Elementary hole excitations in CuO_2 planes

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The Hamiltonian of the generalized Hubbard model is considered. With some reasonable assumptions regarding the energy parameters of the model, the magnetic subsystem of spins localized at the copper atoms can be described by an effective antiferromagnetic Hamiltonian. The free holes move along a zone formed as a result of hybridization of the copper ion levels and bonding orbitals of the closest oxygen ions. The quasiparticle (magnetic polaron) spectrum is found for the antiferromagnetic ordering of the magnetic subsystem. In a first approximation the bottom of the spectrum coincides with the boundary of the magnetic Brillouin zone. Possible mechanisms for formation of bound states of such quasiparticles are analyzed.

1. INTRODUCTION

Among the many experimental papers on the physical properties of high temperature superconductors, several favor the idea of formation as a result of doping of the oxygen hole band. This is equivalent to the generally accepted idea of the absence of Cu^{3+} ions in the CuO_2 planes. According to this concept, in the absence of doping the fundamental state of the copper and oxygen ions is Cu^{2+} and O^{2-}; i.e., on each copper ion there is exactly one hole in a d-orbital, if we accept as the vacuum the state with filled orbitals (Cu^{+},O^{2-}). The crystal field of the tetragonal symmetry splits the copper d-orbital series, so that the energy of an electron on a $d_{x^2-y^2}$ orbital is maximal and this state is singly occupied. In turn, the p_x oxygen orbital, having a nearest-neighbor copper ion in the x-direction, has a lower energy in the crystal field than the nonbonding p_y and p_z orbitals, which may favor the appearance of free holes on these orbitals. However, a sufficiently strong hybridization of the $d_{x^2-y^2}$ and p_x states of copper and oxygen can form an electronic level lying higher than the nonbonding ones; then the holes will occupy this level first. We can convince ourselves of this by examining the simplest two-site Hamiltonian, taking account of the hybridization of $d_{x^2-y^2}$ and p_x states and intrasite repulsion:

$$H=\sum_{\sigma}[-t(d_{\sigma}^{+}p_{\sigma}+p_{\sigma}^{+}d_{\sigma})+\varepsilon_d n_d^{\sigma}+\varepsilon_p n_p^{\sigma}]$$
$$+U_d n_d^{\uparrow}n_d^{\downarrow}+U_p n_p^{\uparrow}n_p^{\downarrow}, \qquad (1)$$

where $d,p(d^{+},p^{+})$ are annihilation (creation) operators for holes on copper and oxygen ions. The principal features of the basic hole state, enumerated above, in the presence and absence of doping impose the following conditions on the energy parameters:

$$\varepsilon=\varepsilon_p-\varepsilon_d>0, \quad U_d>\varepsilon. \qquad (2)$$

According to the values of Ref. 2, $U_d \gg \varepsilon,t,U_p$. We will take $U_d=\infty$ for simplicity. In this case the minimum energy of two holes in the hybridized (hh) states is:

$$E_{hh}^{(2)}=\varepsilon_d+\varepsilon_p+(\varepsilon+U_p)/2-[(\varepsilon+U_p)^2/4+2t^2]^{1/2}. \qquad (3)$$

To answer the question of which orbitals form the hole band, we must compare this energy with the energy of two holes, one of which is in the hybridized state with energy $E_h^{(1)}$, described by the Hamiltonian (1), and the second is on a nonbonding orbital with energy $\varepsilon_p',\varepsilon_p'<\varepsilon_p$. In this case we have

$$E_{nh}^{(2)}=\varepsilon_p'+E_h^{(1)},$$
$$E_h^{(1)}=\varepsilon_d+(\varepsilon+U_p')/2-[(\varepsilon+U_p')^2/4+t^2]^{1/2}. \qquad (4)$$

Here U_p' is the Coulomb repulsion of holes occupying different p-orbitals.

Comparison of expressions (3) and (4) shows that $E_{hh}^{(2)}$ can be less than $E_{nh}^{(2)}$. In particular, if $t \ll \varepsilon$ and $U_p=U_p'=0$, this will happen if the inequality $t^2>\varepsilon(\varepsilon_p-\varepsilon_p')$ is fulfilled. When the real environment of a copper atom, surrounded by four oxygen atoms, is taken into account, the energy of the hh-state should be further reduced compared to the energy of the nh-state.

We note that in the case $t/\varepsilon \ll 1$ (this is just the situation studied in the present work) the degree of hybridization is small. Our remarks about sufficiently strong hybridization need not be taken literally. They mean only that the band of hybridized states is much wider than the band formed by overlap of nonbonding orbitals.

In Sec. 2 an effective Hamiltonian describing hopping of holes on oxygen among the hybridized bonds is obtained. In Sec. 3 it is shown that the character of the elementary excitations is connected with the ground state of the system, mainly with the spatial correlation functions in the ground state. In this work it is assumed that the ground state of the undoped system is antiferromagnetic (AFM). It is known that a particle inserted into a magnetic structure reorganizes the structure in its surroundings. But, in contrast to the Hubbard model, in the model considered the problem of a "ferromagnetic pocket" does not arise (see Appendix A). We also assume that the parameter t/ε is not too small, so that the free hole and its reorganized surroundings can be considered as a small polaron.

To determine the spectrum of elementary excitations we apply a variational method. In this work we use the approximation in which the ground state consists of two "rig-

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id" Néel sublattices, and take into account the possibility of flipping of spins of the copper ions nearest to an oxygen site occupied by a hole. It is found that the bottom of the band is a line coinciding with the boundary of the two-dimensional magnetic Brillouin zone, and, as a consequence, the density of states at the lower edge of the band has a square-root singularity. Including zero-point spin oscillations weakly affects this result.

It is obvious that if we expand the class of trial functions increasing the size of the polaron and including a larger number of reversed copper spins relative to the ground state, the hole spectrum found in the small-polaron approximation will be deformed on the scale t^2/ε and the quasi-one-dimensional character of the bottom of the band will be lost. It is natural that stabilization of the spectrum is ensured by the exchange interaction between copper spins, which makes a polaron with a large number of reversed spins energetically unfavorable. It will also be shown that for the model considered, with comparatively small values of the exchange interaction, anomalies in the density of states near the bottom of the hole band, found within the small-polaron model, are qualitatively preserved with increase in the polaron dimension.

In Sec. 4 the possibility of forming bound hole states is analyzed.

2. EFFECTIVE HAMILTONIAN

Under the assumptions taken in Sec. 1, the Hamiltonian describing the hole states is a simple generalization of (1) and has the form

$$H=\sum_{\mathbf{r}}\varepsilon_p n_p(\mathbf{r})+\sum_{\mathbf{R}}\varepsilon_d n_d(\mathbf{R})+U_p\sum_{\mathbf{r}}n_p^{\uparrow}(\mathbf{r})n_p^{\downarrow}(\mathbf{r})$$
$$+U_d\sum_{\mathbf{R}}n_d^{\uparrow}(\mathbf{R})n_d^{\downarrow}(\mathbf{R})$$
$$-t\sum_{\langle\mathbf{r},\mathbf{R}\rangle\sigma}(p_{\mathbf{r}\sigma}^{+}d_{\mathbf{R}\sigma}+d_{\mathbf{R}\sigma}^{+}p_{\mathbf{r}\sigma})+V\sum_{\langle\mathbf{r},\mathbf{R}\rangle}n_p(\mathbf{r})n_d(\mathbf{R}),\qquad n=\sum_{\sigma}n^{\sigma}. \tag{5}$$

The indices **r** and **R** refer to O and Cu sites, respectively. The symbol $\langle\mathbf{r},\mathbf{R}\rangle$ shows that the summation goes over nearest sites of oxygen and copper. The Coulomb repulsion V on neighboring sites is also introduced.

In the usual Hubbard model for a half-filled band in the insulating phase ($U\gg t$ and $\bar{n}_d=1$) the effective exchange (antiferromagnetic) interaction of particles with amplitude $\propto t^2/U$ arises in second-order perturbation theory. In the problem considered here the exchange H_m appears only in fourth-order in the kinetic energy t:

$$H_m=\sum_{\langle\mathbf{R},\mathbf{R}'\rangle}t^4(\varepsilon+V)^{-2}[4(2\varepsilon+U_p)^{-1}+2U_d^{-1}](2\mathbf{S}_{\mathbf{R}}\mathbf{S}_{\mathbf{R}'}+{}^1/_2). \tag{6}$$

In Fig. 1, two of the virtual processes leading to the expression (6) are shown.

It is known that the ground state of a spin system described by the Hamiltonian (6) in the three-dimensional case is close to the AFM Néel state, and in one dimension is

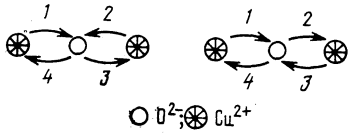

FIG. 1. Two types of virtual processes contributing to the exchange interaction (6); the numbers denote the order of hole hops.

an RVB-type state.[3] In two dimensions the type of spin system ground state is unknown. In the present work, we will assume that it is a two-sublattice state.

It is more important for our purposes to obtain the effective Hamiltonian H_f describing hopping of free holes along the oxygen sublattice. It is obtained in second-order perturbation theory. In Fig. 2 the virtual processes are shown which lead to the expression

$$H_f=\sum_{\mathbf{R},\mathbf{a}_1,\mathbf{a}_2}H_f(\mathbf{R},\mathbf{a}_1,\mathbf{a}_2),\qquad H_f(\mathbf{R},\mathbf{a}_1,\mathbf{a}_2)$$
$$=-t^2(U_d-\varepsilon-2V)^{-1}\sum_{\sigma}X_{\mathbf{R}+\mathbf{a}_2}^{\sigma,0}X_{\mathbf{R}+\mathbf{a}_1}^{0,\sigma}+t^2\{\varepsilon^{-1}+(U_d-\varepsilon-2V)^{-1}$$
$$-\delta_{\mathbf{a}_1,\mathbf{a}_2}[\varepsilon^{-1}-(\varepsilon+U_p)^{-1}]\}\sum_{\sigma_1,\sigma_2}X_{\mathbf{R}+\mathbf{a}_2}^{\sigma_2,0}X_{\mathbf{R}+\mathbf{a}_1}^{0,\sigma_1}Z_{\mathbf{R}}^{\sigma_1,\sigma_2}. \tag{7}$$

Here the Hubbard variables are used: $X_{\mathbf{r}}^{\sigma,0}(X_{\mathbf{r}}^{0,\sigma})$ is the creation (annihilation) operator for a hole with projected spin σ on the oxygen site **r**, and the operator $Z_{\mathbf{R}}^{\sigma_1,\sigma_2}$ produces a spin change $\sigma_2\to\sigma_1$ at site **R** of the copper sublattice.

Energies of the excitations described by the effective Hamiltonians (6) and (7) differ in their scale. Theoretically, in setting the parameter t/ε to zero, we arrive at the quantum-mechanical problem of particle (hole) motion superposed on the magnetic ordering created by the hole itself. A similar situation is well known in the Hubbard model: for $U_d=\infty$ a single hole tends to establish a ferromagnetic order in all space.[4] It is also known[5] that for $U_d\gg t$, but $U_d\neq\infty$, spins order ferromagnetically in the neighborhood of a hole. The radius of such a polaron is $\propto(U/t)^{1/4}$ in the two-dimensional case. Outside this neighborhood the ordering is antiferromagnetic. It follows that one should consider that the dimension of the ferromagnetic neighborhood of a hole for real values of the parameter U/t is not large ($R\sim 1$–2 for $U/t\sim 5$). A polaronic mechanism for high-temperature superconductivity is studied in detail in Ref. 6. An oxygen hold described by the Hamiltonian (7) creates a polaronic

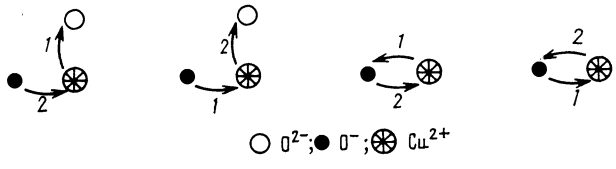

FIG. 2. The contribution of virtual processes to the effective Hamiltonian (7).

state in its surroundings also, but not of the ferromagnetic type. In Ref. 7 a variational approach was used to determine the ground state of a system of a hole on an oxygen + a copper ion spin, in the limiting case $U_d = \infty$ and $U_p = 0$. A tendency was observed toward formation of a nonmagnetic polaron, but it is possible to form a polaron with an unsaturated magnetization (compare with the results of Ref. 8). In Appendix A we show that a ferromagnetic polaron is also energetically unfavorable in the case $U_p \neq 0$.

Our basic goal is to construct a realistic variational function which will reflect the fact that the polaron dimension (even nonmagnetic!) $R \propto (\varepsilon^2/t^2)^{1/4}$, and for reasonable values of ε/t is of the order of one-two lattice constants.

3. VARIATIONAL WAVE FUNCTION AND SINGLE-PARTICLE EXCITATION SPECTRUM

The problem of an oxygen hole described by the Hamiltonian (7) involves a single particle, aside from the fact that the occupation number $n_d(\mathbf{R}) = 1$. The band structure is sensitive to the type of magnetic ordering of the copper sublattice. Here and below we take $U_d = \infty$, so the Hamiltonian (7) takes the form

$$H_f = \sum_{\mathbf{R},\mathbf{a}_1,\mathbf{a}_2,\sigma_1,\sigma_2} \{[\tau_1 - \delta_{\mathbf{a}_1,\mathbf{a}_2}(\tau_1-\tau_2)] X^{\sigma_2,0}_{\mathbf{R}+\mathbf{a}_2} X^{0,\sigma_1}_{\mathbf{R}+\mathbf{a}_1} Z^{\sigma_1,\sigma_2}_{\mathbf{R}}\},$$

$$\tau_1 = t^2\varepsilon^{-1}, \quad \tau_2 = t^2(\varepsilon+U_p)^{-1}. \tag{7'}$$

In Ref. 9 the case $U_d = 2\varepsilon$ was studied, and it was shown that the effective hole Hamiltonian reduces to the usual Hubbard model, with a spectrum of elementary excitations corresponding to the strong-coupling approximation. The correctness of such an approximation depends on the choice of ground state. In the limit $U_d \to \infty$ examined below the Hamiltonian (7') clearly depends on the state of the spin system through the operator Z and, as will be shown below, the spectrum of elementary excitations turns out to be different.

We note that it is energetically favorable to form a singlet state of the spin belonging to the copper ion and the spin of the hole "smeared out" over the oxygen surroundings. If we consider the state of the copper spin subsystem to be antiferromagnetic, then particles (holes) having a given spin projection are localized near sites of the copper sublattice with the opposite magnetization. Effective particle hopping proceeds through just this sublattice.

To construct a Bloch eigenfunction of the strong-coupling Hamiltonian, it is common to use a set of Wannier functions (see, for example, Ref. 9). We will build Bloch functions in the subspace of a set of site functions which are not necessarily orthogonal:

$$|\mathbf{R}\sigma\rangle = \sum_{\mathbf{a}} (f(\mathbf{R},\mathbf{a}) X^{\sigma,0}_{\mathbf{R}+\mathbf{a}} + g(\mathbf{R},\mathbf{a}) X^{-\sigma,0}_{\mathbf{R}+\mathbf{a}} Z^{\sigma,-\sigma}_{\mathbf{R}}) |G\rangle, \tag{8}$$

where $|G\rangle$ is the wave function of the spin system ground state, and $\mathbf{a}$ is the vector connecting nearest Cu and O ions. The function (8), centered near site $\mathbf{R}$, having a particle spin projection σ and accounting for the possibility of copper ion spin flip, is the simplest realization of a magnetic polaron. The coefficients f and g in Eq. (8) can be considered variational. For a simple magnetic lattice, they must depend only on $\mathbf{a}$. For different types of AFM states the set of coefficients is doubled according to the number of magnetic sublattices: $\{f_+, g_+$ and $f_-, g_-\}$.

On the Bloch function ($\mathbf{k}$ belongs to the magnetic Brillouin zone)

$$|\mathbf{k}\sigma\rangle = A_{\mathbf{k}} \sum_{\mathbf{R}} \exp i\mathbf{k}\mathbf{R} |\mathbf{R}\sigma\rangle \tag{9}$$

we must impose orthonormality conditions, equivalent to the relationship

$$1 = A_{\mathbf{k}}^2 \sum_{\mathbf{R},\mathbf{R}'} \exp i\mathbf{k}(\mathbf{R}-\mathbf{R}') \langle\sigma\mathbf{R}'|\mathbf{R}\sigma\rangle. \tag{10}$$

Having chosen $\sigma = -1/2$ to fix the projected particle spin, we will rewrite Eq. (10) in the form:

$$1 = 0{,}5 N_0 A_{\mathbf{k}}^2 \{4(f_+^2 + g_+^2 Z_+^{++} + f_-^2 + g_-^2 Z_-^{++}) + 4\varphi(k)[2f_+f_- + g_+g_-(\langle Z_{\mathbf{R}}^{+-} Z_{\mathbf{R}'}^{-+}\rangle + \langle Z_{\mathbf{R}}^{-+} Z_{\mathbf{R}'}^{+-}\rangle)]\}, \tag{11}$$

where $\mathbf{R}$ and $\mathbf{R}$ are nearest neighbors in the copper sublattice, $Z_+^{++} Z_-^{--} = 1 - Z_+^{--} = \langle Z_R^{++}\rangle$, $\mathbf{R}$ belongs to the "+" sublattice, and $\varphi(\mathbf{k}) = 0.5(\cos 2k_x a + \cos 2k_y a)$. The particle spectrum

$$\varepsilon(\mathbf{k}) = \langle\mathbf{k}|H_f|\mathbf{k}\rangle \tag{12}$$

will be found using the variational functions (8). On the right-hand side of formula (12), the following matrix elements differ from zero:

$$\langle\mathbf{R}|H_f|\mathbf{R}\rangle, \quad \langle\mathbf{R}|H_f|\mathbf{R}+2\mathbf{a}\rangle, \quad \langle\mathbf{R}|H_f|\mathbf{R}+2\mathbf{a}+2\mathbf{a}'\rangle.$$

Expressions for these are presented in Appendix B. We note that these matrix elements are determined through the spin correlation functions taken for the ground state of the antiferromagnet.

Analysis of the spectrum $\varepsilon(\mathbf{k})$ is not difficult to carry out for a "rigid" AFM state of the Ising type, in which $Z_+^{++} = 1$. Then

$$\varepsilon(\mathbf{k}) = \{\tau_1[3f_-^2 + 6f_+g_+ + 6\varphi(\mathbf{k})(f_+ + g_+)f_- + (4\varphi^2(\mathbf{k}) - 1)f_+^2] + \tau_2[f_-^2 + f_+^2 + 2f_+g_+ + 2\varphi(\mathbf{k})(f_+ + g_+)f_-]\} / [f_+^2 + g_+^2 + f_-^2 + 2f_+f_-\varphi(\mathbf{k})]. \tag{13}$$

The essential feature of expression (13), which varies with f_+, g_+ and f_-, is that the bottom of the bend corresponds to $\varphi(\mathbf{k}) = 0$, that is, to a line in $\mathbf{k}$-space (Fig. 3) coinciding with the boundary of the magnetic Brillouin zone. Near this the spectrum has the form

$$\varepsilon(\mathbf{k}) = \varepsilon_0[1 - \beta\varphi^2(\mathbf{k})],$$

with $0 < \beta \sim 1$, and $\varepsilon_0 = \varepsilon_0(\tau_1, U_p)$ as a function of U_p is inside the limits

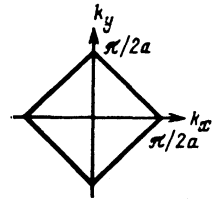

FIG. 3. The boundary of the magnetic Brillouin zone, which coincides with the bottom of the hole spectrum.

$$\varepsilon_0(\tau_1, 0) = -4\tau_1, \quad \varepsilon_0(\tau_1, \infty) = -(1+37^{1/2})\tau_1/2.$$

In the direction perpendicular to the line $\varphi(\mathbf{k}) = 0$, the spectrum is quadratic in $\delta\mathbf{k}$. This means that in the limit of exactly zero particle concentration, the boundary mentioned above is a Fermi surface near which the density of states has a quasi-one-dimensional character with a square-root singularity. This singularity can cause the appearance of instabilities, including superconductivity. A system with a similar excitation spectrum, but of a different nature, was studied in Ref. 10, where it was shown that the Coulomb interaction does not inhibit the superconducting channel. We note that near the bottom of the band the wave functions (8) are close to a spin singlet ($f_+ = -g_+, f_- = g_- = 0$), in other words, the holes on the copper atom and in its oxygen surroundings almost form a singlet pair.

The Heisenberg nature of the magnetic interaction leads to the appearance of "zero-point" fluctuations in the spin correlators, as a result of which expression (13) for the energy spectrum is, naturally, changed: the degeneracy along the whole line of minimal energy disappears, the bottom of the band becomes isolated equivalent points lying in the corners of the magnetic Brillouin zone. In this case the quasi-one-dimensional singularity in the density of states disappears, although the density of states itself remains large near the lower edge of the band on account of the small changes in excitation energy along the nesting line shown in Fig. 3.

To clear up the question of the stability of the quasi-one-dimensional singularity in the density of states $\rho(E)$ in relation to increased polaron size, we must broaden the class of trial functions relative to the functions $|R,\sigma\rangle$ in such a way as to allow the possibility of spin reversals on copper sites other than those nearest to holes. To do this we simultaneously take into account the exchange interaction of spins determined by the Hamiltonian (6). Such an analysis of spectral stability is difficult to carry out analytically. We present the results of a numerical calculation for the case of an Ising-type AFM ground state of the copper subsystem. We will also take $U_d = \infty, U_p = V = 0$ in (6); then the effective exchange interaction differs from the hopping parameter $\tau = t^2/\varepsilon$ by the factor t^2/ε^2, which must be less than unity.

Expanding the basis of variational functions will be accomplished by successive action of the operator H_f of (7) on the function $|R,\sigma\rangle$.

$$H_f^n|R, \sigma\rangle \to \{\Psi\}_n.$$

Here $\{\Psi\}_n$ is a class of orthonormal site functions which is formed by n-fold action of H_f on $|R,\sigma\rangle$: $\{\Psi_n\}$ allows $n+1$ reversed spins on copper ions relative to the ground state. For the cases $n = 1,2,3$, there are created 4, 15, and 46 site functions, respectively. Having built Bloch states out of these functions, we can find the spectrum and the density of states $\rho(E)$ of the lower hole band that interests us.

In Fig. 4a,b plots of the densities of states $\rho(E)$ are shown for $n = 0$ [one trial function (8)] and $n = 3$ (46 trial functions) with a value $t^2/\varepsilon^2 = 0.25$, and in Fig. 4c,d, for $t^2/\varepsilon^2 = 0.125$ and 0.5 with a fixed number (46) of trial functions. It is evident that with $t^2/\varepsilon^2 = 0.25$ the singularity in $\rho(E)$ near the bottom of the band is qualitatively preserved for increase in the polaron dimension. Comparison of the traces in Fig. 4 implies that the description of the small-polaron energy spectrum is adequate if the exchange interaction is not too small.

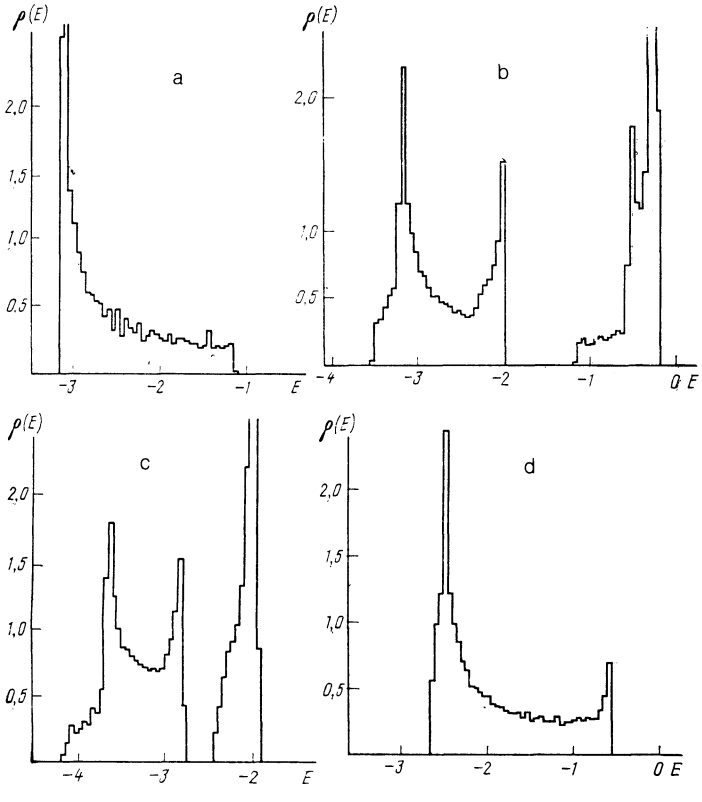

FIG. 4. The form of the density of states $\rho(E)$ of the lower band of the hole spectrum for different values of the number of trial functions and different values of the parameter $x = t^2/\varepsilon^2$: (a) $x = 0.25$ and one function of the form (8); (b) 0.25 and 46 trial functions; (c) 0.125 and 46 functions; (d) 0.5 and 46 functions. Energy, along the abscissa, is measured in units of t^2/ε; the density of states is normalized to a constant.

4. TWO-PARTICLE EXCITATION SPECTRUM

Here we will examine the two-particle singlet states corresponding to a small polaron; we limit ourselves to the case $U_p = \infty$. Unfortunately, an attempt to use the expanded basis of functions $\{\Psi\}_n$ encounters major computational difficulties. Therefore, the chief goal of this part of our work is to demonstrate the dynamic mechanism of hole pairing at small distances. As a basis for describing particles spaced far apart, we will use single-particle hole states corresponding to small polarons. The contribution of large distances ($|\mathbf{R}-\mathbf{R}'| \gg a$) to the asymptotic form of the wave function is:

$$\Phi|G\rangle = g(\mathbf{R}-\mathbf{R}')A_+(\mathbf{R})A_-(\mathbf{R}')|G\rangle, \qquad (14)$$

where the amplitude $g(\mathbf{R}-\mathbf{R}')$ must become exponentially small for $|\mathbf{R}-\mathbf{R}'| \gg a$ in the case of a bound state. The single-particle wave functions $A_\sigma(\mathbf{R})|G\rangle$ must coincide with $|\mathbf{R},\sigma\rangle$ [see Eq. (8)]. According to the comment at the end of the preceding section, these functions must be approximately of the form of a singlet state of two holes on a copper ion and its oxygen surroundings:

$$A_\sigma(\mathbf{R}) = 8^{-1/2}\sum_{\mathbf{a}} (X^{\sigma,0}_{\mathbf{R}+\mathbf{a}} Z_{\mathbf{R}}^{-\sigma,-\sigma} - X^{-\sigma,0}_{\mathbf{R}+\mathbf{a}} Z_{\mathbf{R}}^{\sigma,-\sigma}), \qquad (15)$$

where $\mathbf{R}$ belongs to the " $-\sigma$" sublattice.

When $|\mathbf{R}-\mathbf{R}'|$ becomes of the order of a lattice constant, the two-particle wave function Φ changes. Thus, where both holes are localized near one copper ion, the function Φ takes the form

$$\Phi(\mathbf{R},\mathbf{R}) = \sum_{j=1}^{3} f_j(\mathbf{R}) A^{(j)}_{+-}(\mathbf{R}),$$

where the function $A^{(j)}_{+-}(\mathbf{R})$ describes the formation of a complex of three holes: one on the copper ion at $\mathbf{R}$ and two on the four oxygen ions at $\mathbf{R}+\mathbf{a}$. The index j numbers the three degenerate ground states of this complex with energy $\varepsilon_j = 3\tau_1$ and with spin projection $\pm 1/2$ (the sign depends on the "sign" of the magnetic sublattice $\mathbf{R}$). We give an expression for one of the representations of the degenerate set of functions $A^{(j)}_{+-}(\mathbf{R})$:

$$A^{(1)}_{+-}(\mathbf{R}) = -4\cdot 0^{-1/2}\sum_{l=1}^{3} (-1)^l X^{-0}_{\mathbf{R}+\mathbf{a}_{1+l}} [(X^{+0}_{\mathbf{R}+\mathbf{a}_{2+l}} + X^{+0}_{\mathbf{R}+\mathbf{a}_{4+l}} + 2X^{+0}_{\mathbf{R}+\mathbf{a}_{3+l}}) Z_{\mathbf{R}}^{--} - 2X^{-0}_{\mathbf{R}+\mathbf{a}_{2+l}} Z_{\mathbf{R}}^{+-}], \qquad (16)$$

where $\mathbf{R}$ belongs to the " $-$ " sublattice.

Configurations with two free holes localized near two neighboring copper ions are described by wave functions

$$A_{+-}(\mathbf{R},\mathbf{R}+2\mathbf{a}_s) = 6^{-1/2}\sum_{t\neq s} (X^{+0}_{\mathbf{R}+\mathbf{a}_t} Z_{\mathbf{R}}^{--} - X^{-0}_{\mathbf{R}+\mathbf{a}_t} Z_{\mathbf{R}}^{+-}) \times \sum_{v\neq s} (X^{-0}_{\mathbf{R}+2\mathbf{a}_s-\mathbf{a}_v} Z^{++}_{\mathbf{R}+2\mathbf{a}_s} - X^{+0}_{\mathbf{R}+2\mathbf{a}_s-\mathbf{a}_v} Z^{-+}_{\mathbf{R}+2\mathbf{a}_s}), \qquad (17)$$

where $\mathbf{R}$ belongs to the " $-$ " sublattice. The energy of such a configuration is $\varepsilon_b = -4\tau_1$. The amplitude corresponding to this function will be designated as $p(\mathbf{R},\mathbf{R}+2\mathbf{a}_s)$. We note that the energy of the asymptotic state (14) is equal to $2\varepsilon_g = -6\tau_1$. The increase in energy of the two-particle states with decrease in the interparticle distances ($\varepsilon_f > \varepsilon_b > 2\varepsilon_g$) can be treated as an effective repulsion between holes on the oxygen. Together with this, mechanisms exist for formation of a bound state. One of these is the increased amplitude for particle hops when they come closer to each other. The matrix element for "decay" of the state $A_{+-}(\mathbf{R})$ and the state $A_{+-}(\mathbf{R},\mathbf{R}+2\mathbf{a}_j)$ is equal to $(2/5)^{1/2}\tau_1$, while a free-particle hop has the amplitude $\tau_1/8$. A similar situation for the standard Hubbard model was discussed in Ref. 11, and for the present model with an RVB-type magnetic state, in Ref. 12.

Another important mechanism[13] of attraction results from the Coulomb interaction of a hole on oxygen with holes localized on copper sites. In our model [see the Hamiltonian (5)] this energy is denoted by V. The role of an interaction of this type in binding holes into pairs is indicated in Ref. 14. If two holes on an oxygen are next to one copper ion, as shown in Fig. 5a, then in second-order perturbation theory a term exists which lowers the energy ε_f. The hole hopping process, drawn in Fig. 5a, has the amplitude $t^2/(\varepsilon - V) = \tau_1'$; as a result we get $\varepsilon_f = -3\tau_1'$. One more term from second-order perturbation theory is shown in Fig. 5b and is connected only with virtual hopping of a copper hole. For any configuration of the type shown in Fig. 5b, it is equal to $-2\tau_1' + 6\tau_1 - 4\tau_1''$, where $\tau_1'' = t^2/(\varepsilon + V)$, and becomes negative for $V > \varepsilon/3$. Too large valves $V > \varepsilon/2$ lead to formation of large hole clusters on oxygens and to demixing. The configurations shown in Fig. 5c and d, corresponding to the latter situation, are in resonance with each other.

To find the two-particle spectrum $\varepsilon^{(2)}(\mathbf{q})$ we will solve the variational problem with the Schroedinger equation with the wave function

$$\Phi_q = \Big\{ \sum_{|\mathbf{R}-\mathbf{R}'|>2a} g_q(\mathbf{R},\mathbf{R}') A_+(\mathbf{R}) A_-(\mathbf{R}') + \sum_{|\mathbf{R}-\mathbf{R}'|=2a} b_q(\mathbf{R},\mathbf{R}') A_{+-}(\mathbf{R},\mathbf{R}') + \sum_{j,\mathbf{R}} f_q^{(j)} A^{(j)}(\mathbf{R}) \Big\} |G\rangle. \qquad (18)$$

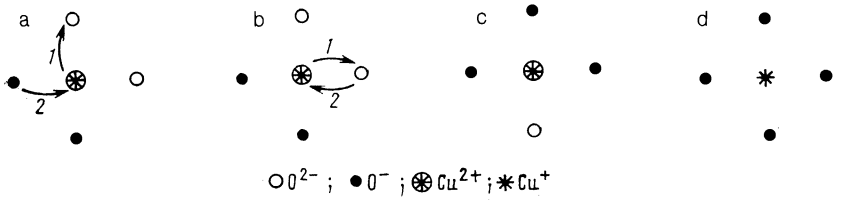

FIG. 5. Copper ions and their oxygen environment; explanation in the text.

Thus, the problem is reduced to the solution of a simultaneous system of equations for the coefficients g, b, and f. Because of the awkwardness of this system, it was solved for the special cases $\mathbf{q}(q, \pm q)$, $\mathbf{q} = (\pi/2a, 0)$ and equivalent points. The dispersion equation has the form

$$[\tilde{\varepsilon}_b - 2\varepsilon_g + 2\tau_1 + f_1(\mathbf{q})]^{-1} = N_0^{-1} \sum_{\mathbf{k}} f_2(\mathbf{k}) / [\varepsilon_{\mathbf{q}}^{(2)} - \varepsilon(\mathbf{k}+\mathbf{q}/2) - \varepsilon(\mathbf{k}-\mathbf{q}/2)] \qquad (19)$$

where

$$\varepsilon(\mathbf{k}) = \varepsilon_g + 4\tau_1[4\varphi^2(\mathbf{k}) - 1], \quad \tilde{\varepsilon}_b = \varepsilon_b + 28\tau_1^2/[5(\varepsilon_{\mathbf{q}}^{(2)} - \varepsilon_f)],$$
$$f_1(q, q) = (4\tau_1 \cos^2 qa)/9, \quad f_1(\pi/2a, 0) = 0,$$

$$f_2(\mathbf{k}) = \begin{cases} 4\sin^2[(k_x+k_y)a]\sin^2[(k_x-k_y)a] & \text{for } q_x = \pm q_y = q, \\ 2\cos^2 2k_x a & \text{for } q_x = \pi/2a, \quad q_y = 0. \end{cases}$$

Here $\tilde{\varepsilon}_b$ describes the renormalization of the energy ε_b due to hybridization with the states A_{+} $(\mathbf{R})$. The energy denominator on the right side of Eq. (19) corresponds to motion of two noninteracting particles with total momentum $\mathbf{q}$. It is not difficult to see that Eq. (19) always has a solution corresponding to free motion of an unbound pair.

We are interested in the other type of solution, which describes bound states of particles. The right side of Eq. (19) has a logarithmic singularity in ε_q^2 at the point $\varepsilon_0^2 = 2\varepsilon_g - 8\tau_1$, corresponding to the bottom of the band for two free particles, which in our model do not depend on the total wave vector. For a decrease $\varepsilon^{(2)} < \varepsilon_0^{(2)}$ the right side of Eq. (19) tends to zero, remaining negative. From this it is easy to see that the condition for existence of a bound state is determined by the inequality

$$\varepsilon_f - \frac{28}{5}\tau_1^2[\varepsilon_b - 2\varepsilon_g + 2\tau_1 + f_1(\mathbf{q})]^{-1} < \varepsilon^{(2)}. \qquad (20)$$

In the case we examine we always have $f_1(q,q) \geqslant 0$. This means that when condition (20) is fulfilled the bottom of the band for a bound state must lie at $q_x = \pi/2a$, $q_y = 0$ and equivalent points, and not in the center of the zone. This fact is connected with the form of the single-particle spectrum.

For the energy parameters of the model presented above (energies and matrix elements τ_1, τ_1') one can persuade oneself that fulfillment of the inequality (20) is equivalent to imposing the condition $V \geqslant \varepsilon/3$.

5. CONCLUSION

We will try to summarize the results obtained above. The Hamiltonian considered here in describing the CuO_2 planes is quite realistic, although it contains several parameters ($U_d, U_p, U_p', \varepsilon, \varepsilon_p, \varepsilon_p', t$) affecting the electronic and magnetic properties of the system. It seems most realistic to assume that all quantities U and ε are larger than the "width" of the band t, and also, that U_d is the largest energy parameter. Reasonable quantum-chemical estimates show that the nonhybridized level ε_p' lies below the hybridized level ε_p. However, a careful analysis of two-hole hybridization demonstrates the reality of the reverse idea, according to which transport occurs through the hybridized oxygen band. In this case, the real dependence of the hole spectrum on the magnetic structure of the copper sublattice is of interest. In this paper we have limited ourselves to considering the AFM state.

Calculation is somewhat simpler for the limit $U_d \to \infty$: most of our results correspond to this situation, although the case of final U_d comparable to ε is doubtless also of interest. In Appendix A we briefly consider this question. We intend to study this case and, in particular, to analyze the assertion in Ref. 9 that the generalized and standard Hubbard models are equivalent for $U_d \sim \varepsilon$. This statement seems to us to be mistaken. In Ref. 9 it was shown that the motion of a hole in a plane can be described as motion of a particle among the sites of a square lattice, with the hopping amplitude for nearest-neighbor sites large compared with the hopping amplitude for non-neighboring sites. On this basis, they neglect the latter amplitudes, which leads to the standard Hubbard model. However, we recall that hopping of a hole from one sublattice to the other is forbidden (in the case of a "rigid" AFM state) or significantly inhibited (in the case of an AFM state with zero-point oscillations or states of the RVB type). This makes hops across sites of the "other" sublattice the chief means of hole motion, which is demonstrated in the present work.

The singularities in the single-particle spectrum found here, in particular its quasi-one-dimensional character, show the importance of analysis of the pairing mechanism because of the strong singularity in the density of states at the edge of the magnetic Brillouin zone. Other mechanisms are connected with formation of a pair of small radius from the quasiparticles—magnetic polarons. This is the situation examined in Sec. 4.

There is another very important question on the form of the hole spectrum in the magnetic RVB state, which is attracting a great deal of interest at present due to the work of Anderson.[3,15] The method used here to construct the variational wave function leads to a universal dependence of its characteristics on the correlators of the magnetic subsystem. We think that the information available on RVB states is still insufficient for calculation of the singularities in the hole spectrum. Nonetheless, according to recent estimates[16] of the RVB and Néel state energies, their difference $\Delta\varepsilon$ is small compared to their own exchange energies. The idea of a magnetic polaron relates also to an RVB structure of the hole environment, the dimension of which, because of the demonstrated small value of $\Delta\varepsilon$, can significantly exceed a lattice constant. Then, for an increase in the free hole concentration the flow of charge through the RVB phase, which should automatically include the Anderson superconductivity mechanism,[15] will become important.

A preliminary study of the one- and two-particle excitations in the RVB phase in the framework of the present model has been carried out in Ref. 12.

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APPENDIX A

Here, we carry out the simplest analysis of a possible magnetic structure arising in the copper sublattice surrounding an oxygen hole. Following Ref. 7, we will neglect the small ($\sim t^4/\varepsilon^3$) exchange interaction of the copper spins and will consider only the Hamiltonian (7). This way is analogous to the approach used by Nagaoka[4] in determining

the spectrum of a single-hole state in the standard Hubbard model. Note that we will not neglect the part of (7) which contains $\tau_3 = t^2 (U_d - \varepsilon - 2V)^{-1}$.

Analysis of the spectrum can easily be carried out for a state of maximal spin.

$$S_{max}=(N_0+1)/2,$$

where N_0 is the number of copper ions. The corresponding wave function has the form

$$\Psi_0 = \sum_{\mathbf{r}} g(\mathbf{r}) X_{\mathbf{r}}^{+0} |F_+\rangle, \tag{A1}$$

where $|F_+\rangle$ is the wave function of the ferromagnetic state of the copper sublattice. The function Ψ_0 satisfies the Schroedinger equation, which can be written for the amplitudes g_h and g_v relating to the horizontal and vertical Cu—O—Cu bonds respectively:

$$Eg_h(\mathbf{r}) = \hat{T}_h g_h(\mathbf{r}) = 2(\tau_2-\tau_1) g_h(\mathbf{r}) + \tau_1 \sum_a [g(\mathbf{r}+\mathbf{a}_x+\mathbf{a}) + g(\mathbf{r}-\mathbf{a}_x+\mathbf{a})]. \tag{A2}$$

The equation for the amplitude g_v is obtained from (A2) by the substitutions $v \leftrightarrow h$ and $x \leftrightarrow y$. We will sometimes drop the indices (h,v), as in Eq. (A2), where the omitted indices can be unambiguously restored.

Fourier-transforming Eq. (A2), we get:

$$(E-2\tau_2+2\tau_1-4\tau_1\cos^2 k_x a) g_h - 4\tau_1 g_v \cos k_x a \cdot \cos k_y a = 0, \tag{A3}$$
$$(E-2\tau_2+2\tau_1-4\tau_1\cos^2 k_y a) g_v - 4\tau_1 g_h \cos k_x a \cdot \cos k_y a = 0.$$

The energy spectrum determined by the system (A3) is:

$$E_1 = -2(\tau_1-\tau_2) + 4\tau_1(\cos^2 k_x a + \cos^2 k_y a), \tag{A4}$$

$$E_2 = -2(\tau_1-\tau_2). \tag{A5}$$

Only in the corners ($\mathbf{k} = (\pm \pi/2a, \pm \pi/2a)$) of the magnetic Brillouin zone do the excitations E_1 become comparable in magnitude to the dispersionless branch E_2.

We will now examine the situation with a nonsaturated magnetic moment:

$$S = S_{max} - 1.$$

This spin deflection can be associated with a spin flip either on a hole on oxygen, or on one of the copper ions. We seek a corresponding wave function in the form

$$\Psi_1 = \sum_{\mathbf{r}} (\varphi(\mathbf{r}) X_{\mathbf{r}}^{-0} + \sum_{\mathbf{R}} g(\mathbf{r},\mathbf{R}) X_{\mathbf{r}}^{+0} Z_{\mathbf{R}}^{-+}) |F_+\rangle. \tag{A6}$$

The analogs of the equations (A2) for the amplitudes $g(\mathbf{r},\mathbf{R})$ look like this:

$$Eg_h(\mathbf{r},\mathbf{R}) = \hat{T}_h g_h(\mathbf{r},\mathbf{R}) + \delta(r, \mathbf{R}-\mathbf{a}_x)[V_{h-}(\mathbf{R}) - G_{h-}(\mathbf{R})] + \delta(\mathbf{r}, \mathbf{R}+\mathbf{a}_x)[V_{h+}(\mathbf{R}) - G_{h+}(\mathbf{R})], \tag{A7}$$

$$Eg_v(\mathbf{r},\mathbf{R}) = \hat{T}_v g_v(\mathbf{r},\mathbf{R}) + \delta(\mathbf{r}, \mathbf{R}-\mathbf{a}_y)[V_{v-}(\mathbf{R}) - G_{v-}(\mathbf{R})] + \delta(\mathbf{r}, \mathbf{R}+\mathbf{a}_y)[V_{v+}(\mathbf{R}) - G_{v+}(\mathbf{R})], \tag{A8}$$

where

$$V_{h-}(\mathbf{R}) = (\tau_1+\tau_3)\sum_{\mathbf{a}} \varphi(\mathbf{R}+\mathbf{a}) - (\tau_1-\tau_2)\varphi_h(\mathbf{R}-\mathbf{a}_x),$$

$$G_{h-}(\mathbf{R}) = (\tau_1+\tau_3)\sum_{\mathbf{a}} g(\mathbf{R}+\mathbf{a},\mathbf{R}) - (\tau_1-\tau_2) g_h(\mathbf{R}+\mathbf{a}_x,\mathbf{R}).$$

The remaining expressions for V and G are easily obtained by an obvious redesignation of indices.

A Fourier transform of the function g in the first variable

$$g(\mathbf{r},\mathbf{R}) = N_0^{-1} \sum_{\mathbf{k}} g(\mathbf{k};\mathbf{R}) \exp i\mathbf{k}\mathbf{r},$$

applied to Eqs. (A7), (A8) gives

$$(\varepsilon - 4\tau_1\cos^2 k_x a) g_h(\mathbf{k};\mathbf{R}) - 4\tau_1 g_v(\mathbf{k};\mathbf{R}) \cos k_x a \cdot \cos k_y a = \{\exp(ik_x a)[V_{h-}(\mathbf{R}) - G_{h-}(\mathbf{R})] + \exp(-ik_x a)[V_{h+}(\mathbf{R}) - G_{h+}(\mathbf{R})]\} \exp(i\mathbf{k}\mathbf{R}), \tag{A9}$$

$$(\varepsilon - 4\tau_1\cos^2 k_y a) g_v(\mathbf{k};\mathbf{R}) - 4\tau_1 g_h(\mathbf{k};\mathbf{R}) \cos k_x a \cdot \cos k_y a = \{\exp(ik_y a)[V_{v-}(\mathbf{R}) - G_{v-}(\mathbf{R})] + \exp(-ik_y a)[V_v(\mathbf{R}) - G_{v+}(\mathbf{R})]\} \exp(i\mathbf{k}\mathbf{R}). \tag{A10}$$

The quantity $\varepsilon = E + 2(\tau_1 - \tau_2)$ is introduced here. The right-hand side of Eqs. (A9) and (A10) contains the amplitudes $g_{h(v)}(\mathbf{R} \pm \mathbf{a}_{x(y)}, \mathbf{R})$, which allows us to write the self-consistency conditions on them as

$$g_{h(v)\pm} = g_{h(v)}(\mathbf{R} \pm \mathbf{a}_{x(y)}, \mathbf{R}) = N_0^{-1} \sum_{\mathbf{k}} \mathrm{Det}^{-1} \{4\tau_1 [V_{v(h)+} + V_{v(h)-} - G_{v(h)+} - G_{v(h)-}] \times \cos^2 k_x a \cdot \cos^2 k_y a + (\varepsilon - 4\tau_1 \cos^2 k_{y(x)} a)[V_{h(v)\pm} - G_{h(v)\pm} + (V_{h(v)\mp} - G_{h(v)\mp}) \cos 2k_{x(y)} a]\}, \tag{A11}$$

where

$$\mathrm{Det} = \varepsilon[\varepsilon - 4\tau_1(\cos^2 k_x a + \cos^2 k_y a)].$$

The structure of the system of four equations (A11) is such that we must look for a solution in the form

$$g_h(\mathbf{R}+\mathbf{a}_x, \mathbf{R}) = A\varphi_h(\mathbf{R}+\mathbf{a}_x) + B\varphi_h(\mathbf{R}-\mathbf{a}_x) + C[\varphi_v(\mathbf{R}+\mathbf{a}_y) + \varphi_v(\mathbf{R}-\mathbf{a}_y)]. \tag{A12}$$

The three remaining functions are obtained from (A12) by an appropriate change of indices.

It is not difficult to determine the coefficients A, B, and C, calculating the sums over $\mathbf{a}$ for $g(\mathbf{R}+\mathbf{a},\mathbf{R})$, $g_h(\mathbf{R}+\mathbf{a}_x,\mathbf{R}) - g_h(\mathbf{R}-\mathbf{a}_x,\mathbf{R})$, and $g_h(\mathbf{R}+\mathbf{a}_x,\mathbf{R}) + g_h \times (\mathbf{R}-\mathbf{a}_x,\mathbf{R}) - g_v(\mathbf{R}+\mathbf{a}_y,\mathbf{R}) - g_v(\mathbf{R}-\mathbf{a}_y,\mathbf{R})$ according to equations (A11) and (A12). As a result of these calculations we get

$$A+B+2C = [1-4(3+\tau_2/\tau_1+4\tau_3/\tau_1)^{-1}(1-I_0)^{-1}]^{-1},$$
$$A+B-2C = \{1+(1-\tau_2/\tau_1)^{-1}[(1-I_0)/4+I_1\tau_1/|\varepsilon|]^{-1}\}^{-1},$$
$$A-B = [1+I_2^{-1}(1-\tau_2/\tau_1)^{-1}]^{-1},$$

where

$$I_0=\int|\varepsilon|[|\varepsilon|+4\tau_1(\cos^2 k_x a+\cos^2 k_y a)]^{-1}(2\pi)^{-2}d^2k,$$

$$I_1=\int 8\cos^2 k_x a\cdot\cos^2 k_y a\cdot[|\varepsilon|+4\tau_1(\cos^2 k_x a+\cos^2 k_y a)]^{-1}(2\pi)^{-2}d^2k,$$

$$I_2=[(1-|\varepsilon|/4\tau_1)+(1+|\varepsilon|/4\tau_1)I_0-I_1].$$

To obtain a closed system of equations to determine the eigen-energies, we need to add the equations for the amplitudes φ:

$$E\varphi_{h(v)}(\mathbf{r})=-\tau_3\sum_{\mathbf{a}}[\varphi(\mathbf{r}+\mathbf{a}_{x(y)}+\mathbf{a})+\varphi(\mathbf{r}-\mathbf{a}_{x(y)}+\mathbf{a})]$$
$$+(\tau_1+\tau_3)\sum_{\mathbf{a}}[g(\mathbf{r}+\mathbf{a}_{x(y)}+\mathbf{a},\mathbf{r}+\mathbf{a}_{x(y)})+g(\mathbf{r}-\mathbf{a}_{x(y)}+\mathbf{a},\mathbf{r}-\mathbf{a}_{x(y)})]$$
$$-(\tau_1-\tau_2)[g_{h(v)}(\mathbf{r},\mathbf{r}+\mathbf{a}_{x(y)})+g_{h(v)}(\mathbf{r},\mathbf{r}-\mathbf{a}_{x(y)})]. \tag{A13}$$

Using the local relation (A12) of the amplitudes g and φ and applying a Fourier transformation to equation (A13) ($\varphi(\mathbf{r})\propto\varphi\exp i\mathbf{Q}\cdot\mathbf{r}$), we obtain an equation that determines the hole band spectrum of the state (A6) in the form

$$\det M=0, \tag{A14}$$

where the 2×2 matrix M has the following matrix elements:

$$M_{11(22)}=|\varepsilon|+2(\tau_1-\tau_2)+4\cos^2 Q_{x(y)}a[(A+B+2C)(\tau_1+\tau_3)-\tau_3]-2(\tau_1-\tau_2)(A+B\cos 2Q_{x(y)}a),$$

$$M_{12}=M_{21}=4[(\tau_1+\tau_3)(A+B+2C)-\tau_3-C(\tau_1-\tau_2)]\cos Q_x a\cos Q_y a.$$

Analysis of the spectrum determined by equation (A14) is rather awkward. Here we will present results for the corners and for the center of the Brillouin zone.

1) $\mathbf{Q}=(\pi/2a,\pi/2a)$. In this case the matrix elements satisfy $M_{12}=M_{21}=0$ and we have

$$|\varepsilon|=2(\tau_1-\tau_2)(A-B-1).$$

The only solution to this equation is $|\varepsilon|=0$, which coincides with the energy of the hole state (A1) at this point (see formulas A4 and A5).

2) $\mathbf{Q}=(0,0)$. The solution of equation (A14) has the following form:

$$|\varepsilon|+2(\tau_1-\tau_2-4\tau_3)=\frac{(3\tau_1+\tau_2+4\tau_3)(1-I_0)/4}{(3\tau_1+\tau_2+4\tau_3)(1-I_0)/4-\tau_1}.$$

For values of the parameters τ_i having a physical significance ($\tau_1\geqslant\tau_2,\tau_3>0$), this equation has at least one solution which splits in two for sufficiently large τ_3 [under the condition $\tau_3>(\tau_1-\tau_2)/4$]. This last fact underscores the necessity of a thorough study of the reconstruction of the magnetic environment of a hole and the hole spectrum in the region of τ_3 indicated. We recall once again that in Ref. 9 the case $\tau_3=\tau_1$ was considered.

APPENDIX B

The quasiparticle spectrum, calculated according to formula (9), is determined, as already shown in Sec. 3, by the following correlators:

$$\langle\mathbf{R}^-|H_I|\mathbf{R}^-\rangle=12\tau_1(f_R^2\langle Z_R^{--}\rangle+2f_R g_R\langle Z_R^{-\cdot}\rangle)+4\tau_2[f_R^2(\langle Z_R^{--}\rangle+\langle Z_{R'}^{--}\rangle)+f_R g_R(2\langle Z_R^{-\cdot}\rangle+\langle Z_R^{+-}Z_{R'}^{-+}\rangle+\langle Z_R^{-+}Z_{R'}^{+-}\rangle)+g_R^2\langle Z_R^{+\cdot}Z_{R'}^{\cdot+}\rangle] \tag{B1}$$

(here, as in the following formulas, $\mathbf{R}$ and $\mathbf{R}'$ signify a pair of the nearest copper sites);

$$\langle\mathbf{R}'^-|H_I|\mathbf{R}\rangle=(3\tau_1+\tau_2)[f_{R'}f_R(\langle Z_R^{--}\rangle+\langle Z_{R'}^{--}\rangle)+f_{R'}g_R(\langle Z_R^{+\cdot}\rangle+\langle Z_{R'}^{\cdot-}Z_R^{-+}\rangle)+g_{R'}f_R(\langle Z_{R'}^{\cdot+}\rangle+\langle Z_{R'}^{+-}Z_R^{-+}\rangle)], \tag{B2}$$

$$\langle\mathbf{R}''^-|H_I|\mathbf{R}\rangle=\tau_1(f_{R''}f_R\langle Z_{R'}^{--}\rangle+g_{R''}f_R\langle Z_{R''}^{+-}Z_{R'}^{-+}\rangle+f_{R''}g_R\langle Z_{R'}^{+-}Z_R^{-+}\rangle+g_{R''}g_R\langle Z_{R''}^{+-}Z_{R'}^{-+}Z_R^{-+}\rangle). \tag{B3}$$

In the last matrix element the "path" was considered by which a hole goes from site $\mathbf{R}$ across $\mathbf{R}'$ to $\mathbf{R}''$.

For an Ising AFM state the matrix elements (B3), with vectors $\mathbf{R}''$ equal to $\mathbf{R}+2\mathbf{a}_x+2\mathbf{a}_y$ and $\mathbf{R}+4\mathbf{a}_x$, are identical. In the case of a Heisenberg state their magnitudes differ slightly, which is the reason for the removal of degeneracy in the energy spectrum along the nesting line.

Below, we produce the values of the magnetic correlators that are needed to calculate the single-particle spectrum for a Heisenberg ground state of the copper sublattice. They have been calculated with the aid of a method applied in Ref. 16 to find the energy of a Heisenberg two-sublattice state. The method consists of using a variational wave function in combination with a Monte-Carlo method, which allows estimation of energy and calculation of the correlator with great accuracy for such essentially quantum systems as the Heisenberg antiferromagnet with spin 1/2. In qualitatively analyzing the hole spectrum it was sufficient to use a single-parameter variational function; we then find $\langle Z_R^{\cdot\downarrow}\rangle=0.9181$ ($\mathbf{R}$ belongs to the "+" sublattice); $\langle Z_R^{\downarrow\cdot}Z_R^{\cdot\uparrow}+Z_R^{\cdot\downarrow}Z_R^{\downarrow\cdot}\rangle=-0.2592$; $\langle Z_R^{\downarrow\cdot},Z_R^{\downarrow\cdot}\rangle=0.0594$.

To calculate numerical values of the correlator

$$K=\langle Z_{R'}^{\cdot++}(Z_R^{+-}Z_{R''}^{-+}+Z_R^{-+}Z_{R''}^{+-})\rangle$$

we must distinguish four cases:

a) $\mathbf{R}'$ belongs to the "+" sublattice, but $\mathbf{R}$ and $\mathbf{R}''$ are next-nearest copper sites; for instance $\mathbf{R}''=\mathbf{R}+2\mathbf{a}_x+2\mathbf{a}_y$; $K=0.0499$;

b) $\mathbf{R}'$ belongs to the "−" sublattice, $\mathbf{R}$ and $\mathbf{R}''$ are the same as in (a); $K=0.0371$;

c) $\mathbf{R}'$ belongs to the "+" sublattice, $\mathbf{R}$ and $\mathbf{R}''$ are next-nearest sites, but horizontally or vertically, for example, $\mathbf{R}''=\mathbf{R}+4\mathbf{a}_x$; $K=0.0206$;

d) $\mathbf{R}'$ belongs to the "−" sublattice, $\mathbf{R}$ and $\mathbf{R}''$ are the same as in (c); $K=0.0371$.

The result of a numerical calculation shows that the degree of splitting of the energy level along the nesting line is very small and amounts to $\sim 0.5\times 10^{-4}\tau_1$; the minima are distributed in the corners of the magnetic Brillouin zone.

[1] J. M. Tranquada, S. M. Heald, A. R. Medenbaugh, and M. Suenaga, Phys. Rev. B35, 7187 (1987); A. Fujimory, E. Takayoma-Muromachi, Y. Uchida, and B. Okai, Phys. Rev. B35, 8814 (1987); N. Nucker, J. Fink, B. Renker, D. Evert *et al.*, Z. Phys. B67, 9 (1987); N. Nucker, J. Fink, J. C. Fuggle, P. J. Durham *et al.*, Phys. Rev. B37, 5158 (1988).

[2] C. M. Varma, S. Schmitt-Rink, and E. Abrahams, Sol. St. Comm. **62**, 681 (1987); V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987); J. E. Hirsch, Phys. Rev. Lett. **59**, 228 (1987).
[3] P. W. Anderson, G. Baskaran, Z. Zou, and T. Hsu, Phys. Rev. Lett. **58**, 2790 (1987).
[4] Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
[5] E. L. Nagaev, Zh. Eksp. Teor. Fiz. **54**, 228 (1968) [Sov. Phys.—JETP **27**, 122 (1968)].
[6] V. L. Pokrovskiĭ, G. V. Uĭmin, and D. V. Khveshchenko, Pis'ma v Zh. Eksp. Teor. Fiz. **46**, 136 (Appendix) (1987) [JETP Lett. **46**, S113 (1988)].
[7] L. I. Glazman and A. S. Ioselevich, Pis'ma v Zh. Eksp. Teor. Fiz. **47**, 464 (1988) [JETP Lett. **47**, 547 (1988)].
[8] S. V. Iordanskiĭ and A. V. Smirnov, Zh. Eksp. Teor. Fiz. **79**, 1942 (1980) [Sov. Phys.—JETP **52**, 981 (1980)].
[9] F. C. Zhang and T. M. Rice, Phys. Rev. **B37**, 3759 (1988).
[10] Yu. V. Kopayev, Pis'ma v Zh. Eksp. Teor. Fiz. **47**, 628 (1988) [JETP Lett. **47**, 726 (1988)].
[11] A. F. Barabanov, L. A. Maksimov, and A. V. Mikheenkov, Fiz. Tverd. Tela **30**, 2518 (1988) [Sov. Phys.—Solid State **30**, 1449 (1988)]; G. V. Uĭmin, L. A. Maksimov and A. F. Barabanov, Pis'ma v Zh. Eksp. Teor. Fiz. **48**, 281 (1988) [JETP Lett. **48**, 312 (1988)].
[12] A. F. Barabanov, R. O. Kuzyan, L. A. Maksimov, and G. V. Uĭmin, in *Superconductivity*, ed. V. I. Ozhogin, Vol. 3, p. 70 (Moscow, 1988).
[13] A. F. Barabanov, L. A. Maksimov, and G. V. Uĭmin, Pis'ma v Zh. Eksp. Teor. Fiz. **47**, 532 (1988) [JETP Lett. **47**, 622 (1988)].
[14] J. E. Hirsch, S. Tang, E. Loh, and D. J. Scalapino, Phys. Rev. Lett. **60**, 668 (1988).
[15] P. W. Anderson, Science **235**, 1196 (1987); G. Baskaran, Z. Zou, and P. W. Anderson, Sol. St. Comm. **63**, 973 (1987); J. M. Wheatley, T. C. Hsu, and P. W. Anderson, Phys. Rev. **B37**, 5897 (1988).
[16] D. A. Huse and V. Elser, Phys. Rev. Lett. **60**, 2531 (1988).

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