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On the accuracy of the single-band mapping of the Emery model and superconductivity

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Abstract. A variational derivation of the effective-single-band Hubbard Hamiltonian for the double-band Emery model is presented. The accuracy of the single-band mapping is analysed for the finite four-site cluster and for the infinite plane. The BCS solutions of the effective problem indicate the possibility of d-channel superconductivity of correlational nature.

1. Introduction

The search for an adequate description of strongly correlated systems, in particular of the cuprate HTSC, is still in progress. In recent work [1–4] a method has been proposed for constructing an effective-single-band Hamiltonian from a multiband model of the CuO_2 plane of HTSC. It is based on perturbation theory for intercluster interactions. A suitable cluster basis contains the d orbital of Cu, and Wannier combinations of the oxygen p orbitals of $x^2 - y^2$ symmetry. Only the lowest states of clusters, with the numbers $i = 0, 1, 2$ of holes in the cluster, have been separated out and put into correspondence with the site states of a single-band (SB) model. The projecting of the original Hamiltonian onto the above subspace leads to the effective Hubbard Hamiltonian, which takes into account all features of the three-band Emery model even for large intercluster fluctuations. Unlike those in the early work [5–10], the new SB mapping applies at arbitrary values of the parameter $t/\delta\epsilon$, where $\delta\epsilon = \epsilon_p - \epsilon_d$ is the energy difference of the p and d orbitals and t is the hopping between them.

A similar SB Hamiltonian (SBH) has been derived [11] via the variational method of local unitary transformations of the original Hamiltonian with subsequent projection onto the SB subspace. In line with the results in [11], the optimal transformation appears to be close to that which diagonalizes the intracluster part of the Hamiltonian.

A study of the accuracy of the SB mapping is very important, since the treatment of the SB model is much simpler than that of thorough multiband models [12, 13]. Therefore a direct estimation of the accuracy may be instructive. Both limits are of interest: the case of hole localization at small doping and the case of large intercluster interactions at large doping.

In the present work the accuracy of the variational SB mapping is studied via comparison of energies obtained by the Hartree–Fock (HF) treatment of the SBH and the double-band Hamiltonian (DBH), obtained with the use of local unitary transformation of the original Hamiltonian. For the finite four-centre system, comparison with the result from exact diagonalization is carried out. Simultaneously the method of unitary transformation is formulated in a more general form than in [12]. Like the nonunitary *ansatz* of Gutzwiller's

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type [14–17], the method provides a direct representation of correlated states. But unlike the methods of [1–4], it also allows one to form a basis for the optimal effective Hamiltonian in a variational way. In such effective problems a study of the BCS solutions gives an indication of the possibility of superconducting pairing of d type due to correlated hopping interactions of a correlational nature.

2. Derivation of the effective-SB and effective-DB Hamiltonians

Consider the simplified Emery model determined by two parameters only: $\delta\epsilon/t$ and U/t. Here $\delta\epsilon = \epsilon_p - \epsilon_d$ and t are the energy difference of the p and d orbitals and the hopping between them, and U is the on-site Coulomb interaction at the Cu. As in [1–4, 11], we use the basis of nonoverlapping cluster orbitals $\{d_n, a_n\}$, where a_n corresponds the Wannier combination of p orbitals of $x^2 - y^2$ symmetry. In this basis the Hamiltonian takes the form [11]

$$H = \sum_n h_n + \sum_{n \neq m} V_{nm} \tag{1}$$

$$h_n = \epsilon_d n_n^d + \epsilon_p n_n^p + 2tF(0) \sum_{n,\sigma} (a_{n\sigma}^\dagger d_{n\sigma} + \text{HC}) + U n_{n\uparrow}^d n_{n\downarrow}^d \tag{2}$$

$$V_{nm} = 2tF(n-m)(a_{n\sigma}^\dagger d_{m\sigma} + \text{HC}) \tag{3}$$

where

$$F(n-m) = \frac{1}{N} \sum_k \mathrm{e}^{\mathrm{i}k(n-m)} F_k \qquad F_k = (s_x^2 + s_y^2)^{1/2} \tag{4}$$

$$s_{x(y)} = \sin(k_{x(y)}/2). \tag{5}$$

The correlated wave functions of the DB approximation are presented as a result of local unitary transformation of the original DB function Φ:

$$\Psi_{DB}(a,d) = W\Phi(a,d) \qquad W = \prod_n W_n. \tag{6}$$

In particular, we will study the transformations of the original uncorrelated Hartree–Fock (HF) states, like in the Gutzwiller *ansatz* [14], where the nonunitary operator W was used. Here the local unitary operators W_n refer to nonoverlapping two-orbital clusters $\{d_n, a_n\}$ [11] and commute with each other. Their parameters are variational ones and are obtained from minimization of the energy:

$$\bar{H}^{DB} = \langle \Psi_{DB} H \Psi_{DB} \rangle = \langle \Phi | W^\dagger H W | \Phi \rangle. \tag{7}$$

Representation (6) is similar to the Gutzwiller *ansatz* [14]. But unlike in [14], the unitary transformation allows one to obtain the effective Hamiltonian of the new DB problem:

$$\tilde{H}(a,d) = W^\dagger H W. \tag{8}$$

It acts in the space of functions $\Phi(a,d)$.

In the SB approximation the correlated state is presented as a transformed SB HF function, for example $\Phi(a)$†:

$$\Psi_{SB}(a,d) = \prod_n W_n(a,d)\Phi(a). \tag{9}$$

† Various SB representations, for example $\Psi_{SB} = W'\Phi(d)$ or $\Psi_{SB} = W''\Phi(b)$ with $b_n = \cos\beta a_n + \sin\beta d_n$, are equivalent, and relations between W' and W'' here or W in (9) are easily obtained.

Then minimization of the energy:

$$\tilde{H}^{SB} = \langle \Psi_{SB} H \Psi_{SB} \rangle = \langle \Phi(a) | W^{\dagger} H W | \Phi(a) \rangle \tag{10}$$

provides a new transformation which is optimal for SB HF functions. The corresponding effective Hamiltonian of the SB problem is obtained by projection of the transformed one onto the subspace of SB functions $\Phi(a)$:

$$\tilde{H}^{SB}(a) = P_a W^{\dagger} H W P_a. \tag{11}$$

Here P_a projects $\tilde{H}(a, d)$ onto the subspace of functions $\Phi(a)$, with zero occupancy of the d orbitals. This may be done without loss of generality.

Note that the HF approach to the new effective-SB or effective-DB problems (8) and (11) may be adequate if they again appear to be strongly correlated problems. But the HF approach is adequate for estimation of the inaccuracy introduced by the SB mapping of the problem. The difference between the SB and DB energies (7) and (10) can be regarded as a measure of such inaccuracy.

Let us give details the operator W_n. In equations (6)–(11) the unitary operator W_n transforms the components of the nth cluster a_n, d_n in the total wave function Φ, and it conserves the hole number i and the spin of the cluster. That is, W_n acts on the states $|i\lambda\rangle$ of the nth cluster (the index n is omitted below) with i holes on it:

$$|1\lambda\sigma\rangle = \{|a_{\sigma}^{\dagger}\rangle, |d_{\sigma}^{\dagger}\rangle\}_{\lambda} \qquad |3\lambda\sigma\rangle = \{|a_{\alpha}^{\dagger} a_{\beta}^{\dagger} d_{\sigma}^{\dagger}\rangle, |d_{\alpha}^{\dagger} d_{\beta}^{\dagger} a_{\sigma}^{\dagger}\rangle\}_{\lambda} \tag{12}$$

$$|2\lambda\rangle = \{|a_{\alpha}^{\dagger} a_{\beta}^{\dagger}\rangle, |d_{\alpha}^{\dagger} d_{\beta}^{\dagger}\rangle, |(a_{\alpha}^{\dagger} d_{\beta}^{\dagger} + d_{\alpha}^{\dagger} a_{\beta}^{\dagger})/\sqrt{2}\rangle, \ldots\}_{\lambda} \tag{13}$$

$$|0\rangle \qquad |4\rangle = |a_{\alpha}^{\dagger} a_{\beta}^{\dagger} d_{\alpha}^{\dagger} d_{\beta}^{\dagger}\rangle.$$

Here α, β are the up- and down-spin projections. Explicit expressions for only singlet components of the double hole cluster states are given, since we suggest that W transforms only these components and retains the triplet ones unchanged.

Any unitary operator W_n with the above properties can be expressed via the Hubbard operators $X^{(n)}_{i\lambda,i\lambda'}$ acting in the cluster basis (12), (13):

$$W_n = \prod_i \left[I + \sum_{\lambda,\nu} (S_{i\lambda,i\nu} - \delta_{\lambda,\nu}) X_{i\lambda,i\nu} \right]. \tag{14}$$

It is determined by a set of unitary matrices $S^{(i)} = S_{i\lambda,i\nu}$. They characterize the rotation among corresponding components of the basis (12), (13) with i holes on the cluster.

According to the definition, the Hubbard operators have only one nonzero matrix element $\langle i\lambda | X_{i\lambda,i'\lambda'} | i'\lambda' \rangle = 1$, and unitarity of W_n follows directly from their properties.

Thus, a general transformation which conserves the hole number and a spin on the cluster is determined by sets of real unitary matrices $S^i = S_{i\lambda,i\mu}$, $i = 1, 2, 3$. Here $S^{(1)}(\alpha_1)$ and $S^{(3)}(\alpha_3)$ are the second-order matrices depending on parameters α_1, α_3 respectively, and $S^{(2)} = S_{2\lambda,2\lambda'}$ is the third-order matrix depending on three parameters (ϕ, β, χ) if we suppose that W_n acts only among the singlet two-hole components (13) of the cluster basis.

Consider now the action of W_n on the arbitrary operator Q_n referring to the nth cluster. Each operator of such kind can be expanded over the Hubbard operators:

$$Q_n = \sum q_{i\lambda,i'\lambda'} X^{(n)}_{i\lambda,i'\lambda'} \tag{15}$$

Therefore, the transformed operator $\tilde{Q}_n$ has a similar form:

$$\tilde{Q}_n = W_n^{\dagger} Q_n W_n = \sum \tilde{q}_{i\lambda,i'\lambda'} X^{(n)}_{i\lambda,i'\lambda'} \tag{16}$$

and the coefficients $\tilde{q}$ are connected to the original expansion coefficients q in equation (15) by a linear transformation:

$$\tilde{q}_{i\lambda,i'\lambda'} = \sum S_{i\lambda,i\mu} S_{i'\lambda',i'\mu'} q_{i\mu,i'\mu'}. \tag{17}$$

As a result, the transformed Hamiltonian of the DB model takes the form

$$\tilde{H}^{DB} = \sum_n \tilde{h}_n + 2t \sum_{n\neq m} F(n-m)(\tilde{a}^{\dagger}_{n\sigma} \tilde{d}_{m\sigma} + \text{HC}). \tag{18}$$

Here the intracluster part $\tilde{h}_n$ depends on the even Hubbard operators $X_{i\lambda,i\lambda'}$. Their expressions in terms of the Fermi operators are given in the appendix. The final form of the transformed operator $\tilde{a}_{n\sigma}$ is

$$\tilde{a}_{n\sigma} = \sum_{i,j} g^a_{i,j} r_i(\sigma) R_j(-\sigma) \tag{19}$$

and $\tilde{d}_{n\sigma}$ has a similar form with the corresponding coefficients $g^d_{i,j}$. Here $r_i(\sigma)$ and $R_j(s)$ are

$$r_i(\sigma) = \{a_{n\sigma}, d_{n\sigma}, a_{n\sigma} n^d_{n\sigma}, d_{n\sigma} n^a_{n\sigma}\}_i \tag{20}$$

$$R_j(s) = \{1, n^a_{ns}, n^d_{ns}, a^+_{ns} d_{ns}, d^+_{ns} a_{ns}, n^a_{ns} n^d_{ns}\}_j. \tag{21}$$

The coefficients $g^{a(d)}_{i,j}$ are determined by $S^{(i)}$ with the use of a relation of the type of (17).

After substitution of $\tilde{h}_n$ and equations (19)–(21) in equation (18), we obtain an explicit expression for the transformed DB Hamiltonian $\tilde{H}$ in terms of the original Fermi operators, involving the dependence of all of the coefficients on the variational parameters $(\alpha_1, \alpha_3, \phi, \beta, \chi)$. Then the average value of the energy

$$\bar{H} = \langle H \rangle = \langle \Psi H \Psi \rangle = \langle \Phi \tilde{H} \Phi \rangle = \langle \tilde{H} \rangle_{HF} \tag{22}$$

is exactly expressed via the single-particle averages

$$\rho^{aa}_k = \langle a^{\dagger}_k a_k \rangle \qquad \rho^{dd}_k \qquad \rho^{ad}_k = \langle a^{\dagger}_k d_k \rangle.$$

Thus the self-consistent HF solutions of the effective-DB problem have been found for some transformation parameters $p_\nu = (\alpha_1, \alpha_3, \phi, \beta, \chi)$ and the energy was subsequently minimized with respect to p_ν. The procedure for obtaining such a solution followed by minimization over parameters has been elaborated.

Now we derive the SB Hamiltonian (11) acting in the space of the SB functions (9) with zero occupancy of the d orbitals. It has a rather simple form:

$$\tilde{H}(a) = \sum_n (E_a a^{\dagger}_{n\sigma} a_{n\sigma} + V_0 n^a_{n\uparrow} n^a_{n\downarrow}) + \tilde{T}(a) \tag{23}$$

$$\tilde{T}(a) = 2 \sum_{i,j} \sum_{n\neq m,\sigma} F(n-m) t_{i,j} (a^{\dagger}_{in\sigma} a_{jm\sigma} + \text{HC}) \tag{24}$$

$$a_{1n\sigma} = a_{n\sigma}(1 - n^a_{n,-\sigma}) \qquad a_{2n\sigma} = a_{n\sigma} n^a_{n,-\sigma}. \tag{25}$$

Here $i, j = 1, 2$ and E_a, V_0, t_{ij} depend on the parameters p_ν of the unitary transformation. Notice that a zero occupancy of d orbitals in $\Phi(a)$ does not mean the same for the total SB function $\Psi(a, d) = W(a, d)\Phi(a)$. It means only that the lowest cluster components are preferentially occupied and the excited cluster configurations are absent. For the SB model with optimal transformation parameters the cluster states

$$W_n|0\rangle \qquad W_n|a^{\dagger}_{n\sigma} 0\rangle \qquad W_n|a^{\dagger}_{n\alpha} a^{\dagger}_{n\beta} 0\rangle \tag{26}$$

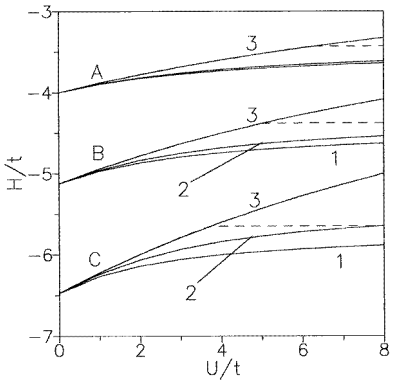

Figure 1. The energy of the four-site complex *adad* as a function of $U = U_d$ at $n = 2$. Curves 1 are the results of the exact diagonalization of the Hamiltonian; they coincide with the results obtained with the optimal double-configurational SB function (28). Curves 2 are the results for the optimally transformed HF function (27), and curves 3 are the same for the pure HF approximation. Dashed curves combined with parts of curves 3 for small U are the energies for Gutzwiller's function. The bunches A, B, C refer to $\delta\epsilon/t = 0, 1, 2$ respectively.

are close to the lowest eigenstates of the intracluster Hamiltonian h_n, and the optimal operator W_n is close to that which diagonalizes h_n. This confirms that the intercluster interactions in the Emery model are small.

A self-consistent HF solution of (23) with minimization over the transformation parameters has also been realized. Now only three parameters are significant, since two of them governing the rotation of the three-hole components or the excited singlet two-hole components do not affect the energy in the SB approach.

3. The four-site complex

First we present the energies for the finite complex of four centres $a_1d_1a_2d_2$ having two sorts of orbital. Let these centres be placed at the vertices of a square and the system be described by the Coulomb interaction $U = U_d$ on two d centres and by the a–d hopping $t = t_{ad}$. To study the accuracy of the SB mapping of such a problem we divide the complex into two clusters $(ad)_2$, and the correlated state $\Psi(ad) = W\Phi(a)$ is presented as transformed SB states $\Phi(a)$ of two types—the HF function Φ^I or the double-configuration function Φ^{II}:

$$\Psi^I(ad) = W\Phi^I \qquad \Phi^I = \prod_\sigma a^\dagger_{g\sigma}|0\rangle \tag{27}$$

$$\Psi^{II}(ad) = W\Phi^{II} \qquad \Phi^{II} = \cos\theta \prod_\sigma a^\dagger_{g\sigma}|0\rangle + \sin\theta \prod_\sigma a^\dagger_{u\sigma}|0\rangle. \tag{28}$$

Here $a_{g(u)} = (a_{1\sigma} \pm a_{2\sigma})/\sqrt{2}$.

Figure 1 presents the energy of the system as a function of U. Curves 1 are the results for the double-configuration SB function (28). It almost coincides with the result of exact diagonalization. The deviation δE is less than $0.0064t$, $0.013t$, $0.018t$ for $\delta E = 0$, t, $2t$. Curves 2 are the results for optimally transformed HF functions (27). Curves 3 are the results of the HF treatment of the original untransformed problem at $W = I$. It is seen that the deviations of curves 1 from the exact results 3 are connected with the HF treatment of the transformed effective Hamiltonian but not with the use of the effective-SB Hamiltonian.

The electronic densities ρ_a, ρ_d, ρ_{ad} coincide with similar accuracy. The corresponding deviations are $\delta\rho_d/\rho_d < 0.01$, $\delta\rho_{ad}/\rho_{ad} < 0.02$ for results obtained with the use of function (28) and by exact diagonalization. At the same time it is seen that the HF treatment of the SB may be adequate.

It is instructive also to compare these results with the energies of the system at $n = 2$ obtained with the use of Gutzwiller's function:

$$\Psi_{Gut} = \prod_{i=1,2} [1 + (\eta - 1)n^d_{i\uparrow} n^d_{i\downarrow}]\Phi_{HF}.$$

The energy is minimized with respect to η in the interval (0,1). It appears that for $U < U_c$ the value $\eta_{min} = 1$ and the energies coincide with the pure HF value. For $U > U_c$ one obtains $\eta_{min} = 0$ and the corresponding energies are shown by dashed curves in figure 1. Thus, for this finite system at $n = 2$ the energies for Gutzwiller's functions are always higher than those for the unitary transformed HF functions.

Table 1. The expansion coefficients of the site states (26) of the SB model in the cluster basis (12), (13) obtained using the cluster perturbation theory or by the variational method of unitary transformations.

	$\delta\epsilon/t$	C^1_1	C^1_2	C^2_1	C^2_2	C^2_3
Cluster	2	0.462	−0.887	0.487	0.294	−0.822
Variation	2	0.559	−0.829	0.477	0.322	−0.818
Cluster	0	0.707	−0.707	0.645	0.198	−0.738
Variation	0	0.714	−0.700	0.621	0.230	−0.749

4. Results for the simplified Emery model

Having in mind the above, we use the HF treatment of the SB and DB problem for estimation of the inaccuracy which is introduced by using the SB approximation in the Emery model (1) with the parameters $U/t = 7, \delta\epsilon = 0, 2, 4$. After minimization over the variational parameters the energies in the SB and DB problems appear to be very close. The deviation is $\delta E \leqslant 0.005t$ for the hole concentration in the range $1 \leqslant n \leqslant 1.8$. If the optimal variational operator W is replaced by the transformation operator W_{cl} which diagonalizes the intracluster Hamiltonian—i.e. minimizes the energy—in neglecting the intercluster interaction, then the deviation of the energy is also very small: $\delta E \leqslant 0.005t$ for the same model for $1 \leqslant n_h \leqslant 1.8$. A good accuracy for the energy near its minimum does not mean that the same accuracy will be achieved for other physical quantities. For example, the superconducting gap in the BCS solution changes by 40% on replacing W by W_{cl}.

The optimal transformations of the original problem to the effective-SB and effective-DB ones are also close to each other but do not coincide completely. Table 1 presents the expansion coefficients c^i_λ of the transformed cluster states (26):

$$W\Phi_i(a_n) = \sum_\lambda c^i_\lambda |i\lambda\rangle \qquad c^i_\lambda = S_{i1,i\lambda} \tag{29}$$

in the basis of the cluster functions (12), (13). These coefficients determine the real structure of the site states of the SB model. The first and third lines in table 1 give the expansion coefficients of the eigenfunctions of the intracluster part h_n of the Hamiltonian. Table 1 shows the difference in structure of the site states of SB models obtained variationally

and by use of the cluster perturbation theory. The variational approach effectively takes into account the corrections to the basis of the SB model introduced by the intercluster interactions.

The self-consistent DB HF solutions appear to be close to the SB solutions. That is, the weight $P^* = \rho_a\rho_d - \rho_{ad}^2$ of the excited cluster configurations in the DB function $\Phi_{HF}(ad)$ appears to be very small in comparison with the weight, $\approx$1, of the lowest configurations (26) incorporated in the SB function. The variational calculations of the effective-DB problem yield $P^* \approx 10^{-4}$ at $\delta\epsilon/t \simeq$ 1–4 and $U_d/t \simeq 7$. Recall that in the effective-DB Hamiltonian $\tilde{H}$ the cluster states with occupied d orbitals symbolize the excited cluster states, unlike to the case for the lowest cluster states (26) of the SB model.

Thus, the effective-SB Hamiltonian derived with the use of optimal unitary transformations or the cluster transformation W_{cl} can be a basis for the study of AF and SC pairing in systems.

5. Admissible types of SC pairing

The relation $V_0/t_{i,j} > 3$–6 for the main parameters of the effective-SB Hamiltonian $\tilde{H}$ for the hole density $n > 1$ and $\delta\epsilon/t =$ 1–4 indicates that the Hamiltonian still leads to a strongly correlated Hubbard problem, and the HF approximation is obviously inappropriate here. Nevertheless, some indications as to the possibility of any type of pairing can be obtained in the band approach to the SB problem. Since such results have a qualitative rather than quantitative character, we restrict the analysis to the simplified model (1), which misses many important interactions of the real CuO_2 plane. We suppose that the main role of these interactions reduces to renormalization of the main effective parameter $\delta\epsilon/t$ of model (1).

In the band approach to the SB problem (23), the AF pairing is determined by the parameter V_0/t which is 0.75 (0.73) or 1.735 (1.75) for the variational (the cluster) transformation parameters for $\delta\epsilon/t = 0$ or 2. The values of the AF gap are then $0.45t$ or $1.55t$, and the AF order with the double magnetic unit cell disappears for $n = 1.15$ or 1.4, respectively.

Now we estimate the possible types of SC pairing in the effective-SB problem based on the simple BCS-like function $\Phi_{BCS}(a)$ without taking into account the AF correlations. The average energy of the SB Hamiltonian (23) over $\Phi_{BCS}(a)$ is

$$\begin{aligned} &\langle H\rangle/N = (2E_a\rho_0 + V_0\rho_0^2 + 2t\theta_0) + \langle H^{SC}\rangle \\ &H^{SC} = k_{00}u_0^\dagger u_0 + \sum_{l\neq 0} k_{0l}(u_0^\dagger u_l + \text{HC}) + \sum_{l\neq 0}\kappa_l u_l^\dagger u_l. \end{aligned} \tag{30}$$

Here the summing is carried out over the vectors $l = (l_x, l_y)$, and ρ_l, u_l are the normal and anomalous averages:

$$\rho_0 = N^{-1}\sum_k \mathrm{e}^{\mathrm{i}kl}\rho_k \qquad \langle u_l\rangle = N^{-1}\sum_k \mathrm{e}^{\mathrm{i}kl}\langle a_{k\alpha}^\dagger a_{-k\beta}^\dagger\rangle$$

$$\theta_0 = N^{-1}\sum_k [F_k - F(0)]\rho_k \qquad \kappa_l = -8\tau F(l)\rho_l \qquad \tau = t_{11} + t_{22} - 2t_{12}.$$

The main constant $k_{00} = V_0 - 8\tau\theta_0 \simeq V_0$ corresponding to the anomalous average of s type is large and positive. This forbids SC pairing of s type. At the same time the last term in equation (30) might provide SC pairing of d symmetry. Since the κ_l decrease sharply with l, it is sufficient to consider only the main first contribution from $l = 1$ in the pairing

interaction of d symmetry:

$$V(\text{SC–d}) = \kappa_1 \beta_1^\dagger \beta_1$$
$$\beta_1^\dagger = N^{-1} \sum_k (\cos k_x - \cos k_y) a_{k\alpha}^\dagger a_{-k\beta}^\dagger \qquad \kappa_1 = -8\tau F(1)\rho_1.$$

The constant κ_1 of the SC pairing of d type depends on the value $\tau = t_{11} + t_{22} - 2t_{12}$ determined by the parameters of the kinetic energy (24) of the SB model. At $U/t = 7$ the constant κ_1 is negative ($\tau,\ \rho_1 < 0,\ F(1) > 0$) over the whole range of doping $1 < n < 1.8$.

However, the value of the constant is very small: $\kappa_1 = -\{0.1\text{–}0.02\}$, and simple BCS solutions of the SB problem (29) give too small a value of the gap: $\Delta \simeq (1\text{–}7) \times 10^{-5} t$ for $U/t = 7$, $\delta\epsilon/t = 2\text{–}4$. One cause of such a small gap may be the neglect of intercluster correlations. A large band width and a small density of states at the Fermi level are typical for the single-particle HF or BCS solutions of the SB problem. In real situations the SB problem (23) corresponds to the large interaction $V_0/t_{ij} > 1$, leading to the hole localization in lower hybrid orbitals of clusters. This can significantly enlarge the density of states in the upper Hubbard band—and the SC gap correspondingly.

Thus the BCS solutions demonstrate that an electronic mechanism of correlational nature may be responsible for the SC pairing of d symmetry with a value of the gap much less than the scale of the electronic parameter t of the original model. Previously Hirsch and Marsiglio [18] had discussed the mechanism of superconductivity due to the correlated hopping interaction (CHI) in the oxygen p-orbital system. The CHI had been postulated in [18, 19], and a small p–p hopping (about 0.06 eV) was needed to describe the proper scale of the gap for SC pairing of s type. Unlike in [18], the term $a_{n\sigma}^\dagger a_{m\sigma} n_{n,-\sigma} n_{m,-\sigma}$ in the effective-SB Hamiltonian (23) derived from the original model with p–d hopping may induce superconductivity of d type with a value of the gap much less than the electronic energy scale t in the system. However, the above-discussed simplified model does not include the important Coulomb interactions (U_p, V_{pd}, etc) which also contribute to the constant of SC–d pairing. So further studies taking into account these interactions and the AF correlations are needed.

6. Conclusions

The variational effective-SB Hamiltonian of the Emery-like problem obtained by local unitary transformation of the original Hamiltonian gives energies as accurate as those from the effective-DB model. The effective-SB model obtained by a variational method appears to be very close to the SB model derived in the cluster perturbation method [1–4]. The calculations of the four-site complex confirm a high accuracy of the SB model, but show that HF treatment of the SB problem may be inadequate. The BCS solutions of the SB model give an indication of the possibility of superconducting pairing of d symmetry of correlational nature.

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Appendix

The intracluster part h_n of the transformed Hamiltonian (18) is expressed in terms of the even Hubbard operators $X^{(n)}_{i\lambda,i\lambda'}$ which are diagonal over the hole number $i = 1, 2, 3$. In terms of the Fermi operator they are (the number n of the cluster is omitted below)

$$X_{1\lambda\sigma,1\lambda'\sigma} = \begin{pmatrix} P_0^d P_\sigma^a & a_{1\sigma}^\dagger d_{1\sigma} \\ d_{1\sigma}^\dagger a_{1\sigma} & P_0^a P_\sigma^d \end{pmatrix}_{\lambda\lambda'}$$

$$X_{3\lambda\sigma,3\lambda'\sigma} = \begin{pmatrix} P_2^d P_\sigma^a & -a_{2,-\sigma}^\dagger d_{2,-\sigma} \\ -d_{2,-\sigma}^\dagger a_{2,-\sigma} & P_2^d P_\sigma^a \end{pmatrix}_{\lambda\lambda'}$$

$$X_{2\lambda,2\lambda'} = \begin{pmatrix} P_2^a P_0^d & a_\uparrow^\dagger a_\downarrow^\dagger d_\downarrow d_\uparrow & \dfrac{1}{\sqrt{2}}\displaystyle\sum_\sigma a_{2\sigma}^\dagger d_{1,-\sigma} \\ & P_0^a P_2^d & \dfrac{1}{\sqrt{2}}\displaystyle\sum_\sigma d_{2\sigma}^\dagger a_{1,-\sigma} \\ & & \dfrac{1}{2}\displaystyle\sum_\sigma (P_\sigma^a P_{-\sigma}^d - a_\sigma^\dagger a_{-\sigma} d_{-\sigma}^\dagger d_\sigma) \end{pmatrix}_{\lambda\lambda'}.$$

The missing elements in the last matrix are the Hermitian conjugate ones $X_{2\mu,2\nu} = (X_{2\nu,2\mu})^\dagger$, and the following notation is used:

$$P_0^a = (1 - n_\uparrow^a)(1 - n_\downarrow^a) \qquad P_2^a = n_\uparrow^a n_\downarrow^a \qquad P_\sigma^a = n_\sigma^a (1 - n_{-\sigma}^a)$$
$$a_{1\sigma} = a_\sigma (1 - n_{-\sigma}^a) \qquad a_{2\sigma} = a_\sigma n_{-\sigma}^a.$$

P_0^d, P_2^d, $d_{1\sigma}$ and $d_{2\sigma}$ are similarly defined.

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