Nonmagnetic spin polaron in a generalized Hubbard model for CuO_2 planes

L. I. Glazman and A. S. Ioselevich

L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR; Institute of Problems of the Technology of Microelectronics and Especially Pure Materials, Academy of Sciences of the USSR

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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 Cu^{2+} 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 Cu^{3+} 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 CuO_2 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 $U_d \to \infty$.

In the Emery model, the Hamiltonian of the holes is

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

where $d^+_{j\sigma}$ and $a^+_{i\sigma}$ 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; $U_p, t_{pd} \ll \epsilon \ll U_d$. For the additional hole we find the new Hamiltonian[1)] $\mathscr{H} = \mathscr{H}_h + \mathscr{H}_{ex}$ from (1) through a unitary transformation[5]:

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

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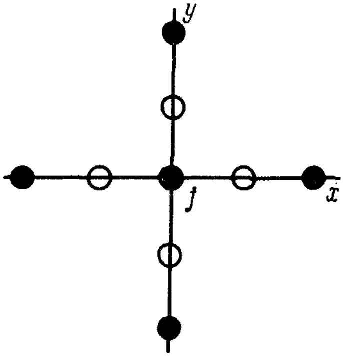

FIG. 1. Fragment of a CuO_2 lattice. ●—Cu; ○—O. For a given j the sites i_1, i_2 in $\langle j i_1 i_2 \rangle$ can be any pair of O sites shown, including coincident sites ($i_1 = i_2$). The lattice constant is $a_0 = 1$.

This Hamiltonian is equivalent to $\mathscr{H}_0$ within $(t_{pd}/\epsilon)^4$. The Hamiltonian $\mathscr{H}_{ex}$ 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 $\mathscr{H}_h$, 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 model[6] 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 polarons[7]), since both the single-site energies and the jump amplitudes depend on the spins in (2).

The state of the Hamiltonian $\mathscr{H}_h$ can be characterized by the total spin $S = S_{\max} - m$, $m \geqslant 0$; 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: $\varphi_m(i, j_1 .. j_{m-1})$ and $\psi_m(i, j_1 .. j_m)$, 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 $\psi_m(i, j_1 ..., j_m)$, 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 $m \geqslant 2$?

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

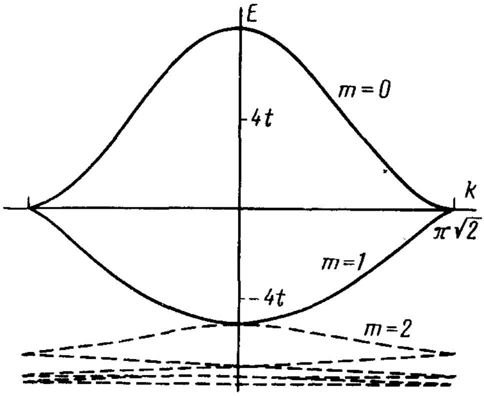

FIG. 2. The dispersion law $E_m(\mathbf{k})$ for $\mathbf{k}$ in the [11] direction. The dashed lines show the suggested form of $E_m(\mathbf{k})$ for $m \geqslant 2$. The plot of $E_m(\mathbf{k})$ in the one-dimensional case is analogous.

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 $\psi_2(ij_1j_2)=e^{i\mathbf{k}\mathbf{k}}\chi(r)$ for $r \geqslant 3$, 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 $\chi(2)/\chi(3)=1+v(Ek)$. 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 $k \geqslant k^*=0.2\pi$. 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, $r_2 \to \infty$ and we have $\delta_2 \to 0$. 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 $r_2 \to \infty$. 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 $k \to k_0$, 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 $\mathscr{H}_h$. 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. Uĭmin 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.

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

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

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

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