+ \quad (19)$$

$$\{b_1(k), b_2(k), b_3(k), b_4(k)\} = \{a_{k\uparrow}, a_{-\bar{k}\uparrow}, a_{-k\downarrow}^+, a_{\bar{k}\downarrow}^+\} \quad k \in F. \quad (20)$$

The full set of such independent operators can be obtained if the vector k varies in half of all the phase volume. For instance let k vary in the 2D region of volume F corresponding to filled states in the half-populated original band (see figure 1).

Then H_L takes the form

$$H_L = \sum_{ij=1}^4 \sum_{k \in F} L_{ij} b_i^+(k) b_j(k) + C_L. \quad (21)$$

The equations for the Hermitian matrix $L_{ij}(k)$ via the weighting functions and OPs are given in appendix 2. Substituting equations (19) and (20) into (18) yields

$$L_{ij} U_{j\lambda}(k) = -U_{j\lambda}(k) E_\lambda(k) \quad (22)$$

which determine the spectrum $E_\lambda(k)$ and the unitary matrix $U_{j\lambda}$ of coefficients in (19).

Now the averages of any product of operators over the Gibbs ensemble of states diagonal in the quasiparticle numbers are

$$\langle b_i^+(k) b_j(k') \rangle = \delta_{kk'} U_{il} f_l U_{lj}^+ \quad \langle b_i^+(k) b_j^+(k') \rangle = \langle b_i(k) b_j(k') \rangle = 0 \quad (23)$$

$$f_l = \{1 + \exp[-\beta E_l(k)]\}^{-1}. \quad (24)$$

Similar averaging of the operators Δ_μ^ν , Δ_3^ν , Γ_{s0}^ν , Z_{s0}^ν after reducing to the form (A13)–(A15) leads to the following self-consistent equations:

$$\underline{\Delta}_\mu^\nu = \kappa_\mu^\nu N^{-1} \sum_{k \in F} \text{Re}[\varphi_\mu^\nu(k) T_{12} - (-1)^\mu \varphi_\mu^\nu(\bar{k}) T_{34}] \quad \mu = 0, 3 \quad (25)$$

$$\underline{\Gamma}_{s0}^\nu = \gamma_s^\nu N^{-1} \sum_{k \in F} [g_\mu^\nu(k) T_{31} + g_\mu^\nu(-\bar{k}) T_{42}] \quad (26)$$

$$\underline{Z}_{s0}^\nu = \zeta_s^\nu N^{-1} \sum_{k \in F} [\chi_s^\nu(-\bar{k}) T_{32} + \chi_s^\nu(k) T_{41}] \quad (27)$$

$$N_h = 1 - N^{-1} \sum_{k \in F} \sum_j \eta_j T_{jj}. \quad (28)$$

Here $\sum_{k \in F}$ is the sum over half the phase volume and

$$T_{ij}(k) = U_{il} f_l U_{lj}^+ \quad (29)$$

$$\{\eta_j\} = \{1, 1, -1, -1\}_j \quad j = 1, \dots, 4.$$

When there is one type of pairing equations (25)–(27) reduce to standard equations.

The energy gain as a result of ordering is equal to the difference between the energies of the normal state (N) and the ordered states of the upper bands with the parameters (8) obtained first from solution of the HF equations (8) at fixed N_h :

$$\Delta H = H_N - \langle H_L \rangle \quad H_N = N^{-1} \sum_{k\sigma} [\varepsilon(k) - \mu] f(\varepsilon - \mu) \quad (30)$$

$$\langle H_L \rangle = N^{-1} \sum_\lambda \sum_{k \in F} E_\lambda(k) + C_L = N^{-1} \sum_j \sum_{k \in F} \varepsilon(k_j) \eta_j T_{jj} - C_L \quad (31)$$

$$\{k_j\} = \{k, -\bar{k}, -k, \bar{k}\} \quad j = 1, \dots, 4. \quad (32)$$

Before solving the self-consistent equations for the OPs it is of interest to understand the nature of each of the three types of ordering ($\underline{\Delta}$, $\underline{\Gamma}$ and \underline{Z}). This can be done by model calculations of the coefficient $Q_M = \lim(j_q/A_q)$ at $q \rightarrow 0$ which is indicative of the Meissner effect (here j_q and A_q are the Fourier transforms of the current and the vector potential of field). Model calculations using equations (A18), (A24) and (A25) in appendix 3 for a system with one type of non-zero OP show the following. For the AF

state, Q_M is equal to zero as typical for the normal state; for SC pairing, $Q_M < 0$ as one expects for the SC state; $Q_M > 0$ for the AA OP which means apparently that the state with AA OP is unstable with respect to rearrangement to CDW or SDW states. Therefore we omit terms with Z operators in our further considerations.

4. Results of the numerical study

The starting point in choosing the parameters was the requirement of a small difference $|\varepsilon_d - \varepsilon_p| < t$ of renormalized HF energies for the half-filled upper band, i.e. similar energies of configurations with one hole in Cu or one hole in O sites. This is a reason to apply the band approach although one expects only a qualitative picture rather than quantitative results by this method since it does not remove the high-energy double-hole configurations in Cu sites. Some indication of the accuracy of the band approach is provided by a comparison [17] of the results of AF studies of the CuO_2 plane obtained by a MF band calculation with those obtained by a Gutzwiller *ansatz* method. Both methods yield qualitatively similar phase diagrams, although the MF method gives enhanced values of the energy gap and the critical doping destroying the AF ordering.

The original set of parameters for the present 2D calculations taken from [9] are

$$t(N_h = 0) = 1.3 \text{ eV} \quad Q = 1.2 \text{ eV} \quad U_d = 10.0 \text{ eV} \quad U_p = 4.0 \text{ eV} \quad (33)$$

together with $\varepsilon_d - \varepsilon_p = 1.2 \text{ eV}$ [9] at $N_h = 0$. Our study is extended also to cases with $\varepsilon_d - \varepsilon_p < 0$ since these models reveal an explicit region of superconductivity. So

$$(\varepsilon_d - \varepsilon_p)_{N_h=0} = -2 - 1.2 \text{ eV}. \quad (34)$$

Other key parameters can be evaluated as $K_d, K_p \approx t, J \sim t^2/I$ where $I = |\varepsilon_d^0 + \varepsilon_p^0|/2$. The main calculations are done for

$$K_d \approx K_p \approx t \quad J = 0 \quad (35)$$

or

$$K_d \approx 0 \quad K_p \approx t \quad J = 0. \quad (36)$$

The calculations also incorporate the reduced values $(U_d, U_p) = (8.0, 3.2) \text{ eV}$ as well as $(10.0, 4.0) \text{ eV}$. The aim of such testing is to compensate the known shortcoming of the MF theory which overestimates the role of large interactions.

Table 3 presents some of the sets of parameters used as well the values of the 'zero' parameters $\varepsilon_d^0, \varepsilon_p^0$ and t_0 corresponding to chosen values of t and ε_d without doping. Here we set $\varepsilon_p = 0$ at $N_h = 0$. The condition $|\varepsilon_d - \varepsilon_p| \sim t$ leads to large value of $|\varepsilon_d^0 - \varepsilon_p^0|$.

Figure 2 presents some typical dependences of the renormalized parameters t and $E_d = \varepsilon_d - \varepsilon_p$ of the upper band upon the hole concentration $N_h = 5 - n_e$ associated with doping. They have been obtained by solution of the HF equations (5)–(8) at fixed $\varepsilon_d^0, \varepsilon_p^0$ and t_0 determined by E_d, t at $N_h = 0$. The variation in E_d with doping plays an important role. When all other parameters are kept equal, the holding of E_d constant leads to an extension of the AF phase region and the disappearance of the SC region.

As a first step the phase diagrams have been studied for transitions from the normal state (N) to each of the states with one separate type of pairing (AF or SC s or SC d). The dependences $T_c(N_h)$ of the transition temperature upon doping for each type of pairing have been obtained from the equations

Table 3. Some variants of the parameters used in calculations together with the values for $t(N_h = 0) = 1.3$ eV, $Q = 1.2$ eV, $J = 0.0$ eV. We set the renormalized energy of the p orbital as $\epsilon_p(N_h = 0) = 0$ eV; thus ϵ_d^0 and ϵ_p^0 are measured from $\epsilon_p(0)$.

No	$E_d(N_h = 0)$ (eV)	U_d (eV)	U_p (eV)	K_d (eV)	K_p (eV)	ϵ_d^0 (eV)	ϵ_p^0 (eV)	t_0 (eV)
1	1.2	10.0	4.0	1.3	1.3	-15.9	-7.7	3.21
2	0.0	10.0	4.0	1.3	1.3	-17.4	-7.9	3.24
3	0.0	8.0	3.2	1.3	1.3	-15.9	-7.2	3.24
4	-1.0	10.0	4.0	1.3	1.3	-18.6	-8.0	3.26
5	-1.0	8.0	3.2	1.3	1.3	-17.0	-7.3	3.26
6	-1.0	10.0	4.0	0.0	2.0	-17.1	-8.4	2.84
7	-1.0	10.0	4.0	0.0	2.2	-17.1	-8.5	3.00
8	-1.3	10.0	4.0	0.0	2.0	-17.5	-8.4	2.82
9	-1.3	10.4	4.0	0.0	2.2	-17.5	-8.5	2.99

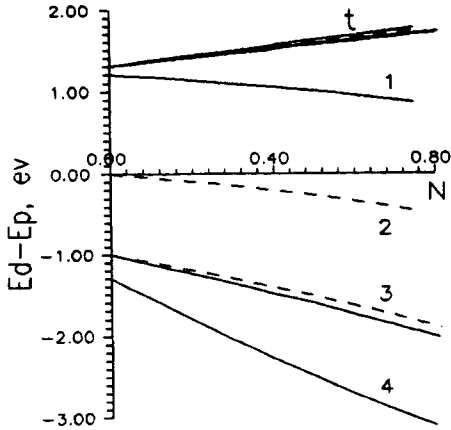


Figure 2. Dependences of the band parameters $E_d(N_h) = \epsilon_d - \epsilon_p$ (curves 1–4) and $t(N_h)$ (curves t) on the hole number $N = N_h$ obtained from solutions of the HF equations (8) for some variants of the parameters from table 3 ($t(N_h = 0) = 1.3$ eV): curves 1, 2, 3 and 4, $E_d(N_h = 0)$ equal to 1.2, 0.0, -1.0 and -1.3 eV, respectively; —, $U_d = 10$ eV, $U_p = 4$ eV; ---, $U_d = 8$ eV, $U_p = 3.2$ eV. The other parameters are from table 3. The p–d transfer integral depends slightly on the parameters chosen.

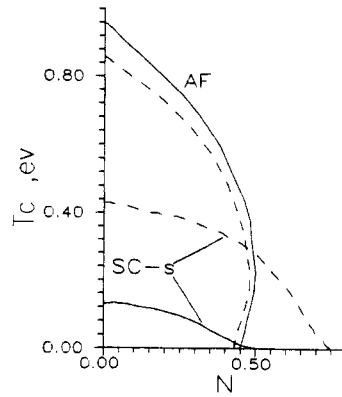


Figure 3. The ‘zero’ phase curves for AF to N and SC to N transition for variants 2 and 3 of the parameters from table 3 ($E_d(N_h = 0) = 0.0$ eV; $K_d = K_p = t(N_h = 0) = 1.3$ eV): —, $U_d = 10$ eV, $U_p = 4$ eV; ---, $U_d = 8$ eV, $U_p = 3.2$ eV. The other parameters are as in table 3.

$$\det(D_{\nu\nu'}) = 0 \quad D_{\nu\nu'} = \delta_{\nu\nu'} - \partial\Delta^\nu / \partial\Delta^{\nu'} \quad \text{at } \Delta^\nu = 0 \quad (37a)$$

or

$$D_{\nu\nu'} = \delta_{\nu\nu'} - \partial\Gamma^\nu / \partial\Gamma^{\nu'} \quad \text{at } \Gamma^\nu = 0. \quad (37b)$$

Here $\nu = 1-5$ for $\Delta^\nu = \Delta_3^\nu$ from table 1 for the N-to-AF transition and $\nu = 1-7$ or

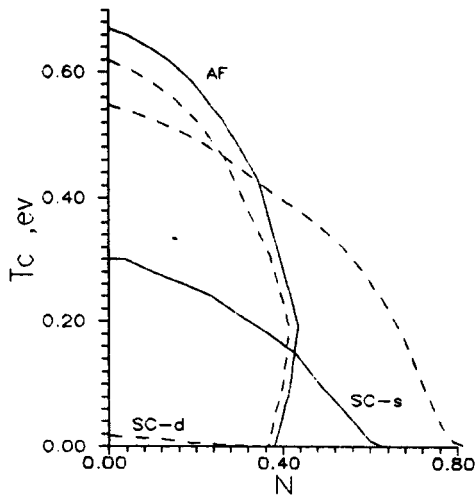


Figure 4. The same as in figure 3 for variants 4 and 5 of parameters from table 3 ($E_d(N_h = 0) = -1$ eV): —, $U_d = 10$ eV, $U_p = 4$ eV; ---, $U_d = 8$ eV, $U_p = 3.2$ eV. The other parameters are as in table 3. The solution for the 'zero' N-SC d boundary exists only for $U_d = 8$ eV and $U_p = 3.2$ eV but lies entirely inside the AF or SC s region.

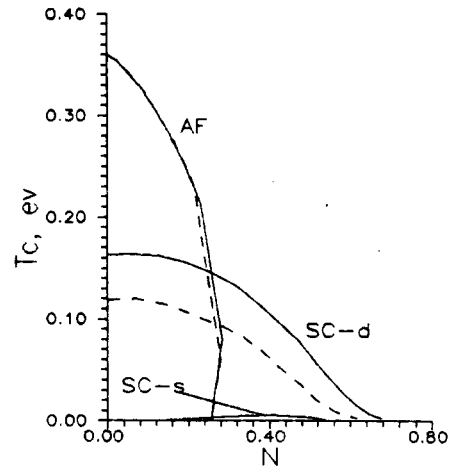


Figure 5. The 'zero' phase boundaries for the AF-to-N and SC-d-to-N transitions for variants 8 (—) and 9 (---) of the parameters from table 3 ($E_d(N_h = 0) = -t(N_h = 0) = -1.3$ eV; $U_d = 10$ eV; $U_p = 4$ eV; $K_d = 0$ eV): —, $K_p = 2.0$ eV; ---, $K_p = 2.2$ eV. The SC s-N boundary appears only at $K_p > 2.1$ eV but lies entirely inside the AF region.

$\nu = 8-11$ for Γ^ν from table 2 for the N-to-SC s or N-to-SC d transitions. The derivatives in (38) are calculated directly as 2D integrals over the phase region $F/8 = \pi^2/4$ owing to symmetry of the integrand. Some inaccuracy of the phase curves at high temperature may be connected with the simplifying assumption that the band parameters are functions of the low-temperature hole concentration instead of the actual concentration. This does not disturb the low-temperature parts of the boundaries.

Figures 3–5 present examples of such phase diagrams for the sets of parameters given in table 3. At $E_d = 1.2$ eV > 0 the N-SC s boundary can occur partly outside the AF region only for very small Coulomb integrals U_d and U_p reduced to values of 5.1 eV and 1.3 eV. However, at $E_d < 0$ there is a doping region where the SC-N boundary can be partly outside the AF-N boundary even for large Coulomb integrals U_d and U_p if the parameters K_d and K_p of the correlated hopping interaction are sufficiently large. Depending on the relation between K_d and K_p , superconductivity of s type occurs if $K_d \approx K_p \approx t$ or of d type if $K_d \ll K_p \approx 1.5t$.

If $K_d = K_p = t$ the SC s phase exists as one can see in figures 3 and 4 for $E_d = 0$, $U_d = 8$ eV, $U_p = 3.2$ eV, and for $E_d = -1.0$ eV, $U_d = 10$ eV, $U_p = 4.0$ eV. The N-SC d boundary lies entirely inside the AF region if it does exist. An increase in the exchange interaction up to $J = 2$ eV leads to extension of the 'zero' N-SC d boundary but it is insufficient to create the SC d phase at $K_d = K_p = t$. A reduction in both the parameters K_d and K_p markedly shortens the range of the SC s solution.

The situation is reversed at $K_d = 0$, $K_p > t$. The 'zero' N-SC s boundary disappears at $K_p < 2.1$ eV, but there is a large SC d region after destruction of the AF order. Figure 5 demonstrates this phenomena for $E_d = -t = -1.3$ eV, $K_d = 0$ and $K_p = 2.2$ eV (full curves) or $K_p = 2.0$ eV (broken curves). Other parameters are as in (34).

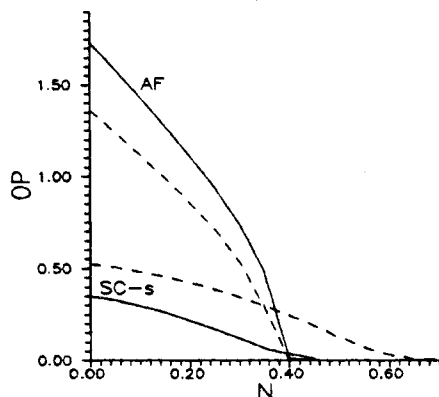


Figure 6. The most representative order parameters as functions of the hole concentration: $\Delta_{\frac{1}{3}}^{\nu=1}(N_h)$ determined from equation (25) and table 1 for the AF solution and $\Gamma_{00}^{\nu=5}(N_h)$ determined from equation (26) and table 2 for the SC s solution for variants 4 (—) and 5 (---) from table 3 ($E_d(N_h = 0) = -1.0$ eV; $K_d = K_p = t(N_h = 0) = 1.3$ eV): —, $U_d = 10$ eV, $U_p = 4$ eV; ---, $U_d = 8$ eV, $U_p = 3.2$ eV. The index ν in Δ^{ν} or Γ^{ν} enumerates the OP according to table 1 or 2.

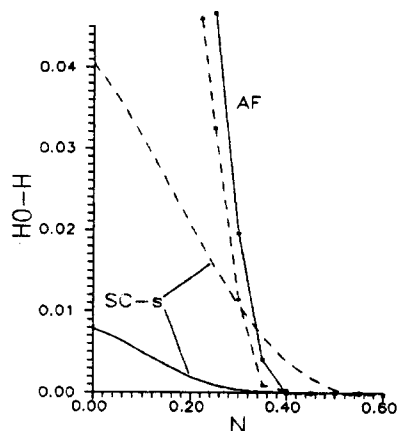


Figure 7. The energy gain during AF or SC s ordering, i.e. the difference ΔH in equation (30) between the energies of the band state and self-consistent MF state with corresponding ordering for variants 4 and 5 of the parameters ($E_d(N_h = 0) = -1.0$ eV; $K_d = K_p = t(0) = 1.3$ eV): —, $U_d = 10$ eV, $U_p = 4$ eV; ---, $U_d = 8$ eV, $U_p = 3.2$ eV.

The reality of the ‘zero’ phase diagram or more exactly of the correct boundaries of the N phase is confirmed by the solutions of the self-consistent equations (25)–(28) for OPs. The iteration procedure for finding the OP works only at a fixed number of particles but not at a fixed chemical potential. Sequential values of the OP converge to the OP values of ‘pure’ solutions corresponding to only AF or only SC ordering (but not mixed ordering) or to zero for the N state. Thus the general solution can be obtained by finding both ‘pure’ solutions and choosing one of them with minimal energy. This accelerates the calculations and allows one to overcome the problem of slow convergence of the iteration procedure near the switching point between AF and SC phases.

Some characteristics of AF and SC solutions at $T = 0.005$ eV = 58 K are presented in figures 6–10 for various sets of parameters. The most representative OP $\Delta_{\frac{1}{3}}^{\nu=1}$ and $\Gamma_{00}^{\nu=4}$ for SCs or $\Gamma_{00}^{\nu=11}$ for SC d are shown in figures 6 and 9. A $\Delta_{\frac{1}{3}}$ -value of 1.5 corresponds to a local magnetic moment on Cu of $(0.3\text{--}0.4)\mu_B$ instead of the observed value of $0.6\mu_B$ [2, 12]. The difference may be connected with the approximation of frozen lower bands.

The energy gain during the AF or SC s ordering as a function of N_h is given in figure 7 for $E_d = -1.0$ eV, $K_d = K_p = t$. It is obtained by use of equations (30)–(32). The crossing of the AF and SC curves is the point of switching of solutions. The energy gain during SC d ordering (e.g. at $E_d = -1.3$ eV, $K_d = 0$, $K_p = 2.0$ eV) is significantly less than for SC s in figure 7. The range of doping where the SC solution has the lowest energy correlates quantitatively with the part of the ‘zero’ SC–N phase boundary outside the region of AF ordering. The energy gaps G for the AF and SC solutions are demonstrated in figures 8 and 10.

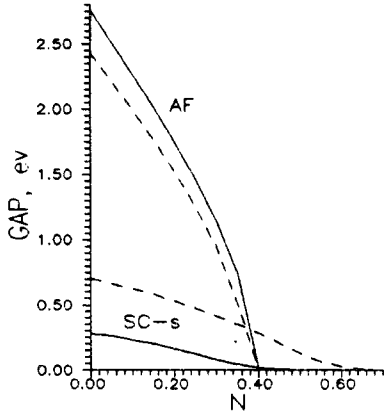


Figure 8. The gap in the energy spectrum as a function of $N = N_h$ for the AF and SC s solutions for variants 4 (—) and 5 (---) of the parameters from table 3 ($E_d(N_h = 0) = -1$ eV; $K_d = K_p = t(N_h = 0) = 1.3$ eV): —, $U_d = 10$ eV, $U_p = 4$ eV; ---, $U_d = 8$ eV, $U_p = 3$ eV. The gap is independent of the k direction.

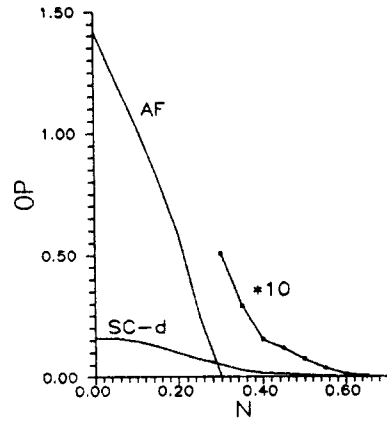


Figure 9. The most representative parameters $\underline{\Delta}_3^1(N_h)$ of the AF solution and $\underline{\Gamma}_{00}^{10}(N_h)$ of the SC d solution for variant 9 of the parameters from table 3 ($E_d(N_h = 0) = -t(N_h = 0) = -1.3$ eV; $U_d = 10$ eV; $U_p = 4$ eV; $K_d = 0$ eV, $K_p = 2.0$ eV). The upper index in the $\underline{\Delta}^i$ or $\underline{\Gamma}^i$ enumerates the OPs according to table 1 or 2. $\underline{\Gamma}_{00}^{10}(N)$ multiplied by ten is also shown.

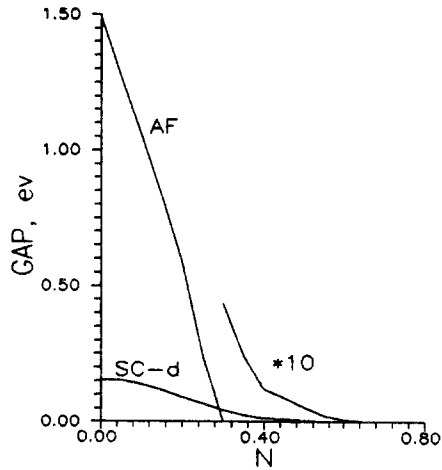


Figure 10. The gap in the energy spectrum for the AF solution as a function of $N = N_h$ and the maximal value of the energy gap for the SC d solution in the direction $k_x = k_y$ for variant 8 of the parameters from table 3 ($E_d(N_h = 0) = -1.3$ eV, $U_d = 10$ eV, $U_p = 4$ eV; $K_d = 0$ eV, $K_p = 2.0$ eV). The SC d gap multiplied by ten is also shown.

In comparison with the s type of superconductivity at $K_d \approx K_p \approx t$ the d type of superconductivity at $K_d = 0, K_p > t$ seems more plausible (if at all) for a description of the real system for the following reasons.

(i) It corresponds to the more realistic, relatively small scale of T_c and of the energy gap, contrary to SC s. However, for both SC s and SC d the MF approach gives the ratio $G/kT_c < 1$ instead of the experimental values of 2.4–8 (see [2]) and the BKS prediction of 3.

(ii) Similar values of K_d and K_p for such different sites as Cu and O are hardly probable.

(iii) Strong correlations of electrons on the Cu site can suppress the influence of first term in the correlated hopping interaction (3b) depending on the Cu occupancy.

5. Conclusions

In the framework of the MF theory applied to the upper band of the well known three-band model the possible types of pairing are classified and the contributions of various local interactions to the corresponding ordering are given in tables 1 and 2. MF calculations indicate possible superconductivity which is responsible for the local interaction $V_K \sim K_d, K_p$ of correlated hopping between Cu and O centres. The SC solution appears only at $E_d = \epsilon_d - \epsilon_p < 0$, i.e. in case of preferential occupation of O sites by holes and it can be of s type for $K_d \approx K_p \approx t$ or of d type at $K_d \ll K_p \approx 1.5t$. The range of doping with superconductivity follows the region of AF ordering but solutions with the coexistence of AF and SC regions have not been found.

If the models considered have any relation to the actual mechanism of superconductivity, then many problems must be solved.

(i) Independent evaluation of the correlated hopping integrals and establishment of their signs are needed.

(ii) The relative energy $E_d = \epsilon_d - \epsilon_p$ of the d orbit must be more exactly estimated.

(iii) The assumption of frozen lower bands in the MF approach must be discarded and the electronic correlations beyond the MF theory must be considered.

(iv) The possibility of the coexistence of SC d and AF ordering with other types of ordering such as SDW of orthorhombic 'p' symmetry which provides variation in the energy gap of the AF state must be studied.

(v) The overlap between the p orbitals in the model must be included.

Appendix 1. Properties of the operators $t_\mu, r_{SM}, z_{SM}, \Delta, \Gamma, Z$ and interpretation of the corresponding ops

The separable form of the first term in the model interaction (11)

$$V_{AF} = \sum_{\nu\mu} K_\mu^\nu D_\mu^\nu (D_\mu^\nu)^\dagger \quad D_\mu^\nu = \sum_k \Phi_\mu^\nu(k) t_\mu(k) \quad (A1)$$

is a consequence of the relations for the Pauli matrices

$$\sum_\sigma (\sigma_\mu)_{\sigma\sigma} (\sigma_{\mu'})_{-\sigma,-\sigma} = 2\delta_{\mu\mu'} (\delta_{\mu 0} - \delta_{\mu 3}) \quad \sum_{\sigma\sigma'} (\sigma_\mu)_{\sigma\sigma'} (\sigma_{\mu'})_{\sigma\sigma'} = 2\delta_{\mu\mu'} \quad (A2)$$

$$\sum_\sigma (\sigma_\mu)_{\sigma,-\sigma} (\sigma_{\mu'})_{\sigma,-\sigma} = 2\delta_{\mu\mu'} (\delta_{\mu,1} + \delta_{\mu,2}).$$

To reduce equation (A1) to a similar form with Hermitian operators Δ_μ^ν we use the relation

$$t_\mu(-\vec{k}) = t_\mu^\dagger(k) \quad (A3)$$

and rewrite D (we omit indices for the moment) as a sum over k ranging through half

the phase volume F inside the 2D Fermi surface of the half-filled upper band (broken region in figure 1):

$$D = \sum_{k \in F} [\Phi(k)t_{\mu}(k) + \Phi(-\bar{k})t_{\mu}^+(k)]$$

$$= \sum_{k \in F} \varphi_+(k)[t_{\mu}(k) + t_{\mu}^+(k)] + \sum_{k \in F} \frac{\varphi_-(k)[t_{\mu}(k) - t_{\mu}^+(k)]}{i}$$

Here $\varphi_+(k) = [\Phi(k) + \Phi(-\bar{k})]/2$, $\varphi_-(k) = i[\Phi(k) - \Phi(-\bar{k})]/2$. Then $DD^+ = \Delta_{\pm}^2 + \Delta_{\pm}^2$ where $\Delta_{\pm} = \sum_k \varphi_{\pm}(k)t_{\mu}(k)$ correspond to weighting functions with definite symmetry

$$\varphi(-\bar{k}) = \varphi^*(k). \quad (\text{A4})$$

Table 1 summarizes such functions corresponding to the real OP Δ_{μ}^{ν} .

To interpret these quantities we compare them with the spin densities $\rho_{\mu}(d, n)$, $\rho_{\mu}(x, n)$, $\rho_{\mu}(y, n)$ or with the total densities $2\rho_0(\alpha, n)$, $\alpha = d, x, y$ of the band electrons on $d_{x^2-y^2}$, p_x or p_y orbitals of the n th site:

$$\rho_{\mu}(d, n) = \frac{1}{2} \sum_{\sigma\sigma'} (\sigma_{\mu})_{\sigma\sigma'} \langle d_{n\sigma}^+ d_{n\sigma'} \rangle \quad \text{etc.} \quad (\text{A5})$$

Here averaging is over the upper band state with all possible collective orderings in accordance with the basic assumption of frozen lower bands.

In a lattice with the AF or CDW doubling of an elementary site, each of the quantities in (A5) has the form

$$\rho_{\mu}(\alpha, n) = \rho_{\mu}(\alpha) + (-1)^n \Delta\rho_{\mu}(\alpha) \quad n = n_x + n_y \quad \alpha = d, x, y$$

$$\Delta\rho_{\mu}(\alpha) = N^{-1} \sum_n (-1)^n \rho_{\mu}(\alpha, n). \quad (\text{A6})$$

In the quasiparticle approximation with the linearized Hamiltonian (16), calculations yield the connection of quantities (A6) with the AF OP:

$$\Delta\rho_{\mu}(d) = \underline{\Delta}_{\mu}^{\nu=1}/\kappa_{\mu}^1 \quad \Delta\rho_{\mu}(x) = \underline{\Delta}_{\mu}^6/\kappa_{\mu}^6 \quad \Delta\rho_{\mu}(y) = \underline{\Delta}_{\mu}^{6'}/\kappa_{\mu}^{6'}. \quad (\text{A7})$$

The upper index in Δ_{μ}^{ν} enumerates the corresponding weighting functions in table 1.

Similarly one can define the extended bond order $p_{j\mu}(n)$, i.e. the spin density ($\mu = 1, 2, 3$) or total density $2p_{j0}(n)$ of each of four Cu–O bonds $j = 1, 2, 3, 4$ of the Cu centre of the n th site:

$$p_{j\mu}(n) = \begin{cases} \sum_{\sigma\sigma'} (\sigma_{\mu})_{\sigma\sigma'} \langle d_{n\sigma}^+ x_{n\sigma'} + x_{n\sigma}^+ d_{n\sigma'} \rangle & j = 1 \\ -\sum_{\sigma\sigma'} (\sigma_{\mu})_{\sigma\sigma'} \langle d_{n\sigma}^+ y_{n\sigma'} + y_{n\sigma}^+ d_{n\sigma'} \rangle & j = 2 \quad \text{etc.} \end{cases} \quad (\text{A8})$$

Symmetric combinations of the bond densities after the separation of alternating parts $\sim (-1)^n$ correspond to the OPs from table 1:

$$\sum_{\mu} p_{j\mu} \rightarrow \Delta_{\mu}^3 \quad \left. \begin{matrix} p_{1\mu} - p_{3\mu} \\ p_{2\mu} - p_{4\mu} \end{matrix} \right\} \rightarrow \Delta_{\mu}^{7(7')} \quad p_{1\mu} - p_{2\mu} + p_{3\mu} - p_{4\mu} \rightarrow \Delta_{\mu}^{10}.$$

One can also construct various combinations of the spin or charge currents within

the elementary site which alternate with n and correspond to states of the orbital antiferromagnet if Δ_μ^2 or Δ_μ^{11} is non-zero or to more complicated structures.

Separability of the anomalous parts of the model interaction (11) over S, M and the symmetry of the r and z operators given by

$$r_{SM}(-k) = (-1)^s r_{SM}(k) \quad z_{SM}(\vec{k}) = (-1)^s z_{SM}(k) \quad (\text{A9})$$

follow from symmetry and the orthogonality properties of the Clebsch–Gordon coefficients. Because of equation (A9) the singlet pairing corresponds only to even weighting functions and the triplet pairing only to odd functions:

$$g_{SM}^\nu(-k) = (-1)^s g_{SM}^\nu(k) \quad \chi_{SM}^\nu(\vec{k}) = (-1)^s \chi_{SM}^\nu(k).$$

This accounts for the arrangement of the weighting functions χ over S in table 2.

Appendix 2. Linearized Hamiltonian

The operators of the number $N_h = 5 - n_c$ of holes and the band energy are expressed via operators b_j (see equation (20)) in the following way:

$$N_h(\mu) = 1 - N^{-1} \sum_j \sum_{k \in F} \eta_j b_j^+(k) b_j(k) \quad (\text{A10})$$

$$\langle H_1 - \mu N \rangle = N^{-1} \sum_j \sum_{k \in F} \eta_j [\varepsilon(k_j) - \mu] b_j^+(k) b_j(k) \quad (\text{A11})$$

$$k_j(k) = \{k, -\vec{k}, -k, \vec{k}\}_j \quad \eta_j = \{1, 1, -1, -1\}_j \quad j = 1, \dots, 4. \quad (\text{A12})$$

To find L_{ij} in (21) it is sufficient to rewrite Δ, Γ, Z via the operators b_j defined by equation (20):

$$\Delta_\mu^\nu = \frac{\kappa_\mu^\nu}{2} \sum_{k \in F} \{[\varphi_\mu^\nu(k) b_1^+(k) b_2(k) - (-1)^\mu \varphi_\mu^\nu(\vec{k}) b_3^+(k) b_4(k)] + \text{HC}\} \quad \mu = 0, 3 \quad (\text{A13})$$

$$\Gamma_{s0}^\nu = \gamma_s^\nu \sum_{k \in F} [g_s^\nu(k) b_3^+(k) b_1(k) + g_s^\nu(-\vec{k}) b_4^+(k) b_2(k)] \quad (\text{A14})$$

$$Z_{s0}^\nu = \zeta_s^\nu \sum_{k \in F} [\chi_s^\nu(-\vec{k}) b_3^+(k) b_2(k) + \chi_s^\nu(k) b_4^+(k) b_1(k)]. \quad (\text{A15})$$

Substituting equations (A13)–(A15) into equation (16) and comparing with (21), one finds the elements L_{ij} of the Hermitian matrix:

$$\begin{aligned} L_{jj} &= \eta_j [\varepsilon(k_j) - \mu] & L_{21} &= \sum_{\nu\mu} \Delta_\mu^\nu \varphi_\mu^\nu(k) & L_{31} &= \sum_{\nu s} \Gamma_{s0}^\nu g_s^\nu(k) \\ L_{41} &= \sum_{\nu s} Z_{s0}^\nu \chi_s^\nu(k) & L_{32} &= \sum_{\nu s} Z_{s0}^\nu \chi_s^\nu(-\vec{k}) & \\ L_{42} &= \sum_{\nu s} \Gamma_{s0}^\nu g_s^\nu(-\vec{k}) & L_{43} &= -\sum_{\nu\mu} (-1)^\mu \Delta_\mu^\nu \varphi_\mu^\nu(\vec{k}). \end{aligned} \quad (\text{A16})$$

Appendix 3. Coefficient Q_M indicative of the Meissner effect

To calculate the coefficient Q_M it is sufficient [19] to find $\langle j_q \rangle$ to second order in $A(r)$:

$$\langle j_q \rangle = -c \frac{\partial}{\partial A_q} \sum_{m \neq m'} F(m) \frac{\langle m H^{(1)} m' \rangle}{E_m - E_{m'}} + \sum_m F(m) \langle m H^{(2)} m \rangle = Q_M A_q. \quad (\text{A17})$$

$$Q_M = Q_I + Q_{II}. \quad (\text{A18})$$

Here m are the states of system diagonal over the number of quasiparticles and $F(m)$ is a distribution function over these states, $H^{(1)}$ and $H^{(2)}$ are the terms of first and second order in the expansion of the electronic Hamiltonian $H_A = \sum_q \varepsilon(k - e/cA) a_{k\sigma}^\dagger a_{k\sigma}$ in the field $A(r) = \sum_q A_q \exp[iqr]$. At $q \rightarrow 0$ they are

$$H^{(1)} = -\frac{e}{c} \sum_{kq} (A_q \nabla) \varepsilon(k) a_{k-\sigma}^\dagger a_{k+\sigma} \quad k_\pm = k \pm q/2 \quad (\text{A19})$$

$$H^{(2)} = \frac{e^2}{c^2} \sum_{kqq'} (A_q \nabla) (A_{q'} \nabla) \varepsilon(k) a^+(k\sigma) a(k+q+q', \sigma). \quad (\text{A20})$$

$H^{(1)}$ can be represented via the quasiparticle operators as

$$H^{(1)} = -\frac{e}{c} \sum_i (A_q)_i \sum_{k \in F} \sum_{nl} W_{nl}^i \beta_l^+(k_-) \beta_n(k_+) \quad (\text{A21})$$

$$W_{nl}^i = \sum_j \eta_j (U^+)_{nj} \nabla_i \varepsilon(k_j) U_{jl} \quad (\text{A22})$$

$$\{k_j\} = \{k, -\tilde{k}, -k, \tilde{k}\} \quad \eta_j = \{1, 1, -1, -1\} \quad j = 1, \dots, 4. \quad (\text{A23})$$

Each operator $\beta_l^+(k_-)$ and $\beta_n(k_+)$ from (A21) contributes to (A17) only for states m in (A17) with occupation numbers $n_l(k_-) = 1$, $n_n(k_+) = 0$ so that

$$E_m - E_{m'} = E_n(k_+) - E_l(k_-) = \begin{cases} (q\nabla) E_l(k) & \text{at } l = n \\ E_l(k) - E_n(k) & \text{at } l \neq n \end{cases}$$

$$F(m) = \tilde{F} f_l(k_+) [1 - f_n(k_-)] = \begin{cases} F_0 - \tilde{F} f'_l (q\nabla E_l) / 2 & \text{at } l = n \\ \tilde{F} f_l (1 - f_n) & \text{at } l \neq n. \end{cases}$$

Here F_0 is an insignificant isotropic term, f_L is the Fermi function, $f'_l = df_l/dE_l$ and \tilde{F} refers to the occupation numbers for momenta other than k_+ , k_- . It has a value of unity after summation. Thus the first term in (A18) is

$$Q_I = -\frac{e^2}{c^2} \sum_{ln} \sum_{k \in F} W_{ln}^i W_{ln}^i \left(\delta_{nl} \frac{df_l}{dE_l} - \frac{f_l(1-f_n)}{E_l - E_n} (1 - \delta_{ln}) \right). \quad (\text{A24})$$

The second term in (A2) is equal to

$$Q_{II} = \frac{1}{2c^2} \sum_{jn} \sum_{k \in F} \eta_j \nabla_i \cdot \nabla_i \varepsilon(k_j) |U_{jn}(k)|^2 f_n. \quad (\text{A25})$$

It is easily verified that, if all ops are zero, then $Q_M = Q_I + Q_{II} = 0$ for arbitrary zone dispersion at any occupancy of the band.

Note added in proof. As has just become known to us, I O Kulik [20] and J E Hirsch and co-workers [21–24] have suggested and elaborated upon similar ideas about the mechanism of SC caused by the correlated hopping interaction (CHI). Many important results have been obtained [21–24] for models described by effective on-site and inter-site parameters. In a more detailed picture [20] the SC is caused by the CHI connected with direct hopping between p orbitals of O sites. Based on a physical argument about the increase in the orbital size during its occupation I O Kulik chooses the sign of the p–p CHI such that the effective p–p transfer integral increases with occupation of these orbitals. In terms of the upper band states spanned on our basis differing from [20] we verify that it is indeed the sign of the p–p CHI that is needed to provide the possibility of SC. This differs from our p–d CHI for which attractive effects in SC are achieved when occupation of p or d orbitals reduces the effective p–d transfer integral. It is very interesting to include the p–p CHI in MF calculations.

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