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Extended Emery models with antiferromagnetic and superconducting pairings

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Abstract. The mean-field (MF) study of electronic pairing in the CuO_2 plane of high-temperature superconductors (HTSC) in the band approach is extended to Emery-like models including p_o–p_σ hopping in addition to p_σ–d hopping and a detailed picture of local interactions. Various types of correlated hopping interactions (CHI) are tested as factors that might induce superconductivity (SC). A classification of the order parameters (OP) for all types of pairing is presented for the upper band of such an extended three-band Emery model. Self-consistent equations for all OP are derived. The MF calculations of phase diagrams show that s-type SC may be induced by p–d or p–p CHI, but such systems (in the MF approach) do not exhibit antiferromagnetism (AF) in the undoped case. In contrast, models with large p–d CHI governed by p occupancy may exhibit both d-type SC and AF at small doping, and there is a range of doping where d-type AF and d-type SC may coexist.

1. Introduction

Although the mechanism of superconductivity (SC) in high-temperature superconductors (HTSC) remains unknown up to now, there are some indications that it may be of electronic nature [1]. A variety of different mechanisms have been discussed (RVB [2], spin-bag [3], pairing of oxygen holes [4–6]). Searching for the possible pairing interaction led Kulik [6] and Hirsch and Marsiglio [4, 5] to the idea that the so-called correlated hopping interaction (CHI) might be responsible for SC. Concerning electrons in the CuO_2 plane of Cu-containing HTSC ($La_{2-x}Ba_xCu_2O_4$, $YBa_2Cu_3O_{6+x}$), they have proposed that CHI between both p_π, p_σ orbitals [6] or p_π orbitals [4, 5] of oxygen is important. The mean-field (MF) study of the latter models has been carried out [4]. It demonstrates that for certain models the CHI can compete with the on-centre Coulomb repulsion and provide the SC with reasonable physical properties (penetration depth, gap ratio, etc). The studies [4, 5] are not concerned with magnetic properties—antiferromagnetic (AF) ordering of nearly undoped materials and their dielectric behaviour.

It is, however, hard to accept that the 3d electrons of Cu are completely localized by the correlation effects. Apart from magnetic data, the local-density approximation (LDA) results [7–9] on the electronic structure in conjunction with correlated models [10] and photoemission data [11] seem to indicate the strong covalency of CuO bonds. Thus a study of tight-binding models similar to Emery models exhibiting AF [12] or both AF and SC are of certain interest even within the simple MF approximation in the band approach. In this way a variety of local interactions in the CuO_2 plane have been

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incorporated [13] for the known three-band Emery model in which the SC is caused by the p–d CHI. The latter modulates the hopping between the nearest-neighbour $O(p_\sigma)$ and $Cu(d_{x^2-y^2})$ orbitals depending on the occupancy of these orbitals. The MF theory in the band approach has been used for the upper (incompletely filled) band with the assumption of two frozen lower (filled) bands. The band approach seems to be reasonable for obtaining some information if effective Hartree–Fock (HF) energies of the p and d orbitals (renormalized by large Coulomb interactions) are close, thus providing strong hybridization of these orbitals. A comparison of itinerant versus localized pictures of HTSC is discussed in [14].

One of the aims of the present work was to extend the previous study [13] to models including this direct $p_\sigma - p_\sigma$ hopping (which is not small, $t_p \approx 0.65$ [15, 16]), as well as $p_\sigma - p_\sigma$ CHI in addition to $p_\sigma - d$ hopping and CHI. The p_π orbitals are not considered since both the LDA [7–9] and experiment [11] give evidence of the p_σ nature of the hole states in oxygen. Some mistakes made in [13] are removed here and the re-examined results for 'pure' Emery models are also given.

Our second aim was to study more thoroughly the compatibility of the SC and AF orderings. For this, calculations of phase diagrams for SC transition on the background of an ordered AF state are also performed.

Our third aim was to estimate roughly the admissible range of the key parameters permitting the models to display both AF and SC properties, though the final predictions of course need a more accurate treatment of correlations than that given by MF theory.

The outline of the paper is as follows. In section 2 the formulation of the HF problem and of the model Bardeen–Cooper–Schrieffer (BCS)-like Hamiltonian with all types of SC and AF pairings [13] is briefly reworded for the extended Emery model. All possible order parameters (OP) are characterized in terms of eigenvectors of the HF problem instead of their explicit analytical expressions [13] accessible only for the 'pure' Emery model. Then the linearized model Hamiltonian and self-consistent equations for the OP are derived together with equations for the phase boundaries $T_c(N_h)$ determining the appearance of some type of SC ordering from disordered normal (N) state or on the background of the AF state. Section 3 discusses more accurate results for re-examined 'pure' Emery models (with removal of some mistakes) and the results for the extended Emery model with $p_\sigma - p_\sigma$ hopping.

2. The Hartree–Fock problem and the model Hamiltonian

Consider the extended Emery model [17–21] in the basis of $Cu(d_{x^2-y^2})$, $O(x = p_\sigma)$, $O(y = p_\sigma)$ orbitals including the $p_\sigma - p_\sigma$ hopping ($\sim t_p$) in addition to $p_\sigma - d$ hopping. As in [13] the electronic representation is used here and $d^+_{n\sigma}, x^+_{n\sigma}, y^+_{n\sigma}$ are the corresponding creation operators. The Hamiltonian of the model is

$$H = H_0(\varepsilon_p^0, \varepsilon_d^0, t^0, t_p^0) + V_U + V_Q + V_J + V_K^I + V_K^{II} + V_X \tag{1}$$

where the one-electron Hamiltonian $H_0(\varepsilon_d, \varepsilon_p, t, t_p)$ is

$$H_0 = \sum_\sigma \sum_{(nm)} \zeta_{nm} [t(d^+_{n\sigma}x_{m\sigma} - d^+_{n\sigma}y_{m\sigma} + \text{HC}) - t_p(x^+_{n\sigma}y_{m\sigma} + \text{HC})]$$
$$+ \sum_{n\sigma} \varepsilon_d d^+_{n\sigma}d_{n\sigma} + \sum_{n\sigma} \varepsilon_p(x^+_{n\sigma}x_{n\sigma} + y^+_{n\sigma}y_{n\sigma}). \tag{2}$$

Here m, n are the site numbers $n = (n_x, n_y), \ldots,$ of the nearest-neighbour p, d or p_x, p_y

orbitals, and $\zeta_{mn} = (-1)^{n-m}$ if the signs of the orbitals are chosen as in [15, 16]; t^0, t_p^0, ε_d^0, ε_p^0 are the 'zero' p–d and p–p hopping integrals and the orbital energies; V_U contains the one-centre Coulomb integrals U_d, U_p on atoms Cu and O; V_Q, V_J correspond to the Coulomb and exchange integrals Q and J for the nearest-neighbour p and d orbitals; terms V_K^I, V_K^{II} and V_X describe the correlated hopping between p and d orbitals or between p_x, p_y orbitals, governed by occupancy of d or p orbitals, respectively:

$$V_K^I = -K_d \sum_{(nm)\sigma} \zeta_{nm}[(d_{n\sigma}^+ d_{n,-\sigma}^+ x_{m,-\sigma} d_{n\sigma} + \text{HC}) - (\ldots)_y] \tag{3a}$$

$$V_K^{II} = -K_p \sum_{(nm)\sigma} \zeta_{nm}[(x_{n\sigma}^+ x_{n,-\sigma}^+ d_{m,-\sigma} x_{n\sigma} + \text{HC}) - (\ldots)_y] \tag{3b}$$

$$V_X = -X_p \sum_{(nm)\sigma} \zeta_{nm}[(x_{n\sigma}^+ x_{n,-\sigma}^+ y_{m,-\sigma} x_{n\sigma} + \text{HC}) + (\ldots)_y]. \tag{3c}$$

Here $(\ldots)_y$ denotes the same as previous brackets for y operators and K_d, K_p, X_p are corresponding hybrid integrals with p, d or p_x, p_y orbitals in the small overlap limit.

The HF approximation is used now to reduce the problem of ordering in the three-band system to that in one upper band that is incompletely filled. The HF Hamiltonian coincides with $H_0(t, t_p, \varepsilon_p, \varepsilon_d)$ but with replacement of parameters t^0, t_p^0, ε_d^0, ε_p^0 by renormalized values

$$\begin{aligned}
\varepsilon_d &= \varepsilon_d^0 + U_d\rho_d + 4(2Q + J)\,\rho_d - 8K_d\rho_{pd} \\
\varepsilon_p &= \varepsilon_p^0 + U_p\,\rho_p + 2\,(2Q + J)\,\rho_p - 4K_p\rho_{pd} - 8X_p\tau \\
t &= t^0 - (Q + 2J)\rho_{pd} - K_d\rho_d - K_p\rho_p \\
t_p &= t_p^0 + 2X_p\rho_p
\end{aligned} \tag{4}$$

where $\rho_d = \langle d_{n\sigma}^+ d_{n\sigma}\rangle$, $\rho_p = \langle x_{n\sigma}^+ x_{n\sigma}\rangle$, $\rho_{pd} = \zeta_{nm}\langle x_{m\sigma}^+ d_{n\sigma}\rangle$, $\tau = \zeta_{nm}\langle x_{n\sigma}^+ y_{m\sigma}\rangle$ are average occupations of p, d orbitals and the bond order values for definite spin projection σ.

The HF band states corresponding to creation operators $a_{k\sigma}^{+\lambda}$, $\lambda = 1, 2, 3$, are expanded on the orbital operators

$$a_{k\sigma}^{+\lambda} = N^{-1/2} \sum_{n,\sigma} e^{ikn}\alpha_j(d_{n\sigma}^+, x_{n\sigma}^+, y_{n\sigma}^+)_j\, B_{j\lambda} \tag{5}$$

$$\alpha_j = \{1, -ie^{ik_x/2}, ie^{ik_y/2}\}_j \qquad j, \lambda = 1, 2, 3 \tag{6}$$

where the real matrix B satisfies the following HF equations:

$$\begin{pmatrix} \varepsilon_d & 2ts_x & 2ts_y \\ 2ts_x & \varepsilon_p & 4t_p s_x s_y \\ 2ts_y & 4t_p s_x s_y & \varepsilon_p \end{pmatrix}_{ij} B_{j\lambda} = \varepsilon^\lambda B_{i\lambda} \tag{7}$$

$$s_x = \sin(k_x/2) \qquad s_y = \sin(k_y/2). \tag{8}$$

If the two lower bands are completely filled and only the upper band $\lambda = 1$ is partly

occupied, then the self-consistent HF equations are expressed via the eigenvectors B_{j1} of the upper band only:

$$\begin{aligned}
&\rho_d = 1 - (1/N)\sum_k (B_{11})^2 (1 - f_1) = n(\mu)/2 - 2\rho_p \\
&\rho_{pd} = -(1/N)\sum_k B_{11}(B_{21}s_x + B_{31}s_y)(1 - f_1)/2 \\
&\tau = (1/N)\sum_k s_x s_y B_{21} B_{31} (1 - f_1) \\
&n(\mu) = 6 - (2/N)\sum_k (1 - f_1) = N_h + 5.
\end{aligned} \tag{9}$$

Here N_h is the number of extra holes. Equations (9) differ from those in [13] by including the p_σ–p_σ hopping and corresponding CHI term.

As in [13] the approximation of frozen lower bands is used now, i.e. only interactions inside the upper band are retained. In such an approximation the BCS-like model Hamiltonian of the upper band is constructed, which incorporates all types of pairings with the large phase volume contribution for the nearly half-filled band. The SC or AF pairing pick out the matrix elements of interaction $\langle k_1\sigma, k_2\sigma' | V | k_4\sigma, k_3\sigma' \rangle$ with $(k_1 k_2 k_3 k_4)$, which are equal to $(k, -k, -k', k')$ or $\{(k, -\tilde{k}' k', -\tilde{k}), (k, -\tilde{k}', -\tilde{k}, k')\}$ or $(k, \tilde{k}, \tilde{k}' k')$ in addition to the usual HF terms. Here $k + \tilde{k} = (\pm\pi, \pm\pi)$, i.e. vector k is

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

The obtained model Hamiltonian $H_{mod} = H_0 + V_{AF} + V_{SC} + V_{AA}$ is thus [13]

$$H_{mod} = H_0 + N\left(\sum \Delta^\nu_\mu \Delta^\nu_\mu / \kappa^\nu_\mu + \sum \Gamma^{+\nu}_{SM} \Gamma^\nu_{SM} / \gamma^\nu_S + \sum Z^{+\nu}_{SM} Z^\nu_{SM} / \zeta^\nu_S\right) \tag{11}$$

where

$$\Delta^\nu_\mu = N^{-1}\kappa^\nu_\mu \sum{}' \varphi^\nu_\mu(k) t_\mu(k) \qquad t_\mu(k) = \frac{1}{2}\sum{}'' (\sigma_\mu)_{\sigma\sigma'} a^+_{k\sigma} a_{k\sigma'} \tag{12}$$

$$\Gamma^\nu_{SM} = N^{-1}\gamma^\nu_{SM} \sum{}' g^\nu_S(k) r^\nu_{SM}(k) \qquad r^\nu_{sm}(k) = (1/\sqrt{2}) \sum{}'' C^{SM}_{\sigma\sigma'} a_{-k\sigma'} a_{k\sigma} \tag{13}$$

$$Z_{SM} = N^{-1}\zeta^\nu_S \sum{}' \chi^\nu_S(k) z_{SM}(k) \qquad z_{SM}(k) = (1/\sqrt{2}) \sum{}'' C^{SM}_{\sigma\sigma'} a_{k\sigma'} a_{k\sigma} \tag{14}$$

Here $\sigma_\mu, \mu = 0, 1, 2, 3$, are the Pauli matrices; $C^{SM}_{\sigma\sigma'}$ is the Clebsch–Gordan coefficient for spins 1/2; Σ, Σ', Σ'' are sums over μ, ν, S, M or over k or over σ, σ' respectively. Index ν numerates all possible operators Δ, Γ and Z. Here Hermitian operators Δ correspond to the spin-density wave (SDW) ($\mu = 1,2,3$) or charge-density wave (CDW) ($\mu = 0$) real OP $\underline{\Delta}^\nu_\mu = \langle \Delta^\nu_\mu \rangle$ [13] and Γ, Z correspond to the SC OP $\Gamma^\nu_{SM} = \langle \Gamma^\nu_{SM} \rangle$ or the alternate anomalous (AA) OP $\underline{Z}_{SM} = \langle Z_{SM} \rangle$. The latter refer to OP of type $\langle a_n a_n \rangle \sim (-1)^n$ and can appear in the region of coexistence of AF and SC. The physical meaning of $\underline{\Delta}$, $\underline{\Gamma}$, $\underline{Z}$ has been discussed in [13].

Constants κ, γ and weight functions φ, g are classified in tables 1 and 2 in terms of the original parameters of the model and the eigenvectors B_{j1} of the upper band determined by solution of equation (7). Similar values ζ, χ have been obtained. The reduction of H_{mod} to separable form (11) follows from the properties of operators t, r, z

Table 1. Constants κ and functions φ in operators Δ_μ^ν in equations (12) responsible for SDW ($\mu = 1, 2, 3$) or CDW ($\mu = 0$) of three different types of symmetry ($\nu = 1$–5 or $\nu = 6$–9 or $\nu = 10, 11$). The φ^ν, κ^ν, $\nu = 8$–14, have their analogues $\nu = 8'$–$14'$ with the same κ^ν and φ^ν obtained by replacement $x \to y$, $B_{21} \to B_{31}$. Here $\eta_\mu = 1$, $\mu = 1, 2, 3$; $\eta_0 = -1$; $A_\mu = Q/2 - \delta_{\mu,0}J$; $\omega_x = -ik_x/|k_x|$; $\tilde{f} = f(\tilde{k})$; $F_x = \omega_x \tilde{B}_{11} B_{12} \tilde{s}_x$; $F_{s(d)} = \tilde{B}_{11}(B_{21} s_x \pm B_{31} s_y)$; $L = \omega_x(B_{21}\tilde{B}_{31}\tilde{s}_x\tilde{s}_y + B_{31}\tilde{B}_{21}s_x s_y)$.

ν	κ_μ^ν	φ_μ^ν	ν	κ_μ^ν	φ_μ^ν
1	$-\eta_\mu U_d$	$B_{11}\tilde{B}_{11}$	8	$-\eta_\mu U_p$	$\omega_x B_{21}\tilde{B}_{21}$
2	$-A_\mu$	$F_s + \tilde{F}_s$	9	$-2A_\mu$	$F_x + \tilde{F}_x$
3	$-A_\mu$	$i(F_s - \tilde{F}_s)$	10	$-2A_\mu$	$i(F_x - \tilde{F}_x)$
4, 5	$\pm\eta_\mu K_d/2$	$2\varphi_\mu^1 \pm \varphi_\mu^2$	11, 12	$\pm\eta_\mu K_p$	$\varphi_\mu^8 \pm \varphi_\mu^9$
6	$-A_\mu$	$F_d + \tilde{F}_d$	13, 14	$\mp 2\eta_\mu X_p$	$\varphi_\mu^8 \pm L$
7	$-A_\mu$	$i(F_d - \tilde{F}_d)$			

Table 2. Constants γ and functions g in operators Γ_{SM}^ν in equations (12) corresponding to singlet SC pairing of s or d types ($\nu = 1$–9 or $\nu = 10$–13). Here $M_{s(d)} = B_2^2 \pm B_3^2$; $R_{s(d)} = B_{11}(B_{12}s_x \pm B_{31}s_y)$; $G = B_{21}B_{31}s_x s_y$.

ν	$\gamma_{S=0}^\nu$	$g_{S=0}^\nu$	ν	$\gamma_{S=0}^\nu$	$g_{S=0}^\nu$
1	U_d	B_{11}^2	10	$U_p/2$	M_d
2	$U_p/2$	M_s	11	$2(Q - J)$	R_d
3	$2(Q - J)$	R_s	12, 13	$\mp K_p$	$M_d \pm R_d$
4, 5	$\mp K_d$	$2g_0^1 \pm R_s$			
6, 7	$\mp K_p$	$g_0^2 \pm R_s$			
8, 9	$\pm 4X_p$	$g_0^2 \pm G$			

[13]. To simplify the expressions, we use the symmetry $B_{11}(-k) = B_{11}(k)$, $B_{j1}(-k) = -B_{j1}(k)$, $j = 2, 3$.

Presence of a CDW or SDW leads to doubling of lattice site or to half momenta site in the reciprocal lattice. Thus the whole upper band is equivalent to two sub-bands at $k \in F$, where F is half of the original phase-space site. In terms of such sub-bands the AF and AA OP $\underline{\Delta}$, $\underline{Z}$ correspond to (e_k, h_k) or (e_k, e_{-k}) pairing between electronic states of different sub-bands and $\underline{\Gamma}$ refer to (e_k, e_{-k}) pairing inside the same sub-bands. The AA OP is non-zero only in the region of coexistence of AF and SC. In particular, the simultaneous AF ordering of spins on Cu sites and the singlet superconducting pairing of d type (SC-d) draw into their gain the unique triplet OP Z_{SM}, $S = 1$, $M = 0$, with the following constant ζ and weight function χ:

$$\zeta = 2(Q - J) \qquad \chi = \tfrac{1}{2}[\tilde{B}_{11}(B_{21}s_x - B_{31}s_y) - B_{11}(\tilde{B}_{21}\tilde{s}_x - \tilde{B}_{31}\tilde{s}_y)] \tag{15}$$

where $\tilde{f} = f(\tilde{k})$ and s_x, s_y are defined by equation (8). Such a selection rule follows from symmetry properties. Note also that each spin $S = 0$ or 1 in Z_{SM} may correspond to

function χ of either symmetry, $\chi(\tilde{k}) = \pm\chi(k)$, since the pairing of electrons from different sub-bands is equivalent to pairing of non-identical particles. In contrast to SDW the CDW + SC-d draw into the gain the singlet OP $\underline{Z}_{S=0}$.

In MF theory only negative constants among κ^ν or γ^ν might provide the energy gain in the course of ordering of some symmetry. Therefore in MF approximation the models with only on-centre and nearest-neighbour Coulomb parameters U_d, U_p, $Q > 0$ could not manifest the SC, and the AF ordering could not help in creating an attractive e–e effect as in the technique in [3].

It is seen from table 2 that an attractive effect may be expected from CHI of p_σ–d or p_σ–p_σ types at K_d, $K_p > 0$, $X_p < 0$. According to definition (3) they correspond to hybrid integrals $K_d = -\langle d_n d_n|\Delta H|x_n d_n\rangle$, $K_p = -\langle x_n x_n|\Delta H|d_n x_n\rangle$, $X_p = -\langle x_n x_n|\Delta H|y_n x_n\rangle$, $\Delta H = H - H_{HF}$, in the small overlap limit. To provide the attractive effect the constants of CHI K_d, K_p or X_p must have signs that are opposite to corresponding adopted signs $t > 0$, $t_p > 0$ [15] of hopping integrals $t = \langle x_n|H|d_n\rangle$, $t_p = -\langle x_n|H|y_n\rangle$.

3. Linearized self-consistent problem

The linearized Hamiltonian obtained from equation (11) [13]

$$H_L = H_0(\varepsilon_p, \varepsilon_d, t, t_p) + N\Big(2\sum_{\nu\mu}\Delta^\nu_\mu\underline{\Delta}^\nu_\mu/\kappa^\nu_\mu + \sum_{\nu SM}(\Gamma^{+\nu}_{SM}\underline{\Gamma}^\nu_{SM} + \text{HC})/\gamma^\nu_S + \sum_{\nu SM}(Z^{+\nu}_{SM}\underline{Z}^\nu_{SM} + \text{HC})/\zeta^\nu_S\Big) + C \tag{16}$$

determines the quasi-particle energies E_λ and operators $\beta^+_{\lambda\sigma}, \beta_{\lambda\sigma}$ such that $[H, \beta_{\lambda\sigma}] = -E_\lambda\beta_\lambda$ (C is constant). In the case of z polarization of SDW ($\mu = 3$) or CDW ($\mu = 0$) and singlet SC pairing, the operators $\beta^+_{\lambda\sigma}$ are linear combinations of four operators $b^+_j(k) = \{a^+_{k\uparrow}, a^+_{\tilde{k}\uparrow}, a_{-k\downarrow}, a_{\tilde{k}\downarrow}\}_j$, $j = 1, \ldots, 4$, and k varies in half of the original phase space $k \in F$ [13].

The new form of H_L and of the quasi-particle operators β_λ in terms of b_j operators are

$$H_L = \sum_{i,j=1}^{4}\sum_{k\in F} L_{ji}b^+_i(k)b_j(k) + C \tag{17}$$

$$\beta_\lambda(k) = \sum_j b_j(k)U_{j\lambda}(k) \qquad \beta^+_\lambda(k) = \sum_j (U^+)_{\lambda j}b^+_j \tag{18}$$

where the unitary matrix U and the quasi-particle spectrum E_λ are determined by

$$L_{ij}U_{j\lambda}(k) = U_{j\lambda}(k)E_\lambda(k). \tag{19}$$

The Hermitian matrix L in turn depends on OP, and its elements are

$$L_{jj} = \eta_j[\varepsilon(k_j) - \mu]\sum_{\nu S} \qquad L_{21} = \sum_{\nu\mu}\underline{\Delta}^\nu_\mu\varphi^\nu_\mu(k) \qquad L_{31} = \sum_{\nu S}\underline{\Gamma}^\nu_{S0}g^\nu_S(k)$$

$$L_{41} = \sum_{\nu S}\underline{Z}^\nu_{S0}\chi^\nu_S(k) \qquad L_{32} = \sum_{\nu S}\underline{Z}^\nu_{S0}\chi^\nu_S(-\tilde{k}) \tag{20}$$

$$L_{42} = \sum_{\nu S}\underline{\Gamma}^\nu_{S0}g^\nu_S(-\tilde{k}) \qquad L_{43} = -\sum_{\nu\mu}(-1)^\mu\underline{\Delta}^\nu_\mu\varphi^\nu_\mu(\tilde{k})$$

where $\{k_j\} = \{k, -\tilde{k}, -k, \tilde{k}\}$, $\{\eta_j\} = \{1, 1, -1, -1\}_j$, $j = 1, \ldots, 4$ and μ is the chemical potential.

Spectrum E_λ and matrix U determine the self-consistent equations for OP $\underline{\Delta}$, $\underline{\Gamma}$, $\underline{Z}$ and for the number of extra holes induced by doping. They are the same as in [13]:

$$\underline{\Delta}^\nu_\mu = \kappa^\nu_\mu N^{-1} \sum \mathrm{Re}[\varphi^\nu_\mu(k)T_{12} - (-1)^\mu \varphi^\nu_\mu(-k)T_{43}] \qquad \mu = 0, 3 \tag{21}$$

$$\underline{\Gamma}^\nu_{S0} = \gamma^\nu_S N^{-1} \sum [g^\nu_S(k)T_{31} + g^\nu_S(-\tilde{k})T_{42}] \tag{22}$$

$$\underline{Z}^\nu_{S0} = \zeta^\nu_S N^{-1} \sum [\chi^\nu_S(-\tilde{k})T_{32} + \chi^\nu_S(k)T_{41}] \tag{23}$$

$$N_h = -N^{-1} \sum_j \sum \eta_j T_{jj}. \tag{24}$$

Here Σ is a sum over $k \in F$, i.e. over half of the phase volume, and

$$T_{ij}(k) = U_{ik} f_\lambda U^+_{kj} \qquad f_\lambda = \{1 - \exp[-\beta E_\lambda(k)]\}^{-1}. \tag{25}$$

The equations for the phase boundaries $T_c(N_h)$ (which determine the appearance of the SC OP of some symmetry from normal state (N) or from ordered AF state) are derived from self-consistent equations on Γ^ν of given symmetry and from solution of the eigenvalue problem (19) with first-order perturbation $\delta L = L - L^{(0)}$ introduced by additional new ordering. Thus at $T \to T_c$ one obtains the linear equations $D_{\nu\nu'} Y_{\nu'} = 0$ for $Y_\nu = \{\underline{\Gamma}, \underline{Z}\}_\nu$. The condition for a non-zero solution is

$$|D_{\nu\nu'}| = \mathrm{Det}|\delta_{\nu\nu'} - \partial Y_\nu / \partial Y_{\nu'}| = 0 \tag{26}$$

where Y_ν include all SC and AA OP that couple each other according to symmetry selection rules. Detailed expressions for derivatives in (26) are given in the appendix.

It may be shown that the SC–N transitions are described by a similar equation for only SC OP $\underline{\Gamma}_\nu$ (decoupled from $\underline{Z}_\nu$), whereas the (SC + AF)–AF transition needs equations that couple $\underline{\Gamma}$ and $\underline{Z}$. In the case of SC-d and SDW on Cu sites only one triplet OP $\underline{Z}$ described by equation (15) must be added. In the appendix some arguments are presented for the possible compatibility of SC-d pairing with SDW on Cu sites or the SC-s one with CDW for the nearly half-filled band.

4. Numerical studies of models

The models to be discussed are completely determined by the effective values of hopping integrals t, t_p and relative energy $E_d = \varepsilon_d - \varepsilon_p$ of the d orbital corresponding to the half-filled upper band ($N_h = 0$) and the parameters U_d, U_p, Q, J, K_d, K_p, X_p of interactions in equation (1). Values E_d, t, t_p are quantities renormalized by interactions according to (4).

As in the previous study [13], the original set of parameters has been taken from [15]. In our electronic representation they are (all values in eV):

$$t(N_h = 0) = 1.3 \qquad t_p(0) = 0.65 \qquad Q = 1.2 \qquad U_d = 10.0$$
$$U_p = 4.0 \qquad J = 0 \tag{27}$$

together with $E_d(0) = -t$ to $t = -1.3$ to 1.3 eV at $N_h = 0$. Note that we use as large hopping as predicted by the LDA calculations, and the insulating features and the narrowing of sub-bands divided by large correlation gap are consequences of the AF pairing in the system. The reduced Coulomb integrals $U_d = 8.0$, $U_p = 3.2$ eV have also

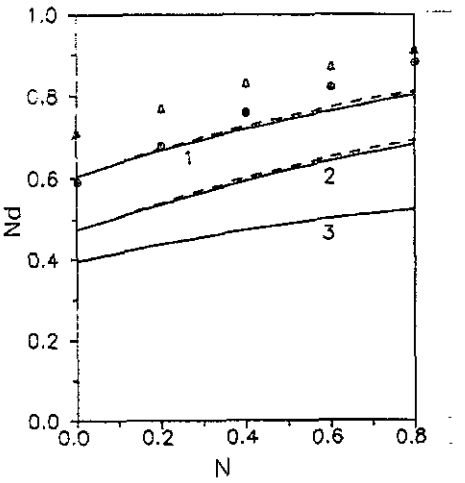

Figure 1. Dependences of the hole number N_d on Cu centre on doping (i.e. on extra hole number $N = N_h$ per Cu_2O unit) for models with $t(0) = 1.3$, $U_d = 10$, $U_p = 4$ (full curves) or $U_d = 8$, $U_p = 3.2$ (broken curves) and with the CHI constants $K_d = X_p = 0$, $K_p = 2$. Curves 1 and 2 refer to models with $E_d(0) = t(0) = 1.3$ and $t_p = 0$ (perfect nesting) or $t_p = 0.65$ (extended Emery models). Curve 3 refers to model $E_d(0) = -t(0) = -1.3$, $t_p = 0$. Points show results [12] with HF or correlated state (upper or lower set of points) for close models but without CHI. All values are in eV.

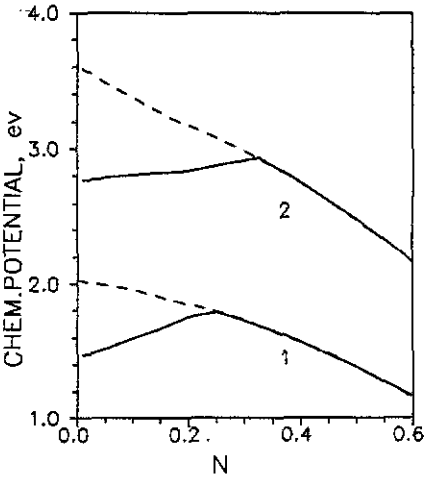

Figure 2. Dependences of chemical potential of electrons in CuO_2 plane on doping. Broken parts of curves refer to normal state in doping region when AF state with double site (full parts of curves) is preferable. $U_d = 8$, $U_p = 3.2$, $K_d = X_p = J = 0$, $K_p = 2$ and $t_p = 0$ or $t_p = 0.65$ (curves 1 and 2 respectively).

been tested to simulate possible reduction of their influence due to correlations. The CHI parameters varied in the range

$$|K_d|, |K_p| \leqslant 2t \qquad |X_p| \leqslant 3t_p. \tag{28}$$

All such parameters determine uniquely the 'zero' values $E_d^0 = \varepsilon_d^0 - \varepsilon_p^0$, t^0, t_p^0 and in turn the upper band parameters at arbitrary doping. There are almost linear dependences [13] of these values on doping $E_d(N_h) \simeq E_d(0) - (2.3 \text{ to } 2.6)N_h$, $t \simeq t(0) + (0.4 \text{ to } 0.5)N_h$, $t_p \simeq t_p(0) + (0 \text{ to } 0.6)N_h$. Our HF results are in line with that for similar models without CHI studied [12]. For example, figure 1 presents some doping dependences $n_d(N_h)$ of the mean hole number on Cu centre, where N_h is number of extra holes per elementary site associated with doping. The small slope of the curves means that for the considered models the extra holes are placed mainly on the p_σ orbitals, leaving the Cu sites with only slightly varying occupancy similar to the behaviour of strongly localized d orbitals.

Now we discuss the ordering in the upper HF band with parameters depending on N_h. Two sorts of calculations have been done.

(i) Calculation of the 'zero' phase diagrams $T_c^0(N_h)$ for transitions from the normal state to the state with only one type of pairing (AF or singlet SC-s or SC-d) using equations of the type

$$\text{Det}|\delta_{\nu\nu'} - \partial\Delta^\nu/\partial\Delta^{\nu'}| = 0 \qquad \text{or} \qquad \text{Det}|\delta_{\nu\nu'} - \partial\Gamma^\nu/\partial\Gamma^{\nu'}| = 0 \tag{29}$$

at $\Gamma^\nu, \Delta^\nu = 0$.

To simplify the calculations we use the assumption that the upper band parameters are functions of the low-temperature hole concentration $N_0 = N(\mu, T = 0)$ instead of the actual one $N(\mu, T)$ at the same μ. At large T_c this gives some inaccuracy of the AF–N phase curves on figures 3 and 6, which present dependences of T_c on N (not N_0). However, the low-temperature boundaries (in particular for SC) are accurate.

(ii) The phase boundaries for SC on the background of the ordered AF state have been obtained from solution of the reduced AF self-consistent problem. The aim was to treat more easily the models with very different scales of T_c for AF and SC. One realizes, however, that the AF state thus obtained with double elementary site may be unstable and it may really exhibit phase transitions, for example, to phases of chemical ordering with periodicity other than double or lead to a discontinuous dependence of the plane charge on doping. Expectation of instability follows from the inverse doping dependence of chemical potential $d\mu/dN_e = -d\mu/dN_h < 0$ inside the AF region. Some typical curves $\mu(N_h)$ are demonstrated in figure 2. Here μ refers to the electronic system of an isolated CuO_2 plane with variable charge. It does not contain the Madelung or other contributions to the energy of the whole crystal.

First of all we present the re-examined results for pure Emery models without p–p hopping ($t_p = 0$), which was studied in [13]. Here we remove some errors missed in [13]. The previous 'zero' temperature T_c^0 for the SC–N transitions have been calculated in [13] with values of the SC coupling constants γ^ν that were greater than the correct ones by a factor 2, and a factor $(-2\eta_\mu)$ from the spin structure was missed in the AF coupling constants κ^ν, connected with CHI. The main revised conclusions about models exhibiting the AF and SC-d remain the same as in [13] besides reducing the 'zero' temperature of the N–SC-d transition. These models are characterized by large p_σ-d CHI governed by the p_σ occupancy: $K_p \geqslant 1.2t$. Figure 3 presents the 'zero' boundaries of SC-d for models with $E_d(0) = -1.3$, $t_p = K_d = X_p = 0$ and $K_p = 2.6 = 2t$, $U_d = 10.0$, $U_p = 4.0$ or $K_p = 2 \simeq 1.5t$, $U_d = 8.0$, $U_p = 3.2$. The whole self-consistent procedure at temperatures 10^{-2} to 0.5×10^{-3} and with high accuracy reveals solutions with AF and SC-d order parameters that are both non-zero in the AF region ($\underline{\Gamma} \ll \underline{\Delta}$). The same conclusion about the coexistence of AF and SC-d for these models is confirmed by the phase diagrams (full curves in figure 4) for SC-d pairing on the background of self-consistent AF state or N state at large N_h. The dotted curve is a result obtained by neglecting AA OP in equation (26).

It is important that a gain of large (~1 eV) electronic interactions can provide the stable small (thermal) scale of the SC-d transition temperature. Thus the puzzling question about the previous too large T_c [13] is now removed.

For another class of models with $K_d \simeq K_p \simeq t \simeq -E_d$ calculations with the corrected coupling constants $\kappa^{4,5} = \pm 2\eta K_d/4$ (in contrast with [13]) in AF OP (see table 2) show strong suppression of AF ordering by the p–d CHI ($3a$) governed by d occupancy. In the undoped CuO_2 plane the AF is observed only for $E_d(0) \geqslant t/2$ for large parameters $U_d = 10$, $U_p = 4$ and it disappears if U_d, U_p reduce down to values 8 and 3.2. The SC-s pairing without any trace of AF ordering actually takes place for most such models and T_c for SC-s varies sharply with $E_d(0)$ from small values to very large ones up to 0.21 eV (see table 3 and discussion below).

This is a typical feature of the SC state of s type induced by any sort of CHI: a great sensitivity of T_c to the parameters of models and the possible unrealistically large values of T_c if the CHI constant increases. Thus an accidental hit to near-threshold values of the CHI parameter is needed to retain a thermal (not electronic) scale of T_c for the SC-s models.

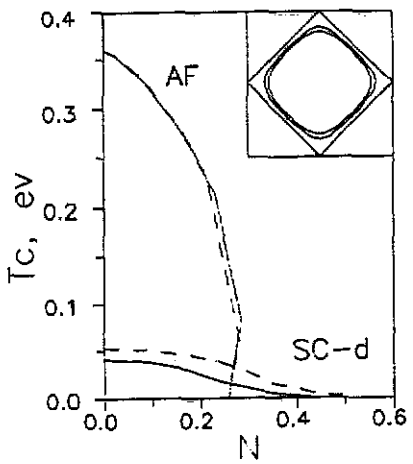

Figure 3. The 'zero' N–SC-d and N–AF phase diagrams for 'pure' Emery models ($t_p = 0$) with parameters $k_d = X_p = J = 0$, $E_d = -1.3$ and $K_p = 2.6$, $U_d = 10$, $U_p = 4$ or $K_p = 2$, $U_d = 8$, $U_p = 3.2$ (full and broken curves). Inset shows the 2D Fermi surfaces of latter system in AF state at $N_h = 0, 0.2, 0.3$.

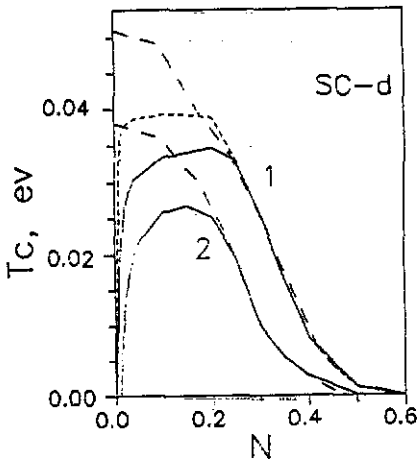

Figure 4. The temperatures of transition to SC-d state for the same models as in figure 3 (1 and 2 refer to $U_d = 10$, $U_p = 4$, $K_p = 2.6$ or to $U_d = 8$, $U_p = 3.2$, $K_p = 2$). The actual (AF + N)–SC-d boundaries are full curves; the 'zero' N-SC-d boundaries (neglecting the AF pairing) are broken curves. The dotted curve is (AF + N)–SC-d boundary calculated with only SC OP without AA OP in AF region.

We now discuss results for the extended Emery models with direct p_σ–p_σ hopping in the range $0 < t_p \leqslant t/2 = 0.65$ eV. Positive signs are taken from LDA data [15, 16].

The possibility of SC pairing depends on the relation of the interaction constants X_p, K_d, K_p with U_d, U_p, Q (see table 2). They are all weighted with corresponding factors depending roughly on the relation of the hole density on the d or p orbitals for states near the Fermi level. The question in principle is: Can the p_σ–p_σ CHI induce the SC as the p_σ–d does for some models? The answer is important in connection with suggestions [4–6] that p–p CHI is responsible for SC. Note that the p_σ–p_σ CHI can contribute only to SC-s (not SC-d) pairing as seen from table 2.

If we depart from AF features and set $t = K_p = K_d = 0$, $\varepsilon_d < \varepsilon_p - 4|t_p|$ to decouple the p_σ and d orbitals, then we come to models with the hole motion on the p_σ lattice only (it is equivalent to previous models [4, 5] of the p_π lattice). In such a model there are no holes on Cu centres but the behaviour of the p_σ hole system does not depend on occupancy of Cu sites. For the upper band in such a model one obtains $\varepsilon_k - \varepsilon_p = 4t_p|s_x s_y| = 2t_p|\cos q_x - \cos q_y|$, $B_{11} = 0$, $B_{21} = B_{31} s_x s_y/|s_x s_y| = 1/\sqrt{2}$ where $q_{x(y)} = (k_x \pm k_y)/2$ are the quasi-momenta in double Brillouin zone corresponding to one O atom in an elementary site of the O lattice. In this way equation (29) for T_c including Γ^ν, $\nu = 2, 8, 9$, from table 2 is reduced to that derived by Hirsch and Marsiglio (equation (12) from [4]). Figure 5 presents a comparison of results for systems of p_σ orbitals only with $U_p = 5$, $t_p(0) = 0.06$ (in our calculations $t = 0$ and $E_d < -2$ provided decoupling of d and p orbitals). In figure 5, 1 and 2 refer to the 3D result [5] for $\Delta t = -X_p = 0.399(U_p + 2Q_p)/16$, $Q_p = 0.346$ and to our result for the close 2D model with $\Delta t_p = -X_p = 0.32(U_p + 2Q_p)/16$, $Q_p = 0$, where Q_p is the Coulomb integral for the nearest-neighbour p_σ orbitals. A small value of $t_p(0)$ was chosen in [4, 5] to provide the near dielectric behaviour of the small doping system.

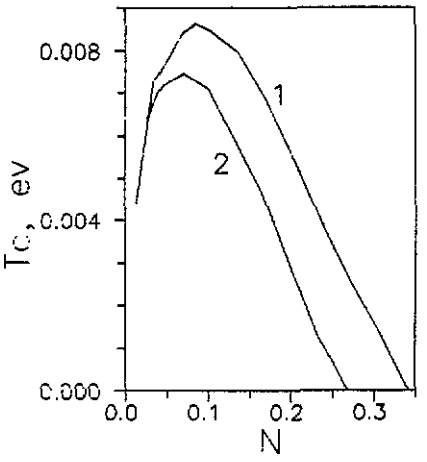

Figure 5. Phase diagram for SC-s caused by the p_σ–p_σ CHI. T_c versus hole number per CuO_2 unit (twice hole number per O atom) for models with oxygen holes only for model with $U_p = 5$, $t_p(0) = 0.06$ and $t = 0$ (latter provides decoupling of d orbitals). Curve 1, 3D result [5] for $\Delta t = -X_p = 0.399(U_p + 2Q_p)/16$ and $Q_p = 0.346$ of Coulomb integral for neighbour p_σ orbitals. Curve 2, our 2D result for $-X_p = 0.32(U + 2Q_p)$ at $Q_p = 0$.

We now turn back to extended Emery models exhibiting the AF ordering and based on parameters (27) with direct p_σ–p_σ hopping $t_p \leqslant 0.65$ eV and retain only the p_σ–p_σ CHI, i.e. set $K_d = K_p = 0$, $|X_p| \leqslant 3|t_p|$. Most of the models, which really show the AF ordering at some doping $N < N_c$, do not exhibit any SC pairing for both versions of Coulomb parameters. The reason is the increase of repulsive contribution from U_d, Q and decrease of the p_σ–p_σ CHI contribution at non-zero hole density on Cu. Thus the p_σ–p_σ CHI alone seems to be inefficient for SC pairing in such models if we require AF ordering for the undoped system. The correlations above MF approximation must be taken to obtain the final verdict on this problem.

A search of SC of s type induced by the combined action of various sorts of CHI reveals two types of rather exotic SC-s models with large CHI integrals. Models of the first type with $K_d \simeq K_p \simeq t$, $X_p = 0$ really display the SC-s pairing, but large K_d (if the corrected AF constants κ^4, $\kappa^5 = \mp 2\eta_\mu K_d$ are used instead of those in [13]) leads to almost entire suppression of the AF ordering by corresponding CHI. Other models with $X_p \leqslant 2t_p$, $K_p \simeq t$, $K_d = 0$ may exhibit the AF and SC-s ordering at some values of E_d. The regions of AF and SC pairing do not overlap. Some typical properties of the phase diagram for these systems are illustrated by table 3. As mentioned above the T_c of SC-s varies sharply with E_d.

In contrast to SC-s models there are models with p–d CHI that can exhibit at various doping both AF and SC with relatively small T_c. These are extended Emery models with $t_p \leqslant 0.65$, $-t < E_d(0) < t$, $K_p \geqslant 1.6$ eV $\simeq 1.2t$, $K_d = X_p = 0$, i.e. systems with the p–d CHI governed by a p_σ occupancy. Their phase diagrams show that the AF ordering is observed in a range of N_h that increases at $E_d > 0$ and decreases at $E_d < 0$ or if p_σ–p_σ hopping of any sign is involved (imperfect nesting).

Table 4 lists the approximate key properties of the magnetic phase. Here N_c is the threshold doping N_h above which the AF order is destroyed, m is the mean magnetic moment on a Cu site, and Δ_X, Δ_S are the values of dielectric gap of undoped CuO_2 plane at points X $(\pi/2, \pi/2)$ and S $(0, \pi)$. It is seen that including p_σ–p_σ hopping acts in some respects just like the decrease of $E_d(0) = \varepsilon_d - \varepsilon_p$. The reason may be in pushing up the antibonding p_σ band by p_σ–p_σ hopping, and this has the same effect as growth of ε_p. Note also that N_c refers to an artificial AF state with double lattice site and no correlations

Table 3. Some characteristics of models exhibiting the SC-s pairing or close to them. N_c is the threshold hole concentration for AF or SC-s pairing if it is possible (else dash); max T_c^0 is maximum value of T_c for SC-s. Models I or II correspond to $K_d = K_p = t = 1.3$, $X_p = 0$, $t_p = 0.65$ or $K_d = 0$, $K_p = 1.54t = 2$, $-X_p = 2t_p = t = 1.3$, and two sets of U_d, U_p. All values in eV.

		$U_d = 10.0$, $U_p = 4.0$			$U_d = 8.0$, $U_p = 3.2$		
	E_d	$-t$	0	t	$-t$	0	t
I	AF: N_c	—	—	—	—	—	—
	SC: N_c	0.37	0.30	—	0.56	0.55	0.36
	max T_c^0	0.01	0.054	—	0.07	0.08	0.03
II	AF: N_c	—	0.33	0.33	—	0.14	0.26
	SC: N_c	0.61	—	—	0.76	2.2	—
	max T_c^0	0.17	—	—	0.30	0.018	—

Table 4. Some characteristics of models exhibiting both the AF and SC-d pairing caused by the p–d CHI with $K_d = X_p = 0$, $K_p = 1.54t = 2$. N_c is the threshold hole concentration for AF pairing; Gap$\{^X_S\}$ and m/m_B are the values of dielectric gap at points X ($k_x = \pi$, $k_y = 0$) or S($\pi/2$, $\pi/2$) and magnetic moment on Cu site for undoped CuO_2 planes; T_c^0 is the maximum value of the 'zero' N-SC-d transition temperature. I and II refer to systems with $t_p = 0$ (perfect nesting) or to extended Emery models with $t_p = 0.65$.

		$U_d = 10.0$, $U_p = 4.0$			$U_d = 8.0$, $U_p = 3.2$		
	E_d	$-t$	0	t	$-t$	0	t
I	N_c	0.27	0.35	0.44	0.25	0.32	0.39
	Gap (eV)	1.5	2.8	4.3	1.2	2.2	3.5
	m/m_B	0.28	0.45	0.61	0.27	0.43	0.6
	$T_c^0/10^{-2}$ (eV)	3.6	2.8	0.9	5.0	3.4	1.4
II	N_c	—	0.24	0.33	—	0.24	0.3
	Gap$\{^X_S\}$ (eV)	0	1.8 1.5	3.4 2.9	0	1.4 1.1	2.7 2.3
	m/m_B	0	0.28	0.47	0	0.26	0.45
	$T_c^0/10^{-2}$ (eV)	0.76	0.64	0.46	0.76	0.95	0.67

above MF have been taken into account. In this connection the model characteristics do not differ drastically from the experimentally observed gap of 2 eV in $LaCu_2O_4$ [22] and 1.7 eV in $YBa_2Cu_3O_6$ [23], and $m = 0.4\mu_B$ in La_2CuO_4 [24] and $m = (0.64$ to $0.66)\mu_B$ in $YBa_2Cu_3O_6$ [24–26].

Figures 6 and 7 show typical phase diagrams for AF and SC-d pairing. In contrast to systems with perfect nesting (figures 3 and 4) in extended Emery models the 'zero' phase SC-N curves show a noticeable suppression of SC pairing at small doping (figure 7). The AF ordering leads to further suppression of SC-d pairing though some region of coexistence of SC-d and AF remains. In this region of doping the triplet alternate anomalous OP described by equation (15) appears; if one neglects it then the T_c changes for SC-d in the region of AF (dotted curve in figure 7). A typical maximum value of the ratio

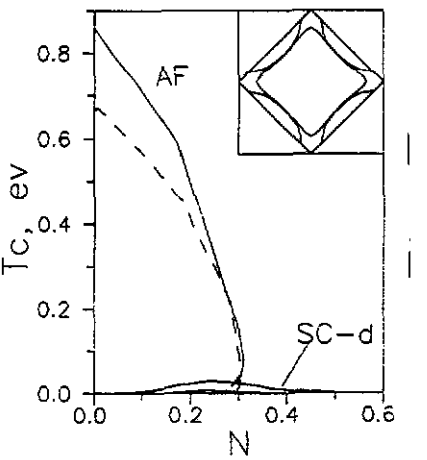

Figure 6. The 'zero' N-AF and NC-SC-d transition temperatures versus hole number for systems with parameters close to those derived in [15]: $E_d(0) = t(0) = 2t_p(0) = 1.3$, $Q = 1.2$, $J = 0$, $K_d = X_p = 0$ (all values in eV) and $U_d = 10$, $U_p = 4$, $K_p = 2.6$ (full curves) or $U_d = 8$, $U_p = 3.2$, $K_p = 2$ (broken curves). Inset shows the 2D Fermi surfaces of latter system in AF state at $N_h = 0, 0.2, 0.3$.

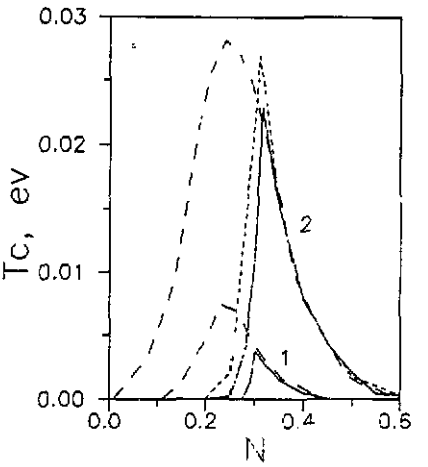

Figure 7. T_c of transition to SC–d state for the same extended Emery models as in figure 6. Curves 1 and 2 refer to $U_d = 10$, $U_p = 4$, $K_p = 2.6$ or $U_d = 8$, $U_p = 3.2$, $K_p = 2$. The actual (AF + N)–SC-d boundaries are full curves; the 'zero' N-SC-d boundaries (neglecting AF pairing) are broken curves. The dotted curve is the (AF + N)–SC-d boundary calculated with only SC-d OP without AA OP in AF region.

$2\Delta/kT_c$ for SC-d gap is about 3.7 at doping corresponding to the maximum of T_c. It is close to the BCS prediction.

5. Summary

In the framework of the MF theory, various electronic pairings have been classified for the upper band of extended Emery models with a detailed picture of local interactions and with parameters close to those extracted [15, 16] from LDA calculations. The self-consistent equations have been derived for all OP. They also determine the equation for T_c of the SC-N, AF-N and even (SC + AF)–AF transitions. The latter allows one to study compatibility of AF and SC. Coupling constants and weight functions in OP (tables 1 and 2) show the role of each interaction in pairing of any sort. The MF calculations confirm the possibility of SC pairing induced by p–d or p–p CHI for sufficiently large CHI constants ($K_d, K_p > 0, X_p < 0$).

The SC of s type may be induced by p–d CHI ($K_d \simeq K_p \simeq t$) or by combined p–d and p–p CHI ($K_p \simeq -X_p \simeq t$). However, as a rule such systems (in MF approach) do not exhibit AF for the undoped case. This shortcoming refers also to models close to that in [5] describing the system of p holes only with the SC-s caused by the p–p CHI. For models with large K_d the AF is suppressed by a corresponding term of the p–d CHI. For models of the p_σ hole systems it is difficult in MF approach to provide sufficient hole density on a Cu site needed for AF ordering. Final conclusions about the possibility to describe both AF at small doping and SC-s need the treatment of correlations above MF.

In departing from above SC-s models, the models with large p–d CHI governed by p_σ occupancy may exhibit both AF at small doping and SC of d type. It is shown that SC-d

and AF may be compatible in some region of doping. Increasing the direct p_σ–p_σ hopping (imperfect nesting) as well as the AF pairing suppress the SC-d at low doping, though a small region with coexistence of AF and SC-d remains. In this region additional triplet alternate anomalous order parameters appear together with singlet SC-d OP and the AF OP.

An important question remains open: how do the correlations renormalize the pairing interactions and change the MF results given above?

Appendix

To calculate the phase boundary of SC on a background of AF from equation (26) the partial derivatives $\partial(\underline{\Gamma}, \underline{Z})/\partial(\underline{\Gamma}, \underline{Z})$ at $\underline{\Gamma} = \underline{Z} = 0$ are needed. They are

$$\partial\underline{\Gamma}^\nu/\partial\underline{\Gamma}^{\nu'} = \gamma^\nu N^{-1} \sum_k {\sum}' \mathcal{F}_{\lambda\lambda'} G^\nu_{\lambda\lambda'} G^{\nu'}_{\lambda\lambda'} \qquad \partial Z^\nu/\partial Z^{\nu'} = \zeta^\nu N^{-1} \sum_k {\sum}' \mathcal{F}_{\lambda\lambda'} L^\nu_{\lambda\lambda'} L^{\nu'}_{\lambda\lambda'}$$

$$\partial\underline{Z}^\nu/\partial\underline{\Gamma}^{\nu'} = (\zeta^\nu/\gamma^{\nu'})\,\partial\underline{\Gamma}^{\nu'}/\partial\underline{Z}^\nu = \zeta^\nu N^{-1} \sum_k {\sum}' \mathcal{F}_{\lambda\lambda'} L^\nu_{\lambda\lambda'} G^{\nu'}_{\lambda\lambda'} \tag{A1}$$

where Σ' is a sum over λ, λ' and

$$G^\nu_{\lambda\lambda'} = g^\nu(U_{3\lambda}U_{1\lambda'} + U_{1\lambda}U_{3\lambda'}) + g^\nu(U_{4\lambda}U_{2\lambda'} + U_{2\lambda}U_{4\lambda'}) \tag{A2}$$

$$L^\nu_{\lambda\lambda'} = \chi^\nu(U_{4\lambda}U_{1\lambda'} + U_{1\lambda}U_{4\lambda'}) + \chi^\nu(U_{3\lambda}U_{2\lambda'} + U_{2\lambda}U_{3\lambda'}) \tag{A3}$$

$$2\mathcal{F}_{\lambda\lambda'} = \begin{cases} (f_\lambda - f_{\lambda'})/(E_\lambda - E_{\lambda'}) & E_\lambda \neq E_{\lambda'} \\ -f_\lambda(1-f_\lambda)/kT & E_\lambda = E_{\lambda'} \end{cases} \tag{A4}$$

$$\chi = \chi(-\tilde{k}) \qquad g = g(-\tilde{k}). \tag{A5}$$

Here $U_{i\lambda}$, E_λ are solutions of equations (16) at $\underline{\Gamma} = Z = 0$.

For state N one has $U_{i\lambda} = \delta_{i\lambda}$ and equations (26) factorize into two independent blocks of equations with decoupled $\underline{Z}$ and $\underline{\Gamma}$ OP. Then T_c for SC–N transition is obtained from $\mathrm{Det}\,|\delta_{\nu\nu'} = -\partial\underline{\Gamma}^\nu/\partial\underline{\Gamma}^{\nu'}| = 0$.

One can obtain a selection rule for non-zero coupling between $\underline{\Gamma}^\nu$, $\underline{Z}^\nu$ on a background of the SDW ($\mu = 3$) or CDW ($\mu = 0$) state using equation (A1) and the matrix U for these states:

$$U = \begin{pmatrix} U_{\mathrm{I}} & 0 \\ 0 & U_{\mathrm{II}} \end{pmatrix} \qquad U_{\mathrm{I}} = \begin{pmatrix} c & s \\ s & -c \end{pmatrix} \qquad U_{\mathrm{II}} = \begin{pmatrix} c & (-1)^\mu s \\ (-1)^\mu s & -c \end{pmatrix} \tag{A6}$$

$$E_\lambda = \{E_-, E_+, -E_-, -E_+\}_\lambda \qquad E^\pm = [\varepsilon - \varepsilon(-\tilde{k})]/2 - \mu \pm (\delta\varepsilon^2 + |L_{21}|^2)^{1/2}$$

where $c = \cos\alpha$, $s = \sin\alpha$, $\tan(2\alpha) = L_{21}/\delta\varepsilon$, $\delta\varepsilon = [\varepsilon(k) - \varepsilon(-\tilde{k})]/2$, and L_{21} is defined by equations (20).

In particular, one obtains that the AF ordering induces the coupling of the SC-d OP with only one triplet AA OP with d symmetry of weight function $\chi(k)$. Another way to obtain the selection rules is to study the generation of operators Z^ν from commutators $[\Delta^\nu, \Gamma^{\nu'}]$ between operators Γ^ν, Δ^ν of given symmetry.

Based on properties of matrix U given by equation (A6) and the symmetry of weight functions, one may expect compatibility of SC-s with CDW or SC-d with SDW for a nearly half-filled band. Such a tendency may be traced for a system with only one SC OP. In such

a case the equation $\mathrm{Det}|1 - \partial\underline{\Gamma}/\partial\underline{\Gamma}| = 0$ with unique OP $\underline{\Gamma}$ is determined mainly by the contribution from the branch $E_-(k)$ of the spectrum. For a system with large SDW (CDW) gap and small doping, one can estimate $c^2 \simeq s^2 \simeq 0.5 + O(|k - k_F|)$ and $g(-\tilde{k}) = \eta g(k) + O(|k - k_F|)$ in the region near the Fermi momentum k_F. Here $\eta = 1$ for extended s symmetry and $\eta = -1$ for d symmetry of $g(k)$. Retaining only the largest term in the equation yields

$$1 + \gamma \sum (2E_-)^{-1} \tanh(\beta E_-/2)\{g(k)[1 + \eta(-1)^{\mu}] + O(|k - k_F|)\} = 0.$$

This expression gives some indication that at sufficiently large negative coupling constant γ the s type of SC might be expected to be compatible with CDW ($\mu = 0$, $\eta = 1$), but not with SDW ($\mu = 3$), whereas the d type of SC may be compatible with SDW ($\mu = 3$, $\eta = -1$). The latter is confirmed by numerical calculations for Emery models, but it is less definitely manifested for extended Emery models with p_σ–p_σ hopping since the imperfect nesting in these models leads to some suppression of SC-d also in the AF region.

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