Effect of exchange on the behavior of a spin polaron in the Emery model

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The effect of exchange interaction on the behavior of a hole in oxygen in the Emery model of a high-temperature superconductor (HTSC) is considered. It is shown that the spin state produced by the hole may be a purely ferromagnetic polaron only up to a certain (small) energy-normalized jump of the critical value of the exchange constant.

In discussions of the problem of high-temperature superconductivity, much consideration has been given to the study of the magnetic states of the new superconductors.[1] This is linked to the fact that the majority of them are antiferromagnets in the non-superconducting state. The antiferromagnetism is suppressed by alloying; that is, by an increase in the concentration of free carriers. The Hubbard model with strong on-site Coulomb repulsion (U_d large)[2] or the generalized Hubbard model is often used in describing the magnetic characteristics of the new superconductors. In the latter case, the approach of Emery[3] is used as the basic approximation, where an additional hole is responsible for the oxygen O^- state. In Refs. 4 and 5, the behavior of a hole on oxygen was studied in the framework of this model, on the assumption that $\tilde{\varepsilon} = \varepsilon_p - \varepsilon_d > 0$ (ε_p is the energy of the O p-orbital; ε_d is the energy of the Cu^{+2} state). According to the estimate of Ref. 3, $\tilde{\varepsilon} \sim 1$ eV.

The problems of the normal states of the HTSC antiferromagnetic phase have also been discussed, in Refs. 6–8, on the basis of a single-band Hubbard model. In particular, Takahashi[6] analyzed the possibility of the formation in cuprates of a ferromagnetic polaron, the existence of which had long been predicted in Ref. 9. Such a polaron can arise for a finite antiferromagnetic exchange constant because a single hole in a half-filled band polarizes a ferromagnetic medium. The balance between the gain in kinetic and loss in exchange energies determines the size of the polaron. Estimates cited in Ref. 6 give the value ~ 0.25 for the ratio $J/t = 4t/U$ above which the large-radius ferromagnetic polaron does not exist. Assuming for the Hubbard model[6,7] $\bar{t} \sim 0.3$ eV, we find $J \sim 900$ K, which is below the measured constant for La_2CuO_4 ($J \sim 1100$ K).[1] Since the numerical estimate was obtained in Ref. 6 on the basis of qualitative reasoning, it could differ from 0.25. However, computer calculations carried out within the Hubbard model on finite units[10] demonstrated antiferromagnetic correlation and the absence of a polaron for the value of the exchange constant obtained from experiment.[1]

We show below that in the Emery model the region of existence of the spin polaron in J is even more narrow.

In Ref. 4 it was shown that in the atomic limit ($U_d \to \infty$, $J \to 0$) the saturated ferromagnetic polaron is not a ground state of the system (for some types of lattices this is possible even in the standard Hubbard model[11]). The authors of Ref. 4 showed that in the limit $J \to 0$ it is more favorable to form a high-spin complex created by the hole, and in principle a state of unsaturated ferromagnetism is not excluded. For $J > 0$, delocalized states of this type on a ferromagnetic or unsaturated ferromagnetic background lead to loss of exchange energy. For a certain range of values of J, this can lead to formation of a large-radius ferromagnetic polaron.

In this study, we determine the region of stability of the polaron state. We note at once that our chosen trial function for the spin polaron with $J \to 0$ (that is, if the polaron radius grows without bound) describes a ferromagnetic background which is not a ground state of the system.[4] This is undoubtedly a defect of the function. However, for finite J, for which we can expect destruction of the ferromagnetic polaron, it correctly reflects qualitatively the dynamics of its decay. In Refs. 6 and 9, the mechanism of polaron destruction lies in the fact that the state formed by the hole and entirely concentrated in the polaronic ferromagnetic well transforms, as J grows, into a state of the continuous spectrum. However, more precisely, the hole, due to the finite well depth, forms a state the wave function of which contains tails which emerge into the Neel surroundings of the ferromagnetic region. In such a case, a delocalized state arises for small values of J. The ratio of the critical values, J_c, for two possible destruction mechanisms of the large-radius spin polaron is weakly sensitive to the choice of the trial wave function.

The reduced Hamiltonian describing the Emery model for p- and d-states is presented in Refs. 3, 5, 12, and 13 and has the form

$$H \equiv H_t + H_J = \frac{t}{2} \sum_{\langle ii'j \rangle} p_{i\sigma}^{+} (1 + 2\mathbf{S}_j \boldsymbol{\sigma}) p_{i'\sigma'} + J \sum_{\langle i_1 i_2 \rangle} \mathbf{S}_{i_1} \mathbf{S}_{i_2}, \tag{1}$$

where σ_α is the Pauli matrix; $p_{i\sigma}$ is the hole destruction operator on the oxygen orbital; S_j are the spin operators, which are expressed in terms of d_j^{+}, d_j, the creation and annihilation operators for Cu holes.

Proposing, further, to also study the antiferromagnetic state, we rewrite Eq. (1) separating out the summation over the magnetic sublattice of the copper spins alone. Also, we will assign states according to combinations transforming as the irreducible representations of the group D_4. This is achieved by introducing the matrix B:

$$B = {}^1/_2 \begin{pmatrix} 1 & 1 & -2^{1/2} & 0 \\ 1 & -1 & 0 & 2^{1/2} \\ 1 & 1 & 2^{1/2} & 0 \\ 1 & -1 & 0 & -2^{1/2} \end{pmatrix}. \tag{2}$$

Here each column forms a basis for a representation A_1, B_1, E of the group D_4. Ultimately, H_1 takes the following form:

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$$H_t=2t\sum_{j\in A} a_{j\sigma}^{+(1)}(1+2S_j\sigma)\,a_{j\sigma'}^{(1)}+\frac{t}{2}\sum_{\gamma\gamma'\alpha\alpha'}\sum_{j\in A} a_{j\sigma}^{+(\alpha)} \times(1+2S_{j+2\hat{x}-\tau_\gamma}\sigma)\,a_{j+\tau_{\gamma'}-\tau_\gamma}^{(\alpha')}B_{\gamma\alpha}B_{\gamma'\alpha'}, \qquad (3)$$

where

$$a_{j\sigma}^{+(\delta)}=\sum_\alpha B_{\alpha\delta}\tilde{p}_{j\sigma}^{+(\alpha)},\quad \tilde{p}_{j\sigma}^{+}=(p_{j+\hat{y}}^{+},p_{j-\hat{x}}^{+},p_{j-\hat{y}}^{+},p_{j+\hat{x}}^{+}),$$
$$\tau_1=2\hat{x}-2\hat{y},\ \tau_2=4\hat{x},\ \tau_3=2\hat{x}+2\hat{y},\ \tau_4=0.$$

The translation vectors τ are written in units of a, the distance between Cu and O spins.

Writing H_1 in the form of a sum over the sublattice A (with constant $2\sqrt{2}a$) is convenient in that the operators $a_{j\sigma}^{(\alpha)}$ anticommute on different sites of this sublattice; all the $a_{j\sigma}^{(\alpha')}$ in the Hamiltonian run over only the A sites, with the sites of the other sublattices linked only to the spin operators $S_{j+2\hat{x}-\tau_\gamma}$.

In analyzing the hole states we choose a trial function with fixed total spin, so that $[H,S_{\rm tot}]=0$ holds.

We will consider a region in the form of a disk of radius R, containing N_R spins belonging to sublattice A (we choose them to be directed downward). Inside the disk the spins of both sublattices are directed in one sense (ferromagnetic ordering). We further suppose that this region is surrounded by a layer in which the tail of the wave function describing the hole in an antiferromagnetic surrounding is nonzero. The second sublattice interacts with the hole by means of two-spin excitations; that is, excitations connected with the reversal of spins of sublattices A and B. Inside the ferromagnetic region, the single-plaquette approximation[4] for the wave function is used, with an envelope that determines the shape of the polaron for a potential well of the oscillatory type. The tail of the wave function of the Néel background is described by a decaying exponential, which corresponds to the usual behavior of a function outside a well of finite depth. Therefore, we finally obtain for the trial function the expression

$$\psi=N_0^{-1}(\psi_f-\psi_a), \qquad (4)$$

$$\psi_f=\sum_{j\leqslant N_R}\left\{a_{j\uparrow}^{+(1)}(1-z_f)^{1/2}-\frac{z_f^{1/2}}{(1+\alpha_f^2)^{1/2}}\left(a_{j\downarrow}^{+(1)}b_j^+ +\frac{\alpha_f}{2}\sum_{\alpha\gamma}B_{\gamma\alpha}a_{j\downarrow}^{+(\alpha)}b_{j+2\hat{x}-\tau_\gamma}^+\right)\right\}\exp(-|\mathbf{j}|^2x_1)|G\rangle, \qquad (5)$$

$$\psi_a=\sum_{j>N_R}\exp\left[-\frac{x^2}{2}-(|\mathbf{j}|-R)x_2\right]\left[a_{j\uparrow}^{+(1)}(1-z_a)^{1/2}-\frac{z_a^{1/2}}{(1+\alpha_a^2)^{1/2}}\left(a_{j\downarrow}^{+(1)}b_j^+ -\frac{\alpha_a}{4}\sum_{\gamma\gamma'\alpha}B_{\gamma\alpha}a_{j\uparrow}^{+(\alpha)}b_{j+\tau_{\gamma'}-\tau_\gamma}^+b_{j+2\hat{x}-\tau_\gamma}^+\right)\right]|G\rangle. \qquad (6)$$

The operators b_j^+ acting on the state $|G\rangle$ reverse the spin on site j. The vectors $\mathbf{j}$ in Eqs. 5 and 6 are normalized to the lattice constant of A ($2\sqrt{2}a$); the parameters x_1 and x_2 determine respectively the shape of the function in the ferromagnetic region and the rate of extinction of the wave function tail in the antiferromagnetic background, with $x_2^2=2R^2x_1$. The function ψ is normalized to unity; the normalizing constant is equal to

$$N_0^2=(1-\beta+\xi)\xi_0;\quad \xi_0=(N_R/x^2)[1-\exp(-x^2)], \qquad (7)$$

where the parameter β is proportional to the number of boundary spins of the region R:

$$\beta={}^1/_2z_f\xi_s,\ \xi_s=(\pi/N_R)^{1/2}x^2\exp(-x^2)[(1-\exp(-x^2)]^{-1}=(\pi/N_R)^{1/2}\xi(x), \qquad (8)$$

$$\xi=\xi(x,x_2)={}^1/_2\xi(x)\exp(-2x_2)(1+2Rx_2)(Rx_2)^{-2}\times[1+2x_2R/R(1+2x_2R)] \qquad (9)$$

We note that in the Néel environment the second sublattice (B) is affected due to two-spin excitations in ψ_a, created locally by the oxygen hole. The values entering in Eqs. (4)–(9) are determined by the conditions for minimum energy.

The average value of the Hamiltonian in the state of Eq. (4) is equal to

$$\varepsilon=\langle\psi|H|\psi\rangle=\left\{t\left[\varepsilon_f+\varepsilon_a\xi+8a_1\left(\frac{z_f(1-z_f)}{1+\alpha_f^2}\right)^{1/2}+4a_2\left(1-z_a-\frac{\alpha_az_a}{1+\alpha_a^2}\right)+\varepsilon_s\right]+\varepsilon_J\right\}\frac{1}{1+\xi}, \qquad (10)$$

$$\varepsilon_f=z_f-8\left[\frac{z_f(1-z_f)}{1+\alpha_f^2}\right]^{1/2}(1+\alpha_f), \qquad (11)$$

$$\varepsilon_a=4(1-z_a)-8\left[\frac{z_a(1-z_a)}{1+\alpha_a^2}\right]^{1/2}-\frac{4\alpha_az_a}{1+\alpha_a^2}+\frac{\alpha_a^2z_a}{4(1+\alpha_a^2)}, \qquad (12)$$

$$a_2=-\frac{\pi}{8N_R}\xi(x)(1-2Rx_2)\exp(-2x_2), \qquad (13)$$

$$a_1=\frac{\pi x^2}{4N_R}[1+\xi(x)],\qquad \varepsilon_s=\beta(\varepsilon_f+\xi\varepsilon_a)+\xi_sa_s(x_2), \qquad (14)$$

$$a_s(x_2)=3\left\{-\frac{5z_f}{4}+1+2\left[\frac{z_f(1-z_f)}{1+\alpha_f^2}\right]^{1/2}\right\}+\beta_1(x_2)\times\left\{\frac{\alpha_az_a}{1+\alpha_a^2}-1+z_a-2[(1-z_f)(1-z_a)]^{1/2}+\alpha_a\left[\frac{z_fz_a}{(1+\alpha_f^2)(1+\alpha_a^2)}\right]^{1/2}\right\}$$
$$\varepsilon_J=4JN_R. \qquad (15)$$

In the expressions cited, ε_j and ε_a describe the contributions from states formed by the hole on a uniform ferromagnetic or antiferromagnetic background. For small values of J, when, as follows from the criteria above, destruction of the large-radius spin polaron takes place, we find values of the constants z_a, α_a, z_f, α_f by minimizing the energy for a uniform ferromagnetic or Néel spin orientation. This goes along with the single-plaquette approximation.[4] We obtain finally, for the constants given, the values $\alpha_a=0.57$, $z_a=0.82$, $z_f=0.46$ and $\alpha_f=1$. The value of the energy $\varepsilon_f=-5.18$ agrees with the result in Ref. 4 and $\varepsilon_\alpha=-3.32$; ε_J is the exchange energy, in which the largest term in N_R is kept. The term ε_s owes its origin to the presence of the boundary around the ferromagnetic region, while a_1 and a_2 describe bulk effects connected with the form of the polaron wave function. The value of $\beta_1(x_2)$ in Eq. (15) is determined as follows:

$$\beta_1(x_2) = \frac{1}{4\pi R}\sum_{j\tau_\gamma\tau_{\gamma'}} \theta(j_1 - N_R)\exp[-(|j_1| - R)x_2], \qquad (16)$$

where

$$\theta(x) = \begin{cases} 1, & x>0 \\ 0, & x\leqslant 0, \end{cases} \qquad j_1 = j+\tau_\gamma-\tau_{\gamma'} > N_R.$$

The equation that determines x_2, following from the condition that ε be optimized, has the form

$$\begin{aligned} &\omega(x,u)f(1+u)/u^3 - (\pi\delta/N_R)[1+\xi(x,u)] = 0, \\ &f = [1+2u^2/R(1+u)]\exp(-2u/R), \end{aligned} \qquad (17)$$

where

$$\omega(x,u) = \varepsilon_a - \varepsilon_f - 4JN_R + \{z_f[\varepsilon_a(1-\xi) - 2\varepsilon_f]/2(1+\xi) - a_s(u)\}\xi_s - 2.82a_1 + 0.69a_2, \qquad (18)$$

$u = Rx_2$, $a_s(u) = 3.39 - 0.7\ \beta_1(u)/3$, $(\beta_1(0) \approx 3)$, and $\xi(x,u)$ is determined in Eq. 9.

All the numerical coefficients are obtained taking account of the values cited above for the parameters z_{af} and α_{af}. The value of δ is a sum of terms connected with the surface energy [the term in β_1 in Eq. (15)] and the kinetic energy [Eq. (13)]. Here, $\delta = 0.44$.

A feature of Eq. (17) is that it always has a positive solution for u (independent of N_R and x), which decreases with a decrease of the function $\omega(x,u)$. This last is the energy which determines the well depth for a state described by the tail of the wave function of Eq. (6). As $\omega(x,u) \to 0$, such a state becomes delocalized and $x_2 \to 0$. A similar behavior of the solution, in fact, follows from Eq. (17). For $u \gg 1$, when almost all the wave function is concentrated inside the disk of radius R, we get the following expression:

$$u^2 = 4N_R\omega(x,\infty)/\pi\delta, \qquad (19)$$

which decays with a decrease in $\omega(x,\infty)$; that is, the region outside the disk, where $\psi_a \neq 0$, grows. The value of u has been expressed in terms of the natural parameter $N_R\omega = \pi R^2\omega$, the effective well depth for a state described by ψ_a. Destruction of the polaron is connected with this parameter tending to zero (while $R \neq 0$). If $\omega(x,u) \to 0$, then Eq. (17) yields a solution with $u \to 0$:

$$u = (8N_R/\pi\delta)\xi^{-1}(x)\omega(x,0), \quad N_R\omega(x,0) \ll 1. \qquad (20)$$

Since as $u \to 0$ the function ξ grows (tends to ∞), then due to the normalization condition the ferromagnetic part of the wave function decreases and, correspondingly, ψ_a increases; that is, the destruction of the large-radius spin polaron in fact takes place.

Minimizing the energy in x and N_R, we obtain equations that determine the forms and dimensions of the ferromagnetic region:

$$\begin{aligned} &\omega(x,u)N_R\frac{\xi}{1+\xi}\frac{1-\exp(-x^2)}{\xi(x)}\frac{d\xi}{d(x^2)} + \Big[\varepsilon_1(u) \\ &+0.27(1-2u)\exp\Big(-\frac{2u}{R}\Big)\Big]\frac{\xi(x)}{x^2}[1-x^2 \\ &-\exp(-x^2)] + 2.21\Big[1+\xi(x)+x^2\frac{d\xi}{d(x^2)}\Big] \\ &\times[1-\exp(-x^2)] = 0, \end{aligned} \qquad (21)$$

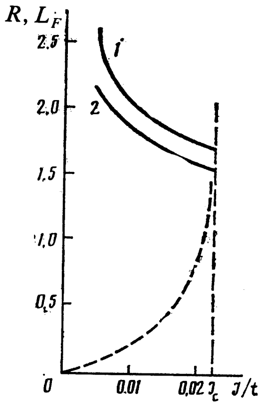

FIG. 1. Dependence of the radii of the ferromagnetic region (R, curve 1) and the ferromagnetic state ($L_F = 2^{1/2}R/x$, curve 2) on the exchange constant J/t. The dashed line shows the qualitative dependence of the parameter $L_a \propto u^{-1}$ on J/t; $J_c = 0.023$. Values on the vertical axis are expressed in units of the lattice constant.

$$\begin{aligned} &-\frac{\omega(x,u)N_R}{(1+\xi)}\xi(x)\exp\Big(-\frac{2u}{R}\Big)(\pi N_R)^{1/2} \\ &+\Big[0.5\varepsilon_1(u) + 0.27(1-2u)\exp\Big(-\frac{2u}{R}\Big)\Big]\xi(x) \\ &+2.21x^2[1+\xi(x)] = 4JN_R^2, \end{aligned} \qquad (22)$$

where

$$\varepsilon_1(u) = \Big[a_s(u) + \frac{z_f}{2}\frac{\varepsilon_f+\varepsilon_a\xi}{1+\xi}\Big](\pi N_R)^{1/2}. \qquad (23)$$

Letting the effective well depth $N_R\omega$ go to zero, we determine the critical value J_c at which destruction of the large-radius ferromagnetic polaron takes place, having solved in this limit Eqs. (21) and (22), together with the condition $\omega(x,u) = 0$. Let us consider that for $u \to 0$

$$\varepsilon_1(0) = [a_s(0) + {}^1/_2 z_f\varepsilon_a](\pi N_R)^{1/2}$$

($a_s(0) = 2.7$) and having substituted in Eqs. (21) and (22) the numerical values of the parameters z_{af}, α_{af}, ε_a, and ε_f, we find numerically the value of J_c (in units of t) and the values of $N_R^c = \pi R_c^2$ and x_c^2 corresponding to it. We finally obtain $J_c = 0.023$, $x_c^2 = 2.2$, and $N_c = 9.1$.

The radius of the hole state in the antiferromagnetic region, $L_a \propto u^{-1}$, grows without bound. In the figure we present the variation of radii of the ferromagnetic state $L_F = \sqrt{2}R/x$ and of the ferromagnetic region R obtained by solution of Eqs. (21) and (22) as a function of J/t. The dashed line describes the qualitative behavior of L_a as $J \to J_c$. The value of J_c found for a choice of $t \approx 1$ eV corresponds to a value $J \approx 200$ K, which is far below the exchange constant characteristic for a HTSC, and also below the value $J_c/t \approx 0.25$ obtained in Ref. 6 on qualitative grounds.

Thus, the analysis carried out shows that in the Emery model, due to the possibility of penetration of a hole into the antiferromagnetic region, it can turn out to be more favorable, for $J > J_c$, to form a delocalized hole state with spin reversal on the copper ions than to preserve a large-radius ferromagnetic polaron, which is linked to a loss of exchange energy. We must note that in the absence of such a mechanism the polaron could still exist. The gain in surface energy leads to a gradual spreading of the wave function of Eq. (6) in the Néel region. The estimates obtained show that the region of values of J for which a large-radius spin polaron is possible is significantly narrower than in the Hubbard model. Therefore, just as in the latter, in the Emery model, apparently, different types of bound states are possible.[6]

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