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"COMB-LIKE" POLARONS AND BIPOLARONS IN HIGH-T_c MATERIALS

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Diagonalization of Hamiltonian composed from d–d exchange interactions between localized d spins of antiferromagnetic cluster and p–d interaction with the spin of carriers indicates a possibility of formation of pure magnetic polarons. The most energetically favorable solution occurs when the carrier density in CuO_2 planes is distributed on every second spin. These "comb-like" polarons have a tendency to bind into pairs (bipolarons) "glued" by the antiferromagnetic medium.

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Conducting electrons in high-T_c superconductors are strongly coupled to the crystal lattice as well as to the system of local spins. As a consequence, the nature of electron pairing is very complicated [1, 2]. Even a consideration of spin interactions alone brings some serious difficulties. Then the main problem is the nature of low-dimensional antiferromagnet (AF) and its response on the effective exchange field caused by carriers (p–d coupling). In this paper we neglect phonon effects and analyze the possibility of a formation of pure magnetic polaron [3, 4]. We show that classical models [3] of AF are not applicable because quantum fluctuations are an essence of the formation of AF polarons and of an AF "glue" [5] which binds AF polarons in Cooper-like pairs. Numerical diagonalization of spin Hamiltonian brings us to the conclusions that: (i) the "comb-like" polarons, i.e., standing wave resulting from an interference of electrons of opposite momenta, where the electron density is localized on every second spin, are characterized by the largest energy of AF polaron formation; (ii) the induction of the local staggered magnetization to which the carrier spin is coupled is ruled out by the quantum fluctuations of AF; (iii) formation of bipolarons can be treated as resulting from an effective indirect Heisenberg exchange between carriers via the AF medium; (iv) the material parameters, which are characteristic of CuO_2 based high-T_c superconductors, are beyond the limit of linear response, the pairing energy is of the order of d–d coupling for small clusters and it vanishes with an increase in the size of AF cluster (AF coherence range). Because of that we postulate that the short AF order is the necessary condition for superconducting phase [6].

Here we examine Hamiltonian, which is a sum of terms describing d–d interaction between localized d-spins in a finite 1D or 2D AF system and the p–d interaction of AF with p carriers

$$\widehat{H} = 2J_{d-d}\sum_{i=1}^{N} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \sum_{i=1}^{N} J_{p-d}(i)\boldsymbol{S}_i \cdot \boldsymbol{\sigma}, \tag{1}$$

where J_{d-d} and J_{p-d} are the exchange constants, which we treat as phenomenological parameters, $\boldsymbol{S}$ is the operator of d-spin, and $\boldsymbol{\sigma}$ — of the carrier spin. We assume that the value of J_{p-d} is proportional to a density of carrier distribution on localized spin i: $J_{p-d}(i) = N_0\alpha|\Psi_{\mathrm{e}}(i)|^2$. Since the sum of carrier density over every elementary cell is normalized, $\sum|\Psi_{\mathrm{e}}(i)|^2 = 1$, the parameter $N_0\alpha$ is equal to the sum of every J_{p-d} constant and it describes the total strength of p–d coupling. We omit a kinetic as well as Coulomb repulsion energy which have to be considered independently basing on the shape of the carrier distribution. The calculations were carried out strictly for finite systems of spins using the Lanczos method of diagonalization. We examine various carrier distributions and different size of AF clusters. Particularly, we probe the class of standing waves $|\Psi_{\mathrm{e}}(i)|^2 = g(ia_0)\cos^2(kia_0 + \phi)$, with an envelope $g(r)$. Inset (a) in Fig. 1 shows the most energetically favorable "comb-like" density of electron distribution. This conclusion results from the inset (b) in Fig. 1 where the polaron susceptibility $\chi_p = 2\Delta E_{\mathrm{ex}}(1e)/(N_0\alpha)^2$ as a function of carrier wave vector, k has a pronounced maximum at $k = \pi/2a_0$. In the latter formula $\Delta E_{\mathrm{ex}}(1e)$ is a gain of energy due to formation of AF polaron defined as the difference between the energy of the ground state of unaffected AF cluster and of the cluster coupled to a carrier. In Fig. 1 the polaron susceptibility for $k = \pi/2a_0$ is plotted as a function of the inverse size of the cluster. The susceptibility decreases with an increase in the number of spins M. It tends, however, to a finite value $\chi_p = (0.135 \pm 0.005)/J_{d-d}$, when extrapolating the infinite AF chain.

The detailed analysis of polaron energy structures and spin correlators shows that the character of the magnetization is different for various k-vectors. For homogeneous distributions ($k = 0$), the only mechanism of polaron formation is breaking of AF coupling and formation of a net magnetic moment. At the maximum of the susceptibility, in turn, the induction of the staggered magnetization is of the Van Vleck type — the perturbation admixes excited states to the ground doublet ($S^* = 1/2$), inducing the staggered moment (see dashed line in Fig. 2a). The fact that the staggered susceptibility is of finite value reflects a pure quantum character of such magnetization. In the absence of quantum fluctuations the susceptibility should diverge.

The "comb-like" polaron (Fig. 1a) acting on every second local spin d induces the staggered moment, i.e., polarizes also the second sublattice which is not affected by this polaron. Because of that another "comb-like" carrier with the opposite spin, which acts on another set of local spins, can be easily bound. In Fig. 2a the energy structure of such bipolaron is plotted. The ground state is a singlet ($S^* = 0$) and the first excited state is a triplet ($S^* = 1$). The singlet corresponds to the antiparallel, while triplet to parallel orientation of the carrier spins, $\boldsymbol{\sigma}$. Because of that, one can say that two carriers are effectively coupled by a Heisenberg

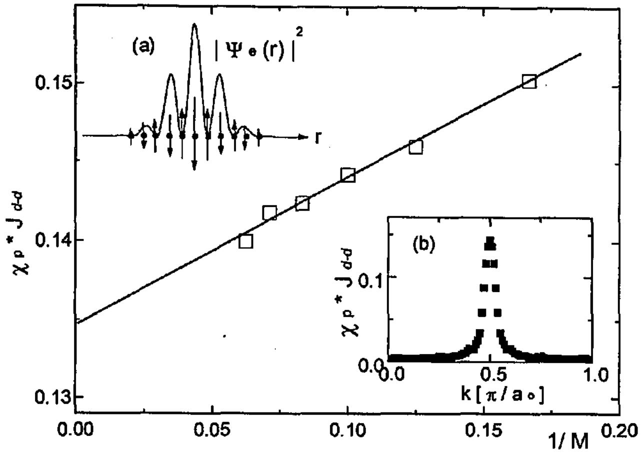

Fig. 1. Polaron susceptibility (normalized by J_{d-d}) as a function of the inverse size of AF cluster M (expressed in number of spins). Insets show: (a) the most energetically favorable shape of polaron — "comb-like" polaron, (b) the polaron susceptibility as a function of wave vector k for $M = 14$.

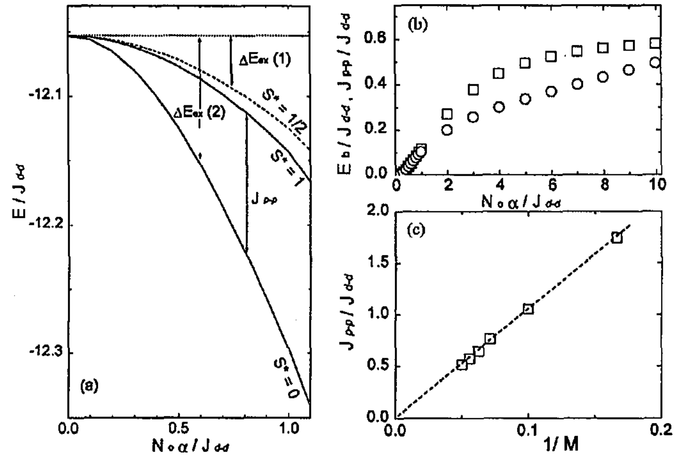

Fig. 2. (a) The energy of the ground state of the "comb-like" magnetic polaron (dashed line) and of two first levels of bipolaron (solid line) which are bound to AF chain of the size $M = 14$ spins as a function of $N_0\alpha$, dotted line is the energy of unaffected AF; (b) the energy of bipolaron formation, E_b (circles), and 3/4 of the effective exchange coupling, J_{p-p} (squares), as a function of $N_0\alpha$; (c) J_{p-p} as a function of inverse size of AF cluster M.

exchange $J_{p-p}\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}$, where AF is a medium which transfers this indirect exchange. The exchange coupling, J_{p-p}, increases with the square of p–d coupling, $N_0\alpha$, for a weak strength, when $N_0\alpha < J_{d-d}$ and it saturates for a larger strength. In Fig. 2 the dependence of the effective electron–electron exchange coupling (actually 3/4 of J_{p-p}) is compared to the binding energy E_b of two "comb-like" polarons, defined as the difference of the energy gain of bipolaron, $\Delta E_{ex}(2e)$ reduced by the double energy gain of monopolaron, $2\Delta E_{\mathrm{ex}}(1e)$. For a weak strength of p–d coupling, E_{b} and $(3/4)J_{p-p}$ are equal showing that the indirect exchange via AF cluster is the only mechanism of bipolaron formation.

With an increase in p–d coupling, when $N_0\alpha > J_{d-d}$, the polaron and the bipolaron energies saturate. In particular, the energy of the pairing E_{b} and of electron–electron effective exchange, J_{p-p}, saturate at value close to J_{d-d} (as shown in Fig. 2b). Because in $\mathrm{CuO_2}$ based high-T_{c} superconductors J_{d-d} is of the order of 70 meV, while the total p–d strength $N_0\alpha$ is an order of magnitude larger, the gain of the magnetic energy due to formation of "comb-like" bipolaron is of the order of J_{d-d}. Thus E_{b} is comparable to the kinetic energy of electrons with $k = \pi/2a$ and larger than electron–electron repulsion energy. The "comb-like" bipolaron is characterized by the most important attributes of Cooper-like pair of d-symmetry: (a) it is a spin singlet, (b) it is formed from electronic states of opposite momenta, (c) only electrons with characteristic k-vectors (AF pocket) can form such pair, so a d-like anisotropy of binding energy is expected.

In Fig. 2c we plot the dependence of the effective exchange coupling J_{p-p} for very strong p–d coupling as a function of size of AF chain. In contrast to the behavior in the case of small $N_0\alpha$ for the strong p–d coupling the energy of polaron pairing vanishes with an increase in the cluster size (compare the data in Fig. 1b and Fig. 2). It brings us to the conclusion that the short AF coherence range, corresponding to the cluster size in our calculations, is the necessary condition for the efficiency of the AF "glue" [5].

In the insulating phase of underdoped $\mathrm{CuO_2}$ planes AF order is destroyed by carriers [6], but it is of a spin glass character. The AF correlation range is short, but the spin coherence range is long, which precludes the pair formation. In the metallic phase the spin coherence is strongly reduced and becomes comparable with the AF correlation range. Thus a transition from insulator to metal is the another necessary condition allowing the formation of magnetic bipolaron. The postulated by us mechanism of metal–insulator transition, however, differs from the Mott transition by the fact that an extra energy gain due to pairing takes place.

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