Dynamics of holes in the extended Hubbard model

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The strong-correlation limit of the extended Hubbard model of plane cuprate perovskites is considered for two ratios of material parameters allowed by the uncertainty of their known values: the Cu-O electron promotion energy is of the order of the Cu-O hybridization at a negligibly small Hubbard repulsion on oxygen sites and the hybridization is much smaller than other energy parameters. By taking into account the antiferromagnetic ordering of lightly doped samples and using the spin-wave approximation, for these two cases effective Hamiltonians are obtained, in which charge and spin degrees of freedom are described by practically independent operators. On the basis of these Hamiltonians it is shown that the low-energy hole dynamics is essentially different in the two cases. In the latter case it can approximately be mapped on the one-band t-J model describing the movement of the Zhang-Rice singlet. However, essential deviations might arise if the oxygen and copper on-site repulsions were comparable. The Hamiltonian in the former case is intrinsically a two-band one which differs from the one-band Hamiltonian in shapes and widths of energy bands and in conditions of the formation of a ferromagnetically ordered region around a hole in the limit of large repulsions.

I. INTRODUCTION

It is generally accepted that the CuO_2 layers play a major role in determining the normal and superconducting properties of the perovskite high-T_c superconductors. It is also widely accepted that these layers can be described by some version of the Hubbard model. However, it is still unclear how much of the detailed electronic structure should be included in the Hamiltonian to represent adequately low-energy properties of these planes. After Anderson's supposition that these properties can be described by the one-band Hubbard model,[1] an attempt was undertaken by Zhang and Rice[2] to confirm this statement using the extended Hubbard model containing $3d_{x^2-y^2}$ Cu and $2p_x$, $2p_y$ O states as the starting point. The conclusion of this paper was criticized from different points of view,[3,4] and among the raised objections the neglect of the ordering of Cu spins and a vague range of applicability of the one-band mapping should be singled out. In connection with these objections it should be noted that the proof of the similarity of the low-energy dynamics of the two models is not only reduced to the demonstration of the fact that the extended Hubbard model possesses a singled-out band of low-lying excitations as it was done in Ref. 2. If the dispersion of the excitations is mainly determined by the interaction with magnons—the case we are concerned with in antiferromagnetically ordered lightly doped samples—it should be shown that this interaction is the same as in the one-band model. One of the aims of the present paper is the determination of some limitations of such mapping.

The second aim of this paper is to find a form of the extended Hubbard Hamiltonian in the case of the strong coupling, which is convenient for calculations. The main problem in the consideration of the Hubbard Hamiltonian and the related $t-J$ Hamiltonian is in a complex form of the lowest eigenstates. It is the same problem one meets in dealing with the Heisenberg Hamiltonian for which the approximate method of overcoming it is known in two- and three-dimensional cases. It is the spin-wave approximation. With reference to the one-band t-J model this approximation has already been introduced in Ref. 5 and 6 and a satisfactory agreement of the results obtained in its framework[6,7] with the exact-diagonalization results for small lattices[8] gives grounds to consider this approximation to be appropriate for the problem. In the Hamiltonians of the spin-wave approximation, obtained below, spin and charge degrees of freedom are described by operators which with a good accuracy can be considered as independent, which makes calculations particularly simple. On the other hand, these Hamiltonians can straightforwardly be compared with the one-band spin-wave Hamiltonian that allows one to prove the possibilities of the one-band mapping.

As it will be shown below the uncertainties in the known values of material parameters allow three possibilities of the parameter ratios. Considering the strong-correlation limit when the repulsion on Cu sites is much larger than other energy parameters (excluding possibly the repulsion on O sites), the extended Hubbard Hamiltonian can be reduced to some generalization of the t-J Hamiltonian. A regular way of performing such a transformation, based on the operator perturbation theory[9] and appropriate for all three cases mentioned above, is discussed in Sec. II. Two of these cases, the case when the Cu-O electron promotion energy is of the order of the Cu-O hybridization at a negligibly small Hubbard repulsion on the oxygen sites and the case when the hybridization is much smaller than other energy parameters, are considered in Secs. III and IV. In these sections the cor-

sponding generalized t-J Hamiltonians are obtained and transformed in accord with the spin-wave approximation; the possibilities of the one-band mapping are elucidated and characteristic shapes of the lowest-energy bands are calculated for reasonable sets of parameters.

II. EFFECTIVE HAMILTONIAN

The object of the subsequent consideration is the Hamiltonian

$$H = U\sum_{\mathbf{m}} n_{\mathbf{m},+1}n_{\mathbf{m},-1} + \frac{U_p}{2}\sum_{\mathbf{m}\delta} n_{\mathbf{m}+\delta,+1}n_{\mathbf{m}+\delta,-1} + \frac{\Delta}{2}\sum_{\mathbf{m}\delta} n_{\mathbf{m}+\delta} + t\sum_{\mathbf{m}\delta\sigma}(d^{\dagger}_{\mathbf{m}\sigma}p_{\mathbf{m}+\delta,\sigma} + \text{H.c.}), \quad (1)$$

where $d^{\dagger}_{\mathbf{m}\sigma}$ and $p^{\dagger}_{\mathbf{m}+\delta,\sigma}$ are the creation operators of electrons in the $3d_{x^2-y^2}$ orbitals of copper and the $2p_\sigma$ orbitals of oxygen, respectively, with spin $\sigma = \pm 1$; $\Delta > 0$ is the Cu-O promotion energy; U and U_p are the Hubbard repulsions on copper and oxygen sites, labeled by the indices $\mathbf{m}$ and $\mathbf{m}+\delta$, respectively; $\delta = (\pm a/2, 0), (0, \pm a/2)$; a is the lattice spacing; t is the Cu-O hybridization; $n_{\mathbf{m}\sigma} = d^{\dagger}_{\mathbf{m}\sigma}d_{\mathbf{m}\sigma}$, $n_{\mathbf{m}} = \sum_\sigma n_{\mathbf{m}\sigma}$. The extended Hubbard Hamiltonian (1) has been introduced and considered in a number of papers.[2,3,10–12]

It is known from the band calculations for a typical representative of cuprate perovskites La_2CuO_4 that $U = 7 - 10$ eV $\gg |t| = 1 - 1.5$ eV. The values of Δ and U_p, usually cited in literature for this crystal, are still controversial, ranging from $\Delta \approx |t|$ and $U_p \approx 0$ to $\Delta \approx U_p \approx 5$ eV (see, e.g., Refs. 13 and 14). In this set of parameters there is at least one small parameter t that allows one to simplify essentially the Hamiltonian. The operator perturbation theory[9] is the most convenient way to do this. For the sake of completeness let us briefly recollect its main results.

Let a Hamiltonian be represented in the form

$$H = H_0 + \epsilon H_1, \quad (2)$$

where $\epsilon \ll 1$ and the Hamiltonian H_0 possesses the degenerate ground state with an energy E_0 separated by a finite gap ΔE from excited states. Let us designate the ground-state eigenvectors of H_0 as $|q\rangle$, their subspace as $\mathcal{L}$, and a projection of an eigenvector C of H onto this subspace as $C_0 = \mathcal{P}C$. $\mathcal{P} = \sum_q |q\rangle\langle q|$. Then, with the accuracy up to the terms of the order of ϵ^4 the eigenvalue E of H, corresponding to C, can be found from the following eigenvalue problem:

$$H_{\text{eff}}C_0 = (E - E_0)C_0, \quad (3)$$

$$\begin{aligned} H_{\text{eff}} = \mathcal{P}\ [&\epsilon H_1 - \epsilon^2 H_1(H_0 - E_0)^{-1}(1-\mathcal{P})H_1 + \epsilon^3 H_1(H_0 - E_0)^{-1}(1-\mathcal{P})(H_1 - E^{(1)})(H_0 - E_0)^{-1}(1-\mathcal{P})H_1 \\ &-\epsilon^4 H_1(H_0 - E_0)^{-1}(1-\mathcal{P})(H_1 - E^{(1)})(H_0 - E_0)^{-1}(1-\mathcal{P})(H_1 - E^{(1)})(H_0 - E_0)^{-1}(1-\mathcal{P})H_1 \\ &-\epsilon^4 H_1(H_0 - E_0)^{-1}E^{(2)}(H_0 - E_0)^{-1}(1-\mathcal{P})H_1]\mathcal{P}, \end{aligned} \quad (4)$$

where $\epsilon E^{(1)}$ and $\epsilon^2 E^{(2)}$ are the first- and second-order corrections in the eigenenergy.

Note that due to the projection operators $(1-\mathcal{P})$ and the supposition about a finite value of ΔE the denominators in (4) are nonzero. The effective Hamiltonian H_{eff} acts in the subspace $\mathcal{L}$ and gives approximate eigenvalues of H for the states C satisfying the condition $\mathcal{P}C \neq 0$ at $\epsilon \to 0$. These states form a low-energy part of the spectrum. Equations (3) and (4) are equivalent to the usual degenerate perturbation theory (see, e.g., Ref. 15).

For further calculations it is convenient to use the definitions of $E^{(1)}$ and $E^{(2)}$ and rewrite H_{eff} with the same accuracy in the form

$$\begin{aligned} H_{\text{eff}} = \mathcal{P}\ [&\epsilon H_1 - \epsilon^2 H_1(H_0 - E_0)^{-1}(1-\mathcal{P})H_1 + \epsilon^3 H_1(H_0 - E_0)^{-1}(1-\mathcal{P})H_1(H_0 - E_0)^{-1}(1-\mathcal{P})H_1 \\ &-\epsilon^3 H_1(H_0 - E_0)^{-2}(1-\mathcal{P})H_1\mathcal{P}H_1 - \epsilon^4 H_1(H_0 - E_0)^{-3}(1-\mathcal{P})H_1\mathcal{P}H_1\mathcal{P}H_1 \\ &+\epsilon^4 H_1(H_0 - E_0)^{-2}(1-\mathcal{P})H_1(H_0 - E_0)^{-1}(1-\mathcal{P})H_1\mathcal{P}H_1 \\ &+\epsilon^4 H_1(H_0 - E_0)^{-1}(1-\mathcal{P})H_1(H_0 - E_0)^{-2}(1-\mathcal{P})H_1\mathcal{P}H_1 \\ &-\epsilon^4 H_1(H_0 - E_0)^{-1}(1-\mathcal{P})H_1(H_0 - E_0)^{-1}(1-\mathcal{P})H_1(H_0 - E_0)^{-1}(1-\mathcal{P})H_1 \\ &+\epsilon^4 H_1(H_0 - E_0)^{-2}(1-\mathcal{P})H_1\mathcal{P}H_1(H_0 - E_0)^{-1}(1-\mathcal{P})H_1]\mathcal{P}. \end{aligned} \quad (5)$$

The terms of the third and the fourth order in (5) contain non-Hermitian addends. However, this non-Hermiticity influences only the fifth-order corrections. As will be seen later, in application to the considered problem Eq. (5) reduces to some generalization of the t-J Hamiltonian.

From the ranges of parameters cited above it is clear that the transfer term in (1) should be included in H_1. If for a moment the remaining part of the Hamiltonian will be considered as H_0, one can determine the possible values of the gap ΔE separating the states of the subspace $\mathcal{L}$ (one $d_{x^2-y^2}$ electron per Cu atom and one or two p_σ electrons per O atom) from excited states:

$U_p+\Delta = U-\Delta_h$, $U-U_p-\Delta = \Delta_h$ and $U-\Delta = U_p+\Delta_h$. Here Δ_h is the Cu-O promotion energy in the hole representation. These expressions give estimations of the possible values of denominators in (4) and (5). If any of these values is comparable with $|t|$, the corresponding terms should be attributed to H_1 to make the perturbation theory applicable. The values of parameters reported in Refs. 13 and 14 allow three possibilities: (i) $U_p+\Delta \approx |t|$, (ii) all denominators are much larger than $|t|$, and (iii) $U-U_p-\Delta \approx |t|$. The third case allows an essential decrease of the Cu momentum, in comparison with its zero-point fluctuation value, in an undoped crystal due to a strong Cu-O hybridization. The uncertainty of the known value of the momentum[16] does not permit to exclude this possibility. Nevertheless, the further consideration is limited by the first two cases. Some peculiarities of the third case have qualitatively been discussed in Ref. 11.

III. THE CASE $\Delta \approx |t|$

Considering case (i), let us suppose additionally that $U_p = 0$.[13] It is clear that in this case the first term in (1) should be chosen as H_0, ϵ is t or Δ, and H_1 is the sum of the third and fourth terms divided by ϵ (here and below U is taken as a unit of energy). At a number of electrons less than or equal to $5N$, where N is the number of Cu sites, the subspace $\mathcal{L}$ consists of states without doubly occupied Cu sites.

In spite of the complex form of Eq. (5) the corresponding calculations are comparatively simple. Neglecting unessential terms of the third order and keeping from the terms of the fourth order only the term describing the Cu-Cu superexchange, one finds

$$\begin{aligned} H_{\text{eff}} = {} & 2t\mathcal{P}\sum_{\mathbf{m}\sigma}(d^{\dagger}_{\mathbf{m}\sigma}\pi_{\mathbf{m}\sigma}+\text{H.c.})\mathcal{P} \\ & +\frac{\Delta}{2}\sum_{\mathbf{m}\delta} n_{\mathbf{m}+\delta} + 8t^2\sum_{\mathbf{m}}(\mathbf{S}_{\mathbf{m}}\mathbf{s}_{\mathbf{m}} - \tfrac{1}{4}N_{\mathbf{m}}n_{\mathbf{m}}) \\ & +4t^4\sum_{\mathbf{ma}}(\mathbf{s}_{\mathbf{m}}\mathbf{s}_{\mathbf{m}+\mathbf{a}} + \tfrac{1}{4}n_{\mathbf{m}}n_{\mathbf{m}+\mathbf{a}}), \end{aligned} \tag{6}$$

where the operators $\pi_{\mathbf{m}\sigma} = \frac{1}{2}\sum_{\delta} p_{\mathbf{m}+\delta,\sigma}$ are introduced by analogy with,[2]

$$\begin{aligned} & N_{\mathbf{m}\sigma} = \pi^{\dagger}_{\mathbf{m}\sigma}\pi_{\mathbf{m}\sigma}, \quad N_{\mathbf{m}} = \sum_{\sigma} N_{\mathbf{m}\sigma}, \\ & S^{\sigma}_{\mathbf{m}} = \pi^{\dagger}_{\mathbf{m}\sigma}\pi_{\mathbf{m},-\sigma}, \quad S^{z}_{\mathbf{m}} = \frac{1}{2}(N_{\mathbf{m},+1} - N_{\mathbf{m},-1}), \end{aligned} \tag{7}$$

and the operators $s^{\sigma}_{\mathbf{m}}$ and $s^{z}_{\mathbf{m}}$ are analogously determined through $d_{\mathbf{m}\sigma}$, $\mathbf{a} = (\pm a, 0)$, $(0, \pm a)$.

The operators $\pi_{\mathbf{m}\sigma}$ are not orthogonal ($\{\pi_{\mathbf{m}\sigma}, \pi^{\dagger}_{\mathbf{m}'\sigma'}\} = \frac{1}{4}\delta_{\sigma\sigma'}\sum_{\delta\delta'}\delta_{\mathbf{m}+\delta,\mathbf{m}'+\delta'}$) and, as in Ref. 2, it is convenient to introduce new operators satisfying the usual commutation relations,

$$\begin{aligned} \phi_{\mathbf{k}\sigma} &= \beta_{\mathbf{k}}\frac{1}{\sqrt{N}}\sum_{\mathbf{m}} e^{i\mathbf{km}}\pi_{\mathbf{m}\sigma} \\ &= \tfrac{1}{2}\beta_{\mathbf{k}}[p^{x}_{\mathbf{k}\sigma}(1+e^{i\mathbf{kx}}) + p^{y}_{\mathbf{k}\sigma}(1+e^{i\mathbf{ky}})], \end{aligned} \tag{8}$$

where $\beta_{\mathbf{k}} = \{1+\frac{1}{2}[\cos(\mathbf{kx})+\cos(\mathbf{ky})]\}^{-1/2}$, $p^{z}_{\mathbf{k}\sigma} = N^{-1/2}\sum_{\mathbf{m}}\exp(-i\mathbf{km})p_{\mathbf{m}-\mathbf{z}/2,\sigma}$, $\mathbf{x} = (a,0)$, $\mathbf{y} = (0,a)$. It follows from (8) that

$$\pi_{\mathbf{m}\sigma} = \lambda_0\phi_{\mathbf{m}\sigma} + \lambda_1\sum_{\mathbf{a}}\phi_{\mathbf{m}+\mathbf{a}\sigma} + \cdots, \tag{9}$$

where $\lambda_{\mathbf{m}} = N^{-1}\sum_{\mathbf{k}}\exp(i\mathbf{km})\beta^{-1}_{\mathbf{k}}$, $\lambda_0 \approx 0.96$, $\lambda_1 = \lambda_{\mathbf{a}} \approx 0.14$. Due to the fast decrease of $\lambda_{\mathbf{m}}$ with the growth of $|\mathbf{m}|$ only two terms written out in (9) will be considered below. Since the operators $\phi_{\mathbf{m}\sigma}$ do not form the complete set of oxygen operators for a lattice with two oxygen atoms per unit cell, they should be supplemented by the following set of operators:[12]

$$\psi_{\mathbf{k}\sigma} = \tfrac{1}{2}\beta_{\mathbf{k}}[p^{y}_{\mathbf{k}\sigma}(1+e^{-i\mathbf{kx}}) - p^{x}_{\mathbf{k}\sigma}(1+e^{-i\mathbf{ky}})]. \tag{10}$$

In the new notations the effective Hamiltonian acquires the following form:

$$\begin{aligned} H_{\text{eff}} = {} & 2t\lambda_0\mathcal{P}\sum_{\mathbf{m}\sigma}(d^{\dagger}_{\mathbf{m}\sigma}\phi_{\mathbf{m}\sigma}+\text{H.c.})\mathcal{P} + \Delta\sum_{\mathbf{m}\sigma}(\phi^{\dagger}_{\mathbf{m}\sigma}\phi_{\mathbf{m}\sigma} + \psi^{\dagger}_{\mathbf{m}\sigma}\psi_{\mathbf{m}\sigma}) \\ & +2t\lambda_1\mathcal{P}\sum_{\mathbf{ma}\sigma}(d^{\dagger}_{\mathbf{m}\sigma}\phi_{\mathbf{m}+\mathbf{a}\sigma}+\text{H.c.})\mathcal{P} + 8t^2\sum_{\mathbf{m}}(\mathbf{S}_{\mathbf{m}}\mathbf{s}_{\mathbf{m}} - \tfrac{1}{4}N_{\mathbf{m}}n_{\mathbf{m}}) + 4t^4\sum_{\mathbf{ma}}(\mathbf{s}_{\mathbf{m}}\mathbf{s}_{\mathbf{m}+\mathbf{a}} + \tfrac{1}{4}n_{\mathbf{m}}n_{\mathbf{m}+\mathbf{a}}). \end{aligned} \tag{11}$$

The operators $\mathbf{S}_{\mathbf{m}}$ and $N_{\mathbf{m}}$ are expressed through $\phi_{\mathbf{m}\sigma}$ with the help of (9). As can be seen from Eq. (11), the operators $\psi_{\mathbf{m}\sigma}$ describe a conservative subsystem and will not be considered below since the corresponding levels are positioned far above the states of interest. A Hamiltonian analogous to (11) has earlier been obtained in Ref. 12 with the help of unitary transformations.

The further transformation of (11) is based on the antiferromagnetic ordering of spins on Cu sites, described by the Heisenberg term H_H in (11) and observed experimentally in lightly doped samples.[16] In this case a convenient way for the consideration of spin-spin and spin-hole interactions is the spin-wave approximation. As was told above, it allows one to obtain a form of the Hamiltonian

in which spin and charge degrees of freedom are with a good accuracy independent, which essentially simplifies calculations. On the other hand, this form of the Hamiltonian can straightforwardly be compared with the one-band spin-wave Hamiltonian, which allows one to verify the possibility of the one-band mapping.

In the presence of holes the spin-wave approximation can be introduced with the help of the following formulas:[6]

$$s_{\mathbf{m}}^{+1} = \Phi_{\mathbf{m}} b_{\mathbf{m}} P_{\mathbf{m}}^{+1} + b_{\mathbf{m}}^{\dagger} \Phi_{\mathbf{m}} P_{\mathbf{m}}^{-1}, \; s_{\mathbf{m}}^{-1} = (s_{\mathbf{m}}^{+1})^{\dagger},$$

$$\Phi_{\mathbf{m}} = \sqrt{1 - b_{\mathbf{m}}^{\dagger} b_{\mathbf{m}}}, \; s_{\mathbf{m}}^{z} = e^{i\mathbf{\Pi m}} \left(\frac{n_{\mathbf{m}}}{2} - b_{\mathbf{m}}^{\dagger} b_{\mathbf{m}} \right), \tag{12}$$

where $\mathbf{\Pi} = (\pi/a, \pi/a)$, $P_{\mathbf{m}}^{\sigma} = \frac{1}{2}[1 + \sigma \exp(i\mathbf{\Pi m})]$. It is easy to check that on the considered basis of states without doubly occupied Cu sites the operators $s_{\mathbf{m}}^{\sigma}$ and $s_{\mathbf{m}}^{z}$ in (12) satisfy the usual commutation relations of spin operators on the condition that the operators $b_{\mathbf{m}}$ satisfy the following commutation relations:

$$[b_{\mathbf{l}}, b_{\mathbf{m}}^{\dagger}] = \delta_{\mathbf{lm}} n_{\mathbf{m}}, \; [b_{\mathbf{l}}, b_{\mathbf{m}}] = 0. \tag{13}$$

The spin-wave approximation reduces to the neglect of the terms of the third and higher orders in $b_{\mathbf{l}}$, arising from the substitution of (12) into H_H.[9] This is justified for the states with a small number of spin flips. There are two sources of the spin flips—zero-point spin fluctuations and holes. A comparison of their effect shows that the applicability conditions of the spin-wave approximation in lightly doped samples is the same as in an undoped case.

The quadratic form obtained from H_H can be diagonalized by the unitary transformation[6]

$$T = \exp\left[\sum_{\mathbf{k}} \alpha_{\mathbf{k}} (b_{\mathbf{k}} b_{-\mathbf{k}} - b_{\mathbf{k}}^{\dagger} b_{-\mathbf{k}}^{\dagger}) \right],$$

$$\alpha_{\mathbf{k}} = \tfrac{1}{8} \ln\left(\frac{1 + \gamma_{\mathbf{k}}}{1 - \gamma_{\mathbf{k}}} \right), \; \gamma_{\mathbf{k}} = \tfrac{1}{4} \sum_{\mathbf{a}} e^{i\mathbf{ka}}, \tag{14}$$

which takes into account that in accord with (13) the operators $b_{\mathbf{k}} = N^{-1/2} \sum_{\mathbf{l}} b_{\mathbf{l}} \exp(i\mathbf{kl})$ satisfy the boson commutation relations with the accuracy up to the terms of the order of n/N, n is the number of holes. Transformation (14) is equivalent to the Bogolyubov transformation[9] but more convenient because the transformed Hamiltonian $T^{\dagger} H_H T$ has a simpler ground state. For example, in the absence of holes this state is $|\mathcal{N}\rangle$, one of two classical Néel states of Cu spins. Thus, transformation (14) allows one to take comparatively simply into consideration transversal spin fluctuations, which is the main merit of the spin-wave approximation.

The state $|\mathcal{N}\rangle$ is determined by the conditions $b_{\mathbf{m}}|\mathcal{N}\rangle = 0$ and contains occupied oxygen orbitals corresponding to the operators $\phi_{\mathbf{m}\sigma}^{\dagger}$. For this state the creation operator of the hole on the Cu site can be determined by the following formula:

$$h_{\mathbf{m}}^{\dagger} = \sum_{\sigma} P_{\mathbf{m}}^{\sigma} d_{\mathbf{m}\sigma}. \tag{15}$$

Supposing in the spirit of the spin-wave approximation $\Phi_{\mathbf{m}} = 1$ (and, consequently, $b_{\mathbf{m}}^{\dagger}$ is simply the spin-flip operator), from (12) and (15) one finds

$$\begin{aligned} [b_{\mathbf{m}}^{\dagger}, d_{\mathbf{m}'\sigma}] &= -P_{\mathbf{m}}^{-\sigma} d_{\mathbf{m},-\sigma} \delta_{\mathbf{mm}'}, \\ [b_{\mathbf{m}}^{\dagger}, d_{\mathbf{m}'\sigma}^{\dagger}] &= P_{\mathbf{m}}^{\sigma} d_{\mathbf{m},-\sigma}^{\dagger} \delta_{\mathbf{mm}'}, \\ [b_{\mathbf{m}}^{\dagger}, h_{\mathbf{m}'}^{\dagger}] &= 0, \; [b_{\mathbf{m}}^{\dagger}, h_{\mathbf{m}'}] = b_{\mathbf{m}}^{\dagger} h_{\mathbf{m}} \delta_{\mathbf{mm}'}. \end{aligned} \tag{16}$$

By making use of (16) it is easy to verify that the action of the three first terms on the right-hand side (rhs) of (11) on the states $b_{\mathbf{m}_1}^{\dagger} \cdots b_{\mathbf{m}_\nu}^{\dagger} \phi_{\mathbf{m}\sigma} |\mathcal{N}\rangle$, $b_{\mathbf{m}_1}^{\dagger} \cdots b_{\mathbf{m}_\nu}^{\dagger} d_{\mathbf{m}\sigma} |\mathcal{N}\rangle$, and their many-hole generalizations is equivalent to the action of the following operator:

$$-\sum_{\mathbf{m}} [2t\lambda_0 (h_{\mathbf{m}}^{\dagger} h_{\mathbf{m},+1} + h_{\mathbf{m}}^{\dagger} h_{\mathbf{m},-1} b_{\mathbf{m}} + \text{H.c.}) + \Delta \sum_{\sigma} h_{\mathbf{m}\sigma}^{\dagger} h_{\mathbf{m}\sigma} + 2t\lambda_1 \sum_{\mathbf{a}} (h_{\mathbf{m}+\mathbf{a}}^{\dagger} h_{\mathbf{m},-1} + h_{\mathbf{m}+\mathbf{a}}^{\dagger} h_{\mathbf{m},+1} b_{\mathbf{m}+\mathbf{a}} + \text{H.c.})], \tag{17}$$

where $h_{\mathbf{m},+1}^{\dagger}$ and $h_{\mathbf{m},-1}^{\dagger}$ are the oxygen hole creation operators $\phi_{\mathbf{m}\sigma}$ with the spins directed, respectively, parallel and antiparallel to the electron spin on the Cu site $\mathbf{m}$ in the state $|\mathcal{N}\rangle$. A constant term is omitted in (17).

After introducing operators (15) and representing the first-order terms in the form (17), unitary transformation (14) applied to these terms can easily be carried out. The difference $T^{\dagger} h_{\mathbf{m}}^{\dagger} T - h_{\mathbf{m}}^{\dagger}$ gives small corrections to the processes of the magnon creation and destruction, which are already present in (17) and, therefore, the difference can be neglected. Thus, the unitary transformation is reduced to the substitution of $b_{\mathbf{k}}$ by

$$\tilde{b}_{\mathbf{k}} = T^{\dagger} b_{\mathbf{k}} T = b_{\mathbf{k}} \cosh(2\alpha_{\mathbf{k}}) - b_{-\mathbf{k}}^{\dagger} \sinh(2\alpha_{\mathbf{k}}) \tag{18}$$

in Eq. (17). The k representation of the operators $h^{\dagger}_{\mathbf{m}}$ is analogous to the operators introduced in Ref. 5 and their combination $h^{\dagger}_{\mathbf{m+a}}h_{\mathbf{m}}$ in the t-J model, to the hole translation operator in Ref. 6.

One-site terms in (17), which do not contain magnon operators, can be diagonalized and Hamiltonian (11), after the unitary transformation, can be represented in the form

$$\tilde{H} = T^{\dagger}H_{\mathrm{eff}}T = \sum_{\mathbf{m}}\sum_{i=1}^{3}\varepsilon_i c^{\dagger}_{\mathbf{m}i}c_{\mathbf{m}i} - 2t\lambda_0\sum_{\mathbf{m}}[(c^{\dagger}_{\mathbf{m}1}\sin\theta + c^{\dagger}_{\mathbf{m}3}\cos\theta)c_{\mathbf{m}2}\tilde{b}_{\mathbf{m}} + \mathrm{H.c.}]$$
$$-2t\lambda_1\sum_{\mathbf{ma}}\{(c^{\dagger}_{\mathbf{m+a},1}\sin\theta + c^{\dagger}_{\mathbf{m+a},3}\cos\theta)[c_{\mathbf{m}2} + (c_{\mathbf{m}1}\cos\theta - c_{\mathbf{m}3}\sin\theta)\tilde{b}_{\mathbf{m+a}}] + \mathrm{H.c.}\} + 4t^4\sum_{\mathbf{k}}\omega_{\mathbf{k}}b^{\dagger}_{\mathbf{k}}b_{\mathbf{k}}, \tag{19}$$

where

$$h_{\mathbf{m}} = c_{\mathbf{m}1}\sin\theta + c_{\mathbf{m}3}\cos\theta,\quad h_{\mathbf{m},+1} = c_{\mathbf{m}1}\cos\theta - c_{\mathbf{m}3}\sin\theta,\quad h_{\mathbf{m},-1} = c_{\mathbf{m}2},$$
$$\varepsilon_1 = -\frac{\Delta}{2}\left[1 + \sqrt{1 + \left(\frac{4t\lambda_0}{\Delta}\right)^2}\right],\quad \varepsilon_2 = -\Delta,\quad \varepsilon_3 = -\frac{\Delta}{2}\left[1 - \sqrt{1 + \left(\frac{4t\lambda_0}{\Delta}\right)^2}\right], \tag{20}$$
$$\theta = \tfrac{1}{2}\arctan\frac{4t\lambda_0}{\Delta},\quad \omega_{\mathbf{k}} = 4\sqrt{1-\gamma^2_{\mathbf{k}}}.$$

The second-order terms, which introduce small corrections in the definition of operators $c_{\mathbf{m}i}$, are omitted in (19).

When $2\lambda_0|t| \lesssim \Delta$, $\varepsilon_2 - \varepsilon_1$ and terms in (19), which mix the states of bands 1 and 2 with the states of band 3, are much less than $\varepsilon_3 - \varepsilon_1$. This allows one to neglect a contribution of the latter band to the lowest hole-magnon states and to rewrite the corresponding part of the Hamiltonian in the form

$$\tilde{H} = \sum_{\mathbf{m}}\sum_{i=1}^{2}\varepsilon_i c^{\dagger}_{\mathbf{m}i}c_{\mathbf{m}i} - 2t\lambda_0\sin\theta\sum_{\mathbf{m}}(c^{\dagger}_{\mathbf{m}1}c_{\mathbf{m}2}\tilde{b}_{\mathbf{m}} + \mathrm{H.c.}) - t\lambda_1\sin(2\theta)\sum_{\mathbf{ma}}(c^{\dagger}_{\mathbf{m+a},1}c_{\mathbf{m}1}\tilde{b}_{\mathbf{m+a}} + \mathrm{H.c.})$$
$$-2t\lambda_1\sin\theta\sum_{\mathbf{ma}}(c^{\dagger}_{\mathbf{m+a},1}c_{\mathbf{m}2} + \mathrm{H.c.}) + 4t^4\sum_{\mathbf{k}}\omega_{\mathbf{k}}b^{\dagger}_{\mathbf{k}}b_{\mathbf{k}}. \tag{21}$$

From Eq. (20) it follows that $[c_{\mathbf{m}2}, b_{\mathbf{m}'}] = [c_{\mathbf{m}2}, b^{\dagger}_{\mathbf{m}'}] = 0$. Analogous commutators with $c_{\mathbf{m}1}$ can also be accepted to be equal to zero, since the Cu component in this operator is small at $2\lambda_0|t| \lesssim \Delta$. Besides, as it can be verified in the course of calculations, the noncommutativity of this component with magnon operators reveals itself only in high-order processes for the states forming the low-energy part of the spectrum at reasonable values of parameters. The neglect of this noncommutativity does not essentially change the results for this part of the spectrum. Thus, the operators $c_{\mathbf{m}i}$ and $b_{\mathbf{m}}$ connected with charge and spin degrees of freedom can with a good accuracy be considered here as independent.

The third and the last terms on the rhs of Eq. (21) form the Hamiltonian of the t-J model in the spin-wave approximation.[5,6] Other terms lead to the magnon-assisted and zero-magnon mixing of the states of bands 1 and 2. This mixing is not small, since the energy distance between the bands $\varepsilon_2 - \varepsilon_1 \approx 4(t\lambda_0)^2/\Delta$ is of the order of mixing terms. Figure 1 demonstrates the effect of the mixing on the energy band spectrum. The band of states with the z projection of the total spin S_z equal to 1/2, which is the lowest one for the used sets of parameters in both models, is chosen for demonstration. Calculations were carried out with the help of the recursion method described in Ref. 6. Thanks to the antiferromagnetic ordering of spins the wave vectors of states considered can be limited by the magnetic Brillouin zone—the zone of the doubled direct lattice. The bands in parts (a)–(c) of the figure correspond to the full Hamiltonian (21), while part (d) corresponds, to the t-J Hamiltonian constructed from the terms of Eq. (21) pointed out above and the part of the first term with $i = 1$. For the sets of parameters of parts (b) and (c) the shape of the energy band of the t-J model is similar to the one shown in the part (d) (with corresponding shifts and scale changes of the energy axis). This shape has little in common with the shapes of the bands in the parts (a)–(c) and it is impossible to choose the sets of parameters for which the band of the t-J model has such shapes.[7] Besides, for the sets of parameters (a) and (b) the bandwidths of the extended Hubbard model are by an order of magnitude smaller than those of the t-J model and are substantially shifted to lower energies. The second term on the rhs of Eq. (21) plays the main role in the creation of these differences.

The second difference between the two models lies in

the conditions of the formation of a ferromagnetically ordered region around a hole. It is known[17] that such a region is formed due to the gain in the hole kinetic energy in the ferromagnetic surrounding. In our picture the region looks like a cloud of magnons positioned on one of the sublattices in the vicinity of a hole. This spin configuration provides a minimal (for a given size of a distorted region) value of the hole transport term in the t-J Hamiltonian—the third term in Eq. (21). This gain is partly compensated by the growth of the magnon energy that limits the size of the magnon cloud. The Hamiltonian (21) contains an additional transport term, the fourth on the rhs, which can provide the hole movement without destroying the antiferromagnetic ordering. As a result, the presence of this term will hinder the formation of the ferromagnetically ordered region, changing the critical values of the parameters connected with the rise and growth of the region or even destroying it altogether. The same effect is had by the second term on the rhs of (21)—an optimal spin configuration for it differs from the ferromagnetic ordering. In this paper I limit myself to this qualitative discussion since calculations for the states with $S_z > 1/2$ need a more elaborate program than the one used for the states with $S_z = 1/2$ and the low-energy part of the spectrum, which is of the most interest, is formed by the latter states for the values of parameters cited above.

Thus, in the considered case $\Delta \approx |t| \ll U$ the extended Hubbard model cannot be reduced to the t-J model.

IV. THE CASE $|t| \ll U_P + \Delta$, $U - U_P - \Delta$

In this case the three first terms on the rhs of (1) should be included in H_0, $\epsilon = t$, and H_1 is the last term divided by ϵ (as above, $U = 1$). The subspace $\mathcal{L}$ contains states with singly occupied Cu sites and singly and doubly oc-

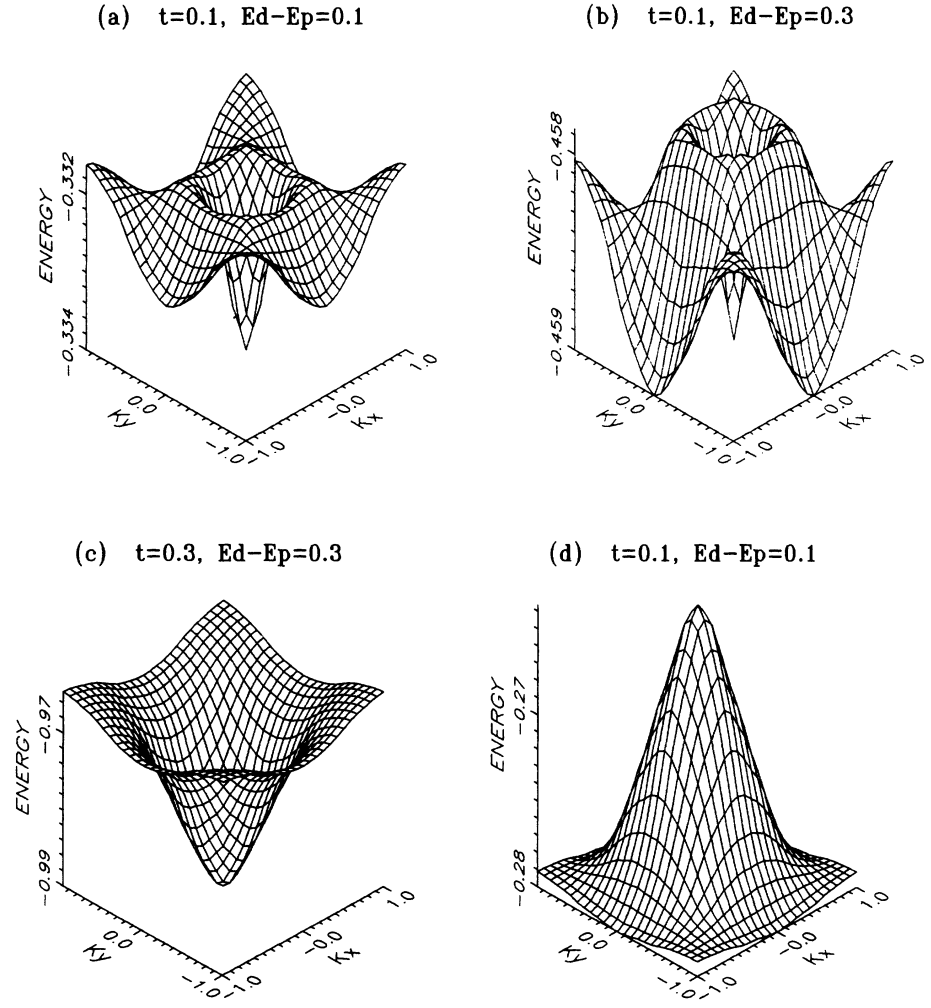

FIG. 1. Energy bands of the states with $S_z = 1/2$. Parts (a)–(c) demonstrate bands in the particular case of the extended Hubbard model described by Hamiltonian (21) (the case $|t| \approx \Delta \ll U$); part (d) shows the band of the t-J model. $Ed - Ep = \Delta$. The repulsion on Cu sites U and $\pi/(\sqrt{2}a)$, where a is the lattice spacing, are taken as units of energy and wave vector length.

cupied O sites (this subspace differs from the subspace in the preceding section—the states with unoccupied Cu sites are excluded).

The first-order term in (5) vanishes: by acting on the states belonging to the subspace $\mathcal{L}$ H_1 yields the states with an unoccupied or doubly occupied Cu site. The action of the left projection operator $\mathcal{P}$ on these states gives zero. Again, neglecting the unessential terms of the third order and keeping from the fourth-order terms only the one describing the Cu-Cu superexchange, one finds

$$H_{\text{eff}} = \tau \sum_{\mathbf{m}} N_{\mathbf{m}} + \mathcal{I} \sum_{\mathbf{m}} \mathbf{s}_{\mathbf{m}} \mathbf{S}_{\mathbf{m}} - \mathcal{I}' \sum_{\mathbf{m}\delta} \mathbf{s}_{\mathbf{m}} \mathbf{s}_{\mathbf{m}+\delta} + \frac{J}{2} \sum_{\mathbf{ma}} \mathbf{s}_{\mathbf{m}} \mathbf{s}_{\mathbf{m}+\mathbf{a}}, \tag{22}$$

where

$$\tau = 2t^2 \left(\frac{1}{U_p + \Delta} - \frac{1}{U - U_p - \Delta} \right),$$

$$\mathcal{I} = 8t^2 \left(\frac{1}{U_p + \Delta} + \frac{1}{U - U_p - \Delta} \right),$$

$$\mathcal{I}' = 2t^2 \left(\frac{1}{U - U_p - \Delta} - \frac{1}{U - \Delta} \right), \tag{23}$$

$$J = \frac{4t^4}{(U - U_p - \Delta)^2} \left(\frac{1}{U} + \frac{2}{2U - U_p - 2\Delta} \right),$$

$N_{\mathbf{m}}$ and $\mathbf{S}_{\mathbf{m}}$ are determined by Eq. (7), $\mathbf{s}_{\mathbf{m}}$ and $\mathbf{s}_{\mathbf{m}+\delta}$ are analogously determined through the operators $d_{\mathbf{m}\sigma}$ and $p_{\mathbf{m}+\delta,\sigma}$, respectively. Analogous Hamiltonians have been obtained earlier by other methods in a number of papers (see, e.g., Refs. 11, 18, and 19).

At the beginning let us assume $U_p = 0$, the case considered in Refs. 2 and 19. In this case the third term on the rhs of Eq. (22) vanishes. Again it is convenient to introduce operators (8) and Eq. (22) can be rewritten in the form

$$H_{\text{eff}} = \mathcal{I}\lambda_0^2 \sum_{\mathbf{m}} \mathbf{s}_{\mathbf{m}} \mathcal{S}_{\mathbf{m}} + 2\tau\lambda_0\lambda_1 \sum_{\mathbf{ma}\sigma} \phi^\dagger_{\mathbf{m}+\mathbf{a},\sigma} \phi_{\mathbf{m}\sigma} + \tfrac{1}{2}\mathcal{I}\lambda_0\lambda_1 \sum_{\mathbf{ma}\sigma} (s^z_{\mathbf{m}} \sigma \phi^\dagger_{\mathbf{m}\sigma} \phi_{\mathbf{m}+\mathbf{a},\sigma} + s^\sigma_{\mathbf{m}} \phi^\dagger_{\mathbf{m},-\sigma} \phi_{\mathbf{m}+\mathbf{a},\sigma} + \text{H.c.}) + \frac{J}{2} \sum_{\mathbf{ma}} \mathbf{s}_{\mathbf{m}} \mathbf{s}_{\mathbf{m}+\mathbf{a}}, \tag{24}$$

where $\mathcal{S}_{\mathbf{m}}$ is the spin operator built from fermionic operators $\phi_{\mathbf{m}\sigma}$ [see (7)].

To obtain a form of Hamiltonian (24) more convenient for calculations and comparison with the Hamiltonian of the t-J model let us again introduce the spin-wave approximation with the help of Eqs. (12) and (13). Neglecting the possibility of occupying one site by two oxygen holes in the states described by ϕ operators, it is also convenient to introduce the following hole-creation operators:

$$a^\dagger_{\mathbf{m}0} = \frac{1}{\sqrt{2}} \sum_\sigma P^\sigma_{\mathbf{m}} (\phi_{\mathbf{m}\sigma} + b^\dagger_{\mathbf{m}} \phi_{\mathbf{m},-\sigma})(1 - b^\dagger_{\mathbf{m}} b_{\mathbf{m}}),$$

$$a^\dagger_{\mathbf{m}1} = \frac{1}{\sqrt{2}} \sum_\sigma P^\sigma_{\mathbf{m}} (\phi_{\mathbf{m}\sigma} - b^\dagger_{\mathbf{m}} \phi_{\mathbf{m},-\sigma})(1 - b^\dagger_{\mathbf{m}} b_{\mathbf{m}}),$$

$$a^\dagger_{\mathbf{m}2} = b^\dagger_{\mathbf{m}} \sum_\sigma P^\sigma_{\mathbf{m}} \phi_{\mathbf{m}\sigma}, \tag{25}$$

$$a^\dagger_{\mathbf{m}3} = \sum_\sigma P^\sigma_{\mathbf{m}} \phi_{\mathbf{m},-\sigma} (1 - b^\dagger_{\mathbf{m}} b_{\mathbf{m}}).$$

The states, created by these operators under the action upon the Néel state $|\mathcal{N}\rangle$, contain a spin singlet and triplets with spin projections 0 and ± 1, formed by two electrons remained in d and ϕ states on the site $\mathbf{m}$ (as can be seen from (24), at $U_p = 0$ ψ states form a conservative subsystem and are not considered here). The choice of signs in the two first formulas of (25) is dictated by the supposition that the state $|\mathcal{N}\rangle$ is built from the site states of the form $\sum_\sigma P^\sigma_{\mathbf{m}} d^\dagger_{\mathbf{m}\sigma} \phi^\dagger_{\mathbf{m}\sigma} \phi^\dagger_{\mathbf{m},-\sigma} |v\rangle$, where $|v\rangle$ is the site vacuum state. Singlet and zero-projection triplet states differ from those considered in Ref. 2 by their connection with the definite magnetic ordering. The states $a^\dagger_{\mathbf{m}i}|\mathcal{N}\rangle$ and their generalizations containing spin flips on the sites $\mathbf{m}' \neq \mathbf{m}$ diagonalize the first term on the rhs of (24). Since $\lambda_0 \gg \lambda_1$, this term is much larger than the second and third terms, which gives grounds to expect this representation to be convenient.

From (25) it can be shown that on the basis of the states mentioned

$$\{a_{\mathbf{m}'i'}, a^\dagger_{\mathbf{m}i}\} = \delta_{\mathbf{m}\mathbf{m}'} \delta_{ii'}. \tag{26}$$

From Eqs. (14), (18), and (25) it can also be shown that the differences $T^\dagger a^\dagger_{\mathbf{m}i} T - a^\dagger_{\mathbf{m}i}$ give small corrections to the terms already presented in the Hamiltonian, which allows one to neglect them. By taking this into account and using (26), it can be verified that Hamiltonian (24) after transformation (14) can be represented in the form

$$\tilde{H} = T^{\dagger} H_{\mathrm{eff}} T = \mathcal{I}\lambda_0^2 \sum_{\mathbf{m}} \left(-\tfrac{3}{4} a^{\dagger}_{\mathbf{m}0} a_{\mathbf{m}0} + \tfrac{1}{4} \sum_{i=1}^{3} a^{\dagger}_{\mathbf{m}i} a_{\mathbf{m}i} \right)$$
$$-\lambda_0\lambda_1 \sum_{\mathbf{ma}} [(\tfrac{3}{4}\mathcal{I} + \tau) a^{\dagger}_{\mathbf{m+a}0} a_{\mathbf{m}0} \tilde{b}_{\mathbf{m+a}} - (\tfrac{1}{4}\mathcal{I} + \tau) a^{\dagger}_{\mathbf{m+a}1} a_{\mathbf{m}0} \tilde{b}_{\mathbf{m+a}}$$
$$+(\tfrac{1}{4}\mathcal{I} + \tau) \tilde{b}^{\dagger}_{\mathbf{m}} a^{\dagger}_{\mathbf{m+a}1} a_{\mathbf{m}0} + \sqrt{2}(\tfrac{1}{4}\mathcal{I} + \tau) \tilde{b}^{\dagger}_{\mathbf{m}} a^{\dagger}_{\mathbf{m+a}2} a_{\mathbf{m}0} \tilde{b}_{\mathbf{m+a}}$$
$$+\sqrt{2}(\tfrac{1}{4}\mathcal{I} + \tau) a^{\dagger}_{\mathbf{m+a}3} a_{\mathbf{m}0} + (\tfrac{1}{4}\mathcal{I} - \tau) a^{\dagger}_{\mathbf{m+a}1} a_{\mathbf{m}1} \tilde{b}_{\mathbf{m+a}}$$
$$+\sqrt{2}(\tfrac{1}{4}\mathcal{I} - \tau) \tilde{b}^{\dagger}_{\mathbf{m}} a^{\dagger}_{\mathbf{m+a}2} a_{\mathbf{m}1} \tilde{b}_{\mathbf{m+a}} - \sqrt{2}(\tfrac{1}{4}\mathcal{I} - \tau) a^{\dagger}_{\mathbf{m+a}3} a_{\mathbf{m}1}$$
$$-2(\tfrac{1}{4}\mathcal{I} - \tau) \tilde{b}^{\dagger}_{\mathbf{m}} a^{\dagger}_{\mathbf{m+a}3} a_{\mathbf{m}2} + \mathrm{H.c.}] + \frac{J}{2} \sum_{\mathbf{k}} \omega_{\mathbf{k}} b^{\dagger}_{\mathbf{k}} b_{\mathbf{k}}. \tag{27}$$

Hamiltonian (27) contains as a part the t-J Hamiltonian—the first term in the square brackets, its Hermitian conjugate, and the last term. Thanks to the inequality $\lambda_0 \gg \lambda_1$, the distance between the lowest, singlet band and triplet bands is much larger than the mixing terms in (27). Thus, after Ref. 2, one can conclude that the one-band t-J model describes satisfactorily low-lying states of the extended Hubbard model in the considered case. To demonstrate this the lowest-energy bands of the states with $S_z = 1/2$ were calculated for these two models with the help of the recursion method. Results are shown in Fig. 2. The shapes of the bands are similar and their positions and bandwidths are close. The same results were also obtained for other parameter sets corresponding to the case. In the course of calculations it can be checked that noncommutativity of the operators $a_{\mathbf{m}i}$ and $b_{\mathbf{m}}$ plays a minor role in determining eigenenergies and eigenvectors of (27) and can be neglected. Again charge and spin degrees of freedom can be considered as independent.

Let us return to Hamiltonian (22) in the case $U_p \neq 0$ when $\mathcal{I}' \neq 0$. One can be convinced that the term with this coefficient reduces the energy distance between the singlet and triplet states and introduces new processes of their mixing. Thereby, the conditions for the one-band mapping get worse, especially in the case $U_p \to U$ when $\mathcal{I}'/\mathcal{I}$ tends to its maximal value which is approximately equal to 1/4. The estimations show that in this case great differences between the results of the extended and one-band models are possible. This conclusion is in agreement with the results of Ref. 3 where a particular situation of the case $U_p \to U$ was considered when U_p and U tend to infinity and Δ_h remains finite. It was shown that on a small lattice the extended Hubbard model and the corresponding $J/t \to 0$ extrapolation of the t-J model have different ground states. In the infinite correlation limit the one-hole ground state of the latter model is the ferromagnetically ordered Nagaoka state[20] with a maximal possible value of the total spin for a given lattice, while for the former model the spin was much smaller. For the values of the parameters of papers[14] the ratio $\mathcal{I}'/\mathcal{I} \approx 0.1$ and an estimation shows that this value is

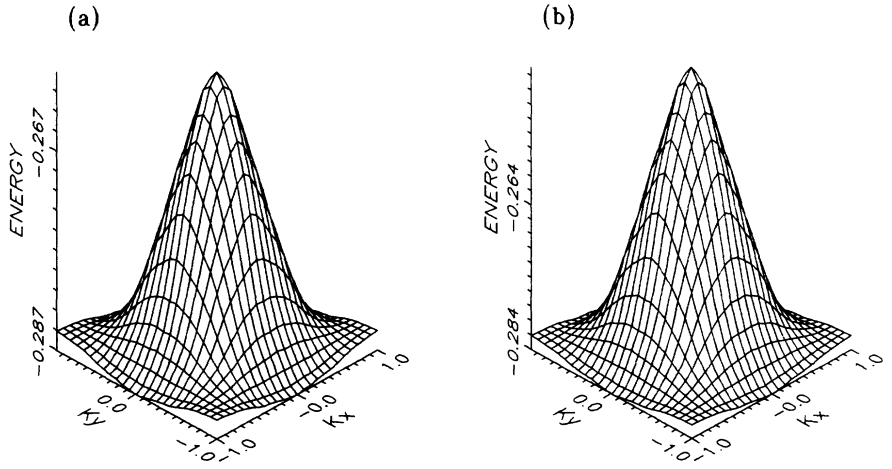

FIG. 2. Energy bands of the states with $S_z = 1/2$ obtained in the particular case of the extended Hubbard model described by Hamiltonian (27) [the case $|t| \ll \Delta, U - \Delta$ (a)] and in the t-J model (b). $t = 0.1$, $\Delta = 0.5$. The units of energy and wave-vector length are the same as in Fig. 1.

too small to change the conclusion about the possibility of the one-band mapping. However, the presence of the third term on the rhs of Eq. (22) has also another consequence which looks essential even at such small values of $\mathcal{I}'/\mathcal{I}$. This term contains addends describing the mixing of ϕ and ψ states, which may make its contribution to a non-negligible occupation of the $3d_{3z^2-r^2}$ Cu orbitals by the holes, observed in recent x-ray-absorption experiments.[21]

Now we can compare the elementary excitations corresponding to different ratios of the parameters, considered in Secs. III and IV. In the latter case the perturbation series for the effective Hamiltonian starts from the second-order terms. For reasonable sets of parameters the leading role in the formation of elementary excitations is played by one of these terms—the first term on the rhs of Eq. (24). This term is responsible for the formation of the Zhang-Rice singlets[2] and the lowest hole states are built from site states of this type, $2^{-1/2}(\phi^{\dagger}_{\mathbf{m},-1}d^{\dagger}_{\mathbf{m},+1}-\phi^{\dagger}_{\mathbf{m},+1}d^{\dagger}_{\mathbf{m},-1})|v\rangle$. In the situation of Sec. III the perturbation series starts from the first-order, hybridization terms, and in this case it is these terms that form hole states, while the second-order terms are only small corrections. As a result, the picture of Zhang-Rice singlets is not appropriate here. The lowest hole states are complex combinations of the site states $\sum_{\sigma}P^{\sigma}_{\mathbf{m}}(\sin\theta\phi^{\dagger}_{\mathbf{m},\sigma}\phi^{\dagger}_{\mathbf{m},-\sigma}-\cos\theta d^{\dagger}_{\mathbf{m},\sigma}\phi^{\dagger}_{\mathbf{m},-\sigma})|v\rangle$ and $\sum_{\sigma}P^{\sigma}_{\mathbf{m}}d^{\dagger}_{\mathbf{m},-\sigma}\phi^{\dagger}_{\mathbf{m},\sigma}|v\rangle$, surrounded by a magnon cloud.

V. CONCLUSION

In the previous sections the strong-correlation limit of the extended Hubbard model, presumably describing the hole dynamics in the copper oxide planes of the high-temperature superconductors, has been considered. The ranges of the known values of parameters allow three characteristic situations with different small parameters. With the help of the operator perturbation theory the extended Hubbard Hamiltonian has been transformed to the generalizations of the t-J Hamiltonian for two of these cases, when the Cu-O electron promotion energy is of the order of the Cu-O hybridization and when the hybridization is the only small parameter. By the antiferromagnetic ordering of lightly doped samples taking into account and using the spin-wave approximation, the effective Hamiltonians have been obtained on the basis of what the low-energy hole dynamics has been shown to be essentially different in the two cases considered. In the latter case it can be described by the one-band t-J model, the Hamiltonian of which in the spin-wave approximation has been obtained in Refs. 5 and 6, while in the former case the dynamics is described by Hamiltonian (21) which cannot be reduced to the one-band Hamiltonian. It should be emphasized that in both Hamiltonians hole and magnon operators are practically independent, which essentially simplifies the calculations. The results of such calculations, the lowest-energy bands, are shown in Figs. 1 and 2.

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