

Nonmagnetic spin polaron in a generalized Hubbard model for CuO₂ planes

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States of an additional particle are analyzed in a generalized Hubbard model which is equivalent to a Kondo lattice with spin-dependent amplitudes for intersite transitions. A hole forms bound complexes with lattice spins. The ground state is substantially different from the magnetic polaron formed by an electron.

The discovery of high-temperature superconductivity revived interest in models with a strong Coulomb interaction, which may determine both the magnetic and superconducting properties of cuprites.¹ In an undoped cuprite, the copper ions are in the Cu²⁺ state (one hole in the *d* shell), and the *p* shell of the O is completely filled. The assumption that the lowest energy of the additional hole corresponds to the state Cu³⁺ leads to an ordinary Hubbard model on a square Cu lattice. In this model, in the case of strong Coulomb repulsion *U_d*, a hole forms a saturated ferromagnetic polaron.² Such a polaron, which greatly increases the effective spin of the carrier, is not observed in cuprites. Attempts to explain the situation have been based on the suggestion that the actual values of *U_d* are not sufficiently large.^{1,3}

In another model which describes a CuO₂ plane, the Emery model,⁴ the additional hole corresponds to an O⁻ lowest state. We will show that in this model a ferromagnetic polaron is not the ground state of the additional hole, even in the limit *U_d* → ∞.

In the Emery model, the Hamiltonian of the holes is

$$\mathcal{H}_0 = -\epsilon \sum d_{j\sigma}^+ d_{j\sigma} + U_d \sum d_{j\uparrow}^+ d_{j\uparrow} d_{j\downarrow}^+ d_{j\downarrow} + U_p \sum a_{i\uparrow}^+ a_{i\uparrow} a_{i\downarrow}^+ a_{i\downarrow} + t_{pd} \sum_{\langle ij \rangle} (d_{j\sigma}^+ a_{i\sigma} + a_{i\sigma}^+ d_{j\sigma}), \quad (1)$$

where *d_{jo}*⁺ and *a_{io}*⁺ are the operators which create a hole in the Cu and O shells; $\epsilon = \epsilon_p - \epsilon_d > 0$; and ϵ_p , *U_p*, ϵ_d , and *U_d* are the one-particle and Hubbard energies at O and Cu sites. The energy is reckoned from the ϵ_p level. The basic assumption of the model is the inequality $\epsilon < U_d$. We ignore the repulsion *U_p*, and we assume that the value (*t_{pd}*) of the energy of the *p-d* hybridization is small; *U_p*, *t_{pd}* ≪ ε ≪ *U_d*. For the additional hole we find the new Hamiltonian¹⁾ $\mathcal{H} = \mathcal{H}_h + \mathcal{H}_{ex}$ from (1) through a unitary transformation⁵:

$$\mathcal{H}_h = t \sum_{\langle j_1 i_2 \rangle} a_{i_1 \sigma_1}^+ (2S_{j_1 \sigma} + 1/2) a_{i_2 \sigma_2}, \quad \mathcal{H}_{ex} = J \sum_{\langle j_1 j_2 \rangle} S_{j_1} S_{j_2}. \quad (2)$$

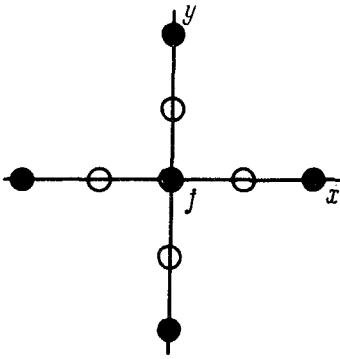


FIG. 1. Fragment of a CuO_2 lattice. ●—Cu; ○—O. For a given j the sites i_1, i_2 in $\langle j i_1 i_2 \rangle$ can be any pair of O sites shown, including coincident sites ($i_1 = i_2$). The lattice constant is $a_0 = 1$.

This Hamiltonian is equivalent to \mathcal{H}_0 within $(t_{pd}/\epsilon)^4$. The Hamiltonian \mathcal{H}_{ex} with $J \sim t_{pd}^4/\epsilon^3 > 0$ corresponds to a superexchange of the spins S_j of the nearest Cu ions. As in Ref. 2, we will examine the hole Hamiltonian \mathcal{H}_h , since $t \sim t_{pd}^2/\epsilon \gg J$. The sites i_1 and i_2 between which transitions are possible are shown in Fig. 1. A fundamental distinction between hole Hamiltonian (2) and the effective Hamiltonian for an additional particle in the ordinary Hubbard model⁶ is that the possible motions of the hole are limited by the operator $2S\sigma + 1/2$, rather than by a Guzwiller projection operator. This system also differs from an ordinary Kondo lattice (where there are also magnetic polarons⁷), since both the single-site energies and the jump amplitudes depend on the spins in (2).

The state of the Hamiltonian \mathcal{H}_h can be characterized by the total spin $S = S_{\max} - m$, $m \geq 0$; its projection S_z ; and the wave vector \mathbf{k} . We denote by E_m the minimum energy corresponding to the given value of m . We will show that in an infinite lattice the strict inequality $E_{m+1} < E_m$ holds for any finite m .

A ferromagnetic state corresponds to $m = 0$ and an eigenfunction of the type $\psi_0(i)$, where i is the position of the hole (with spin up). The corresponding dispersion law has two branches: $E_0^{(1)}(\mathbf{k}) \equiv 0$, $E_0^{(2)}(\mathbf{k}) = 4t(1 + \frac{1}{2} \cos k_x + \frac{1}{2} \cos k_y)$, (Fig. 2). Eigenfunctions with $m > 0$ have two components: $\varphi_m(i, j_1 \dots j_{m-1})$ and $\psi_m(i, j_1 \dots j_m)$, where i in the function φ_m is the coordinate of a spin-down hole, and in ψ_m it is the coordinate of a spin-up hole, and j_l are the coordinates of the "magnons": flipped Cu spins. To determine $E_m(k)$, we use the single-plaquette approximation, which corresponds to the variational function $\psi_m(i, j_1 \dots j_m)$, which vanishes if i is not a neighbor of at least one of the j_l . For $m = 1$ we can easily calculate the lower branch in the single-plaquette approximation $E_1(\mathbf{k}) = t\{0.5 - [16.25 + 8(\cos k_x + \cos k_y)]^{1/2}\}$. The value $E_1 = -5.18t$ is reached at the center of the band.²⁾ At the point $k_x = k_y = \pi$, the branches $E_0(\mathbf{k})$ and $E_1(\mathbf{k})$ merge. The "1-complex" which is found corresponds to the bound state of a hole and a single magnon. Are there bound m -complexes with $m \geq 2$?

Let us verify the existence of a 2-complex. In the single-plaquette approximation, the equations for $\psi_2(ij_1j_2)$ at $r = |(j_1 - j_2)_x| + |(j_1 - j_2)_y| \geq 3$ describe an immobile magnon and a 1-complex which does not interact with this magnon. The boundary

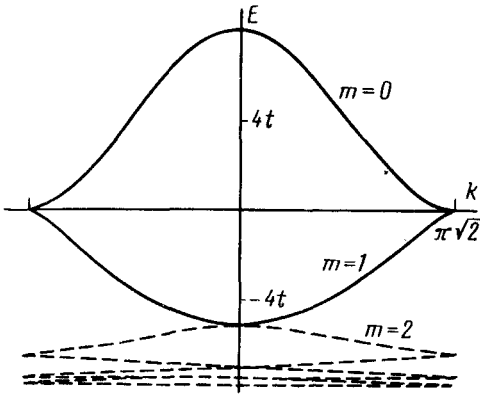


FIG. 2. The dispersion law $E_m(\mathbf{k})$ for \mathbf{k} in the $[11]$ direction. The dashed lines show the suggested form of $E_m(\mathbf{k})$ for $m \geq 2$. The plot of $E_m(\mathbf{k})$ in the one-dimensional case is analogous.

conditions on these equations follow from the solution of the Schrödinger equation at $r < 3$. We narrow the class of functions of the single-plaquette approximation by setting $\psi_2(ij_1j_2) = e^{ik\mathbf{j}}\chi(r)$ for $r \geq 3$, where \mathbf{j} is that site of the sites j_1, j_2 beside which there is no hole. The boundary conditions determine the relationship $\chi(2)/\chi(3) = 1 + v(E\mathbf{k})$. A bound 2-complex arises if $v(E_1, k) > 0$. Calculations for small values of k show that we have $v(E_1, k) \approx -0.022 + 0.058 k^2$ and $v > 0$ as early as $k \geq k^* = 0.2\pi$. The small value of $v(E_1, 0)$ apparently indicates that in the exact solution $E_1(\mathbf{k})$ and $E_2(\mathbf{k})$ touch at the point $\mathbf{k} = 0$ (Fig. 2). These approximations do not allow us to find the maximum binding energy of the 2-complex, $\delta_2 = E_1 - E_2$, or the corresponding value $\mathbf{k} = \mathbf{k}_0$. However, the important point as far as we are concerned is the fact that a bound state exists. Going beyond the scope of the single-plaquette approximation reduces E_1 and E_2 , but the 2-complex remains bound. To show this, we assume that as the variational function is improved, the radius of the 2-complex becomes infinite, $r_2 \rightarrow \infty$ and we have $\delta_2 \rightarrow 0$. We then single out a certain region of r with a radius $r^* \ll r_2$, and we return to the single-plaquette approximation in it. This approach (in the first place) does not alter the part of the energy shift E_2 which is formed by the region $r \sim r_2$ and which coincides with the shift E_1 , and (second) it returns us to our old boundary condition. The latter condition corresponds to a finite value of r_2 , which contradicts the assumption $r_2 \rightarrow \infty$. In other words, the 2-complexes found in the single-plaquette approximation are also in the exact solution, $\delta_2 > 0$.

We can prove that complexes with $m > 2$ exist. In the single-plaquette approximation, a 2-complex is weakly bound and is equivalent to a particle (a 1-complex) in the field of a point attractive center (a magnon). The radius of a 3-complex, r_3 , is determined by the binding of the particle with two centers, which are separated by a distance r . The interaction of a particle with two point potentials leads to the boundary condition $\ln r_3 + \ln r_3/r = [v(k)]^{-1}$. To estimate r and r_3 , we note that the centers are delocalized due to the interaction with the particle, and we have $k - k_0 \sim r^{-1}$. Expanding $v(k)$ in the limit $k \rightarrow k_0$, we find $v(k) = v(k_0)(1 - c(k - k_0)^2)$, $v(k_0) \sim (\ln r_2)^{-1}c \sim 1$, and thus $r \sim (\ln r_2)^{1/2}$, $r_3 \sim (r r_2)^{1/2}$, $E_2 - E_3 \sim (t\delta_2/\ln r_2)^{1/2}$. Corresponding arguments show that there exist complexes with arbitrary m . The fact that they exist remains in force when they go beyond the scope of the single-plaquette

approximation. At $m \gg 1$, the energy of a complex can be estimated by the coherent-potential method: $E_2 - E_m \sim t / \ln r_2$. The mean distances between magnons are $r \sim 1$; i.e., their density ρ is finite, and we have $S = (1 - 2\rho)S_{\max}$. These discussions do not allow us to choose between the singlet ($\rho = 1/2$) and an unsaturated ferromagnet ($0 < \rho < 1/2$) for the ground state.

The properties which we have established for m -complexes in the planar model of CuO_2 remain in force for a one-dimensional chain of alternating Cu-O sites. In particular, the dispersion laws for 0-, 1-, and 2-complexes are qualitatively similar for $D = 1$ and $D = 2$. In the case $D = 1$ we easily find $E_0(k) = 2t(1 + \cos k)$, $E_1(k)$ —the smallest level of the equation $E_3 - \delta t E^2 \cos^2(k/2) + 64t^3 \cos^4(k/2) = 0$, $E_1 = -2t(\sqrt{5} - 1) = -2.47t$. The single-plaquette approximation for a 2-complex in an odd state with $k = \pi$ gives us $E_2 \approx -2.65t$. We can make the following general assertion: E_m is reached at $k = 0$ for odd values of m and at $k = \pi$ for even values. A Néel state is unfavorable. However, a state of hole bound to a domain wall in a Néel chain has an energy $E \approx -2.85t < E_2$.

In summary, the spin state formed by a hole in the two-dimensional Emery model is greatly different from both a saturated ferromagnetic polaron and a Néel state (a variational estimate of the energy of the latter yields $E_N = -4.36t > E_1$). We could make the rigorous assertion that the total spin S of the ground state is macroscopically smaller than S_{\max} . A deviation from a saturated polaron also arises in the ordinary Hubbard model, but only on a nonalternating lattice.² The best of the regular positions of the spins in the polaron corresponds to an unsaturated ferromagnet.⁹ Its specific magnetization depends on the type of lattice. In our case, in contrast, the difference between S and S_{\max} exists for an arbitrary lattice (including an alternating lattice) and is a consequence of the form of the Hamiltonian \mathcal{H}_h . This circumstance may explain why the ground state of the additional hole is also independent of the type of lattice and is a singlet.³ If this suggestion were to be verified, the Emery model might give a microscopic picture of the formation of a spinless hole: a holon. At the same time, an additional electron would form an ordinary magnetic polaron in this model.

We have learned from a communication from G. V. Uimin that this model has been analyzed independently by A. F. Barabanov, L. A. Maksimov, and G. V. Uimin. We thank them for a discussion, and we thank A. G. Aronov for a useful comment.

¹At $\epsilon \gg U_d$, Hamiltonian (1) reduces to the standard Hubbard model. If $U_p \gg \epsilon$, then \mathcal{H}_{ex} and the term with $i_1 = i_2$ in \mathcal{H}_h are suppressed.

²Incorporating $\psi_1(ij) \neq 0$ in the next coordination sphere reduces the value found for E_1 by 0.15t.

³In the case $D = 1$, the actual ground state is clearly a singlet state.⁸

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