New type of antiferromagnetic polaron and bipolaron in HT$_c$ - superconductors

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Abstract:
The possibility of formation of a new type of polaron based on the quantum antiferromagnet (AF) model is reported. We take into account exchange interactions between localized $d$-$d$ spins of the AF, as well as the $p$-$d$ interaction of the AF with $p$-carriers. The energy minimum is found when maximum charge density occurs on every second spin. The formation of such “comb”-like polarons results from the damping of quantum fluctuations and the appearance of Van Vleck-like staggered magnetization. Such polarons tend to form pairs coupled by an AF “glue”.

There are some convincing arguments that occurrence of small polarons and bipolarons is responsible for the formation of a Bose liquid in HT$_c$-superconductors [1, 2]. The mechanism of polaron and bipolaron formation, however, still remains an open question. Theoretical models of this effect invoke the phonons, excitons, plasmons as well as a magnetic “glue” [3, 4].

In this paper we show that the spin exchange interactions alone can lead to the formation of magnetic polarons. Moreover, a specific type of magnetic polarons, called by us the “comb-like” polarons, is characterized by a strong tendency for pair formation. For CuO$_2$-based superconductors their binding energy is comparable to $d$-$d$ coupling, $J_{d-d}$, i.e., of the order of 7.5 meV. We solve numerically the spin Hamiltonian which contains the term of $d$-$d$ coupling between neighboring $d$-spins within the antiferromagnetic (AF) cluster, $2J_{d-d} \mathbf{S}_i \cdot \mathbf{S}_j$, and the term of $p$-$d$ exchange between the $p$-carrier and the $d$-spins, $J_{p-d}(i) \mathbf{S}_i \cdot \sigma$. The $p$-$d$ exchange constants $J_{p-d}(i)$ are assumed to be proportional to the carrier density at the $i$-th spin. The normalization condition of the carrier wave function guarantees that the sum of $J_{p-d}(i)$ does not depend on the distribution, but is equal to a parameter $N_\sigma \alpha$ which describes the strength of the $p$-$d$ coupling. We examine various polaron shapes.

We found “comb-like” polarons, where the electron density is distributed on spins from only one of Neel sublattices, as the most energetically favorable (see
Figure 1: (a) Spatial distribution of carrier density in a “comb-like” bipolaron; (b) Spin polarization of localized $d$-spins, $S_i$, as seen by the carrier $p$-spins, $\sigma$. The staggered magnetization caused by a “comb-like” monopolaron has a similar character, but a smaller amplitude.

The total magnetic moment of such polaron, $S^*$, is equal to $1/2$ and does not change with an increase of $p$-$d$ coupling. The net magnetic moment of $d$-spins remains zero but, because of a nonvanishing correlation between $p$ and $d$-spins, an energy gain due to $p$-$d$ coupling occurs. The correlators $\langle \sigma | S_i \rangle$, i.e., the polarization of $d$-spins seen by the carrier spin, is shown in Fig. 1(b). For a weak $N_o\alpha$ this staggered magnetization increases linearly with $N_o\alpha$. Then the energy gain originating from $p$-$d$ coupling, $\Delta E_{1e}$, increases with the square of $N_o\alpha$, reflecting Van Vleck character of the AF magnetization (see dashed curve in Fig. 2). The induction of the staggered magnetization is related to stabilization of quantum fluctuations of the AF cluster. In the inset in Fig. 2 the energy gain, $\Delta E_{1e}$, is plotted as a function of inverse size of the AF chain. An extrapolation to large size shows that the energy gain tends to a constant value.

The quadratic dependence of $\Delta E_{1e}(N_o\alpha)$ shows the possibility of formation of polaron pairs. In Fig. 2 the energy of the ground singlet, $S^* = 0$, and the first excited triplet of the bipolaron, $S^* = 1$, are shown. The binding energy $E_b$ of such a pair is equal to $\Delta E_{2e} - 2 \Delta E_{1e}$. For a weak $p$-$d$ coupling, $E_b$ is equal to $3/4$ of the singlet-triplet energy distance $J_{p-p}$. The $p$-spins are anti-
ferromagnetically correlated at the singlet, and ferromagnetically at the triplet state. Thus, one can conclude that two carrier spins are effectively coupled by an indirect Heisenberg exchange, $J_{p-p} \sigma \cdot \sigma$, where the AF cluster plays a role of a “glue”.

In CuO$_2$-based superconductors, however, $N_0\alpha \approx 10 J_{d-d}$. As a consequence, the linear response approximation fails. The energy gains, the binding energy, and the $p-p$ exchange all saturate. In the inset in Fig. 2 the saturation value of $J_{p-p}$ is plotted. For a small cluster size it is of the order of $J_{d-d}$, i.e., it is comparable or greater than the binding energy caused by the phononic effect. With an increase of the cluster size the parameter $J_{p-p}$ tends to zero. This allows us to conclude that a short AF coherence range (observed in HTc–materials) is the necessary condition for the existence of an AF “glue”.

Figure 2: Energy levels of the polaron (dashed) and of the bipolaron (solid curves) as a function of $p-d$ coupling $N_0\alpha$. The inset shows the dependence of the energy gain of the polaron, $\Delta E_{1e}$, for a small $N_0\alpha$, and the effective indirect exchange, $J_{p-p}$, between carrier spins in the bipolaron for very large $N_0\alpha$ as a function of inverse cluster size.
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