Elementary excitations in CuO_2 planes

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A generalized Hubbard model is used to derive a one-particle hole spectrum. The features of this spectrum are analyzed for various versions of the ground state of the magnetic subsystem of copper ions. The possible formation of bound hole states is discussed.

The experimental research on high-temperature superconductivity is regularly generating new information, which requires theoretical interpretation. The vigorous campaign which Anderson[1] has mounted for the RVB theory has somewhat overshadowed alternative approaches to an explanation of high-temperature superconductivity, including conventional mechanisms of the BCS type and polaron mechanisms. An approach which has been proposed by Varma *et al.*,[2] Emery,[3] Hirsch,[4] and Zhang and Rice[5] and which uses a generalization of the Hubbard model for a lattice of the CuO_2 type seems promising to us (Fig. 1). The Hamiltonian of this model,

$$\mathcal{H} = \sum_{\mathbf{r}} \epsilon_p n_p(\mathbf{r}) + \sum_{\mathbf{R}} \epsilon_d n_d(\mathbf{R}) + U_p \sum_{\mathbf{r}} n_p^{\uparrow}(\mathbf{r}) n_p^{\downarrow}(\mathbf{r}) + U_d \sum_{\mathbf{R}} n_d^{\uparrow}(\mathbf{R}) n_d^{\downarrow}(\mathbf{R})$$

$$- t \sum_{\langle \mathbf{r}, \mathbf{R} \rangle, \sigma} (p_{\mathbf{r}\sigma}^{+} d_{\mathbf{R}\sigma} + d_{\mathbf{R}\sigma}^{+} p_{\mathbf{r}\sigma}) + V \sum_{\langle \mathbf{r}\mathbf{R} \rangle} n_p(\mathbf{r}) n_d(\mathbf{R}), \qquad (1)$$

includes one-particle levels (ϵ_p,ϵ_d) and intraatomic correlations (U_p,U_d) (the subscripts p and d refer to the O and the Cu, respectively). The jumps occur along hybridized Cu-O orbitals. Here V is the Coulomb repulsion of the holes in the same orbitals.

It is reasonable to assume that in the absence of doping the ground states of the copper and oxygen ions would be Cu^{++} and O^{--}, i.e., that there would be precisely one hole per copper ion. This assertion implies $\epsilon = \epsilon_p - \epsilon_d > 0$. Recent experiments[6] support the suggestion that the free holes which appear in a CuO_2 plane as the result of doping concentrate primarily near the oxygen. There would then be yet another inequality to be satisfied for the parameters of the model:

$$\epsilon + 2V < U_d.$$

The jumping parameter t will be assumed to be smaller than the other parameters, ϵ, U_d, and U_p, so that in a second-order perturbation theory in the kinetic energy t we can construct an effective Hamiltonian which describes hole jumps exclusively along the oxygen sublattice. To bring out the features of the hole band structure, we eliminate from consideration the Cu^{+++} states, i.e., we set $U_d = \infty$. The imposition of this condition is not of fundamental importance, but it is a reasonable approach since

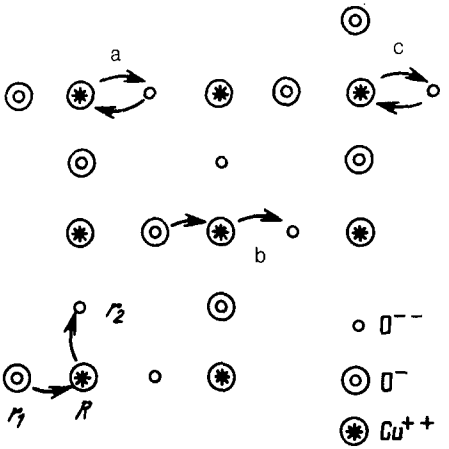

FIG. 1. Schematic diagram of a CuO_2 plane (see the text proper for an explanation).

the estimates of Refs. 2 and 3 indicate that U_d is indeed the largest energy parameter of the problem.

An antiferromagnetic exchange of copper ions in adjacent sites **R** and **R'** arises in fourth-order perturbation theory. It is described by

$$4\frac{t^4}{(\epsilon+V)^2(\epsilon+U_p)}\left(2\mathbf{S}_{\mathbf{R}}\mathbf{S}_{\mathbf{R}'}+\frac{1}{2}\right).$$

The spin correlations in the copper sublattice should evidently be of an antiferromagnetic nature and should influence the hole band spectrum. If there is a finite concentration of oxygen holes, the inverse effect of the band spectrum on the spin state of the copper sublattice will also become important.

Let us return to the question of an effective hole Hamiltonian. Figure 1 shows some virtual processes which cause an effective jump from site $\mathbf{r}_1$ to one of its nearest-neighbor sites $\mathbf{r}_2$. The Hamiltonian for a jump of this sort is

$$\mathscr{H}_{\text{eff}}=(\tau_1-\tau_2\delta_{\mathbf{a}_1,\mathbf{a}_2})p^{+}_{\mathbf{R}+\mathbf{a}_1,\alpha}p_{\mathbf{R}+\mathbf{a}_2,\beta}\left(2\vec{\sigma}_{\alpha\beta}\mathbf{S}(R)+\frac{1}{2}\delta_{\alpha\beta}\right), \tag{2}$$

where $\tau_1=t^2\epsilon^{-1}$, $\tau_2=t^2(\epsilon^{-1}-(\epsilon+U_p)^{-1})$ the vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ connect the nearest Cu and O sites, σ are the Pauli matrices, and $\mathbf{S}(\mathbf{R})$ is the spin vector of copper-sublattice site **R**. For our purposes it is more convenient to express $\mathscr{H}_{\text{eff}}$ in terms of Hubbard variables[7]:

$$\mathscr{H}_{\text{eff}}=(\tau_1-\tau_2\delta_{\mathbf{a}_1,\mathbf{a}_2})X^{\sigma_2 0}_{\mathbf{R}+\mathbf{a}_2}X^{0\sigma_1}_{\mathbf{R}+\mathbf{a}_1}Z^{\sigma_1\sigma_2}_{\mathbf{R}}. \tag{2'}$$

The operator $X^{\sigma 0}$ ($X^{0\sigma}$) generates (annihilates) a particle at an oxygen site, and $Z^{\sigma_1\sigma_2}$ is the operator which represents the spin substitution $\sigma_2\to\sigma_1$ in the copper sublattice.

Bloch functions which determine the one-particle spectrum of Hamiltonian (2') can be constructed from a set of site functions which is complete but not necessarily orthogonal:

$$|\mathbf{R}\sigma\rangle = \sum_{\mathbf{b}} (f_{\mathbf{R},\mathbf{b}} X^{\sigma 0}_{\mathbf{R}+\mathbf{b}} + g_{\mathbf{R},\mathbf{b}} X^{\bar{\sigma} 0}_{\mathbf{R}+\mathbf{b}} Z^{\sigma\bar{\sigma}}_{\mathbf{R}}) |G\rangle , \tag{3}$$

where $|G\rangle$ represents the wave function of the ground state of the spin system, and $\mathbf{b}$ represents the vectors which connect copper and oxygen ions. The coefficients in (3) may be thought of as variational coefficients. For a simple magnetic lattice they should depend on $\mathbf{b}$ alone. For an antiferromagnetic state of copper, the set of coefficients is doubled ($f_{\mathbf{b}}^{+}, g_{\mathbf{b}}^{+}$ and $f_{\mathbf{b}}^{-}, g_{\mathbf{b}}^{-}$).

On the Bloch functions

$$|\mathbf{k}, \sigma\rangle = A_{\mathbf{k}} \sum_{\mathbf{R}} \exp i\mathbf{k}\mathbf{R} \, |\mathbf{R}\sigma\rangle \tag{4}$$

we impose the condition of orthonormality; equivalently, we write

$$1 = A_{\mathbf{k}}^2 \sum_{\mathbf{R}\mathbf{R}'} \exp i\,\mathbf{k}(\mathbf{R}-\mathbf{R}') \langle \sigma\mathbf{R}' | \mathbf{R}\sigma \rangle . \tag{5}$$

We will now present some results calculated for the simplest version of function (3), in which the variational coefficients f and g are nonzero only for the minimal $\mathbf{b}$. In addition to the diagonal matrix elements $\langle \mathbf{R}|\mathscr{H}\mathbf{R}\rangle$, $\langle \mathbf{R}+2\mathbf{b}|\mathscr{H}|\mathbf{R}\rangle$ and $\langle \mathbf{R}+2\mathbf{b}_1+2\mathbf{b}_2|\mathscr{H}|\mathbf{R}\rangle$ are also nonvanishing. The band spectrum

$$\epsilon_{\mathbf{k}} = \langle \mathbf{k} | \mathcal{H} | \mathbf{k} \rangle$$

turns out to depend on the expectation values of the spin projections, $\langle Z_{\mathbf{R}}^{-} \rangle$ and $\langle Z_{\mathbf{R}}^{+} \rangle$, and correlation functions of the type

$$\langle Z^{-+}_{\mathbf{R}} Z^{+-}_{\mathbf{R}+2\mathbf{b}} \rangle, \quad \langle Z^{-+}_{\mathbf{R}} Z^{\sigma\sigma}_{\mathbf{R}+2\mathbf{b}_1} Z^{+-}_{\mathbf{R}+2\mathbf{b}_1+2\mathbf{b}_2} \rangle .$$

Let us briefly review the results of a band calculation for the particular case $U_p = \infty$. For antiferromagnetic states of the band-bottom type, ϵ_0 corresponds to a boundary of the Brillouin zone near which we have

$$\epsilon(\mathbf{k}) - \epsilon_0 \sim (\cos 2k_x a + \cos 2k_y a)^2 .$$

This situation differs from ordinary nesting in that the quadratic dependence of the spectrum leads to a quasi-one-dimensional state density, which in turn makes the system extremely unstable with respect to structural changes. In contrast with the one-dimensional case, on the other hand, the Coulomb interaction does not suppress the superconducting channel.

In units of τ_1, the band bottom ϵ_0 of the ferromagnetic state is $-3\sqrt{2}$; that for an antiferromagnetic state of the Ising type is $\epsilon_0 = (-1-\sqrt{37})/2$, and that for a Heisenberg antiferromagnet is $\epsilon_0 \approx -3.11$. In the paramagnetic case, the band bottom lies above these values. Although a ferromagnetic background would be most advanta-

geous, we need to recall the antiferromagnetic interaction of copper ions. In a competition of this sort, a ferron[8] arises with a typical radius $\sim (U_p \epsilon/t^2)^{1/4}$, which amounts to one or two lattice constants for the actual values of the energy parameters. Fluctuations of this sort, however, are already incorporated in our variational function. In such a situation we need to examine various types of antiferromagnetic ordering and, possibly, states of the RVB type and their effect on the hole spectrum.

In conclusion we would like to point out a mechanism which is manifested in second-order perturbation theory and which leads to a local attraction of holes at short range. Figure 1 (regions a and b) shows virtual processes which make a contribution $-t^2/(\epsilon - V)$, instead of $-t^2/\epsilon$ to the energy. To find the energy of the bound state, we also used a variational approach, but in a different modification: the cluster method. It turns out that for $V/\epsilon \gtrsim 0.36$ a singlet pairing of holes is advantageous. We should point out that values of V which are too large ($V/\epsilon \geqslant 0.5$) cause a spontaneous formation of heavy three-particle bound states. The virtual process shown in region c in Fig. 1 leads to an energy shift $-t^2/(\epsilon - 2V)$, from which we find the inequality written above. This boundary ($V/\epsilon \approx 0.36$) shifts downward in the case $U_p \neq \infty$, since the infinite one-site repulsion in the singlet state is eliminated.

A point which should be noted is that at values of V/ϵ smaller than the critical value a doping may lead initially to a filling of Fermi states up to the energy level of the bosons (the bound holes). Such a possibility might yield an explanation for the low-temperature behavior of the heat capacity, $\sim T$, and certain other physical properties of high-temperature superconductors, including the linear dependence $\rho(T)$ at $T > T_c$.

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