Magnetic polarons in weakly doped high-$T_c$ superconductors.

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We consider a spin Hamiltonian describing $d$-$d$ exchange interactions between localized spins $d$ of a finite antiferromagnet as well as $p$-$d$ interactions between a conducting hole ($p$) and localized spins. The spin Hamiltonian is solved numerically with use of Lanczos method of diagonalization. We conclude that $p$-$d$ exchange interaction leads to localization of magnetic polarons. Quantum fluctuations of the antiferromagnet strengthen this effect and make the formation of polarons localized in one site possible even for weak $p$-$d$ coupling. Total energy calculations, including the kinetic energy, do not change essentially the phase diagram of magnetic polarons formation. For parameters reasonable for high-$T_c$ superconductors either a polaron localized on one lattice cell or a small ferron can form. For reasonable values of the dielectric function and $p$-$d$ coupling, the contributions of magnetic and phonon terms in the formation of a polaron in weakly doped high-$T_c$ materials are comparable.

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I. INTRODUCTION

The role of electron phonon and spin exchange in the formation of polarons, bi-polarons and stripes in CuO$_2$ based high-$T_c$ materials has been a matter of extensive discussion from the very moment high-$T_c$ superconductors were discovered. Experimental observations of the anomalous isotope effect[20] could indicate the role of phonon interactions in the formation of the superconducting state. On the other hand, angularly resolved photoemission[21] (ARPES), transport and tunneling microscopy measurements[22] show $d$-symmetry of the order parameter indicating an important role of exchange. Although some authors underline the role of both mechanisms[23], the solution of full Hamiltonian is complicated and these contributions are usually calculated separately.

The concept of the phonon polaron was introduced by Pekar[24] and Fröhlich decades ago and was adopted to high-$T_c$ superconductors by Alexandrov and Mott[25]. The energy of phonon coupling for high-$T_c$ is estimated to be of the order of a fraction of eV. In another work, Alexandrov[26] proposed that the narrowing of $d$-electron band by the polaron effect and the formation of phonon bipolarons increases the critical temperature to $T_c \approx 100$ K. However, because of the dominant contribution of $d$-symmetry to the order parameter of high-$T_c$ superconductors, exchange interactions are the most often considered ones recently. The modeling of such interactions is difficult because it is necessary to include the role of conducting ($p$) holes as well as localized ($d$) electrons.

In the case of weak $p$-$d$ couplings a linear response of the antiferromagnet (AF) can be assumed. Hence, a phenomenological model of magnetic susceptibility introduced by Millis, Monien, Pines[27] (MMP) can be used.

Zhang and Rice[28] in turn, describe the case of strong hybridization between the $3d$ states of Cu and $2p$ states of O. When the hybridization is much greater than the kinetic energy of the carriers, it is possible to limit the description to the ground singlet state, and in such a case a one band model can be used. This model (called $t$-$J$) is at present the most often used to describe the cuprate superconductors (for a review see[29]). Unfortunately, different techniques of approximations lead sometimes to contradictory solutions of $t$-$J$, as it is in the case of the stripe formation[30]. Also, the dynamics of spin polaron in the framework of $t$-$J$ model was extensively investigated by many authors[31].

However, the spin-fermion model[32], which treats separately the spin of $p$-carrier and $d$-localized spins, seems to be the most appropriate for the case of intermediate $p$-$d$ coupling typical for high-$T_c$ superconductors. Most papers treat the $p$-$d$ interaction as a Kondo exchange. Such an approach allows to show the tendency of stripes to stripe phase formation or $d$-wave pairing. Recently, Balá et al.[33] extended the spin-fermion model starting from the three band Hubbard model. They introduced $p$-$d$ coupling, which is much more complicated than Kondo one, i.e. some exchange couplings between Cu ion and two neighboring oxygen atoms appear. They have considered the formation of magnetic polaron in such a model[34]. They identified all the spectrum of energy states of Zhang-Rice polaron[35] in ARPUS experiments. They found a solution using self-consistent Born approximation (SCBA). However, a comparison of SCBA and exact diagonalization techniques for spin-fermion model has not been carried out yet.
The present paper reports for the first time on calculations of a simple spin-fermion model with exact diagonalization technique for spin Hamiltonian. It broadens the possible range of solutions. The spin-fermion model allows to investigate the cases of strong and intermediate \( p-d \) coupling. Thus a comparison of the phonon and magnetic contributions to the formation of a polaron in weakly doped high-\( T_c \) superconductors for a wide range of parameters is possible. The magnetic exchange interactions are calculated strictly while the phonon contribution is evaluated in the framework of the Fröhlich theory.

In Section 2, we describe the Hamiltonian and the method of finding the ground and excited states of the system. In Section 3, the exchange spin interactions are calculated strictly while the phonon contribution is evaluated in the framework of the Fröhlich theory.

We study a system which consists of spins localized on the \( d \)-shells and mobile \( p \)-like holes. The localized spins are treated within the quantum antiferromagnet model, i.e. none of the Neel sublattices are chosen a priori. We consider finite one- (1D) and two- dimensional (2D) clusters as well as the infinite system. The latter is simulated using periodic boundary conditions (PBC) and an extrapolation to an infinite size. The spin interactions in the system and the kinetic energy of the \( p \) hole is described by the Hamiltonian:

\[
H = 2J_{dd} \sum_{<i,j>} S_i S_j + \frac{1}{2} J_{pd} \sum_{i,\alpha,\beta} S_i c_{i\alpha}^+ \sigma_{\alpha\beta} c_{j\beta} + t_{ij} \sum_{i,j,\alpha} c_{i\alpha}^+ c_{j\alpha},
\]

where \( S_i \) is the effective spin of the nine core \( d \)-electrons (3d\( ^9 \)), the summation was taken under the pairs of neighboring spins \( <i,j> \), \( \sigma_{\alpha\beta} \) are the Pauli matrices of the carrier spin \( s \), \( J_{pd} \) is the Kondo parameter normalized to the volume of elementary cell, \( J_{dd} \) is the exchange integral between \( d-d \) spins, \( t_{ij} \) is the hopping matrix element to the neighbor, \( c_{i\alpha} \) are the operators of creation and annihilation of a hole on the \( i \)-th site, with the projection of spin 1/2 on the quantization axis equal \( \alpha \) respectively. We look for the eigenstates of the Hamiltonian (1) in the form of the product of the orbital wave vector, \( \Psi \), and the spin state vector of local and carrier spins \( X_S \):

\[
\Psi \cdot X_S.
\]

In the space of the single hole occupation at antiferromagnet (AF) sites \( i = 1, ..., N \)

\[
\Psi = \sum_i \varphi(i) u_i,
\]

where \( u_i = |0,0,...,1,0,0...| \) is the occupation vector of the hole at \( i \)-th site and \( \varphi(i) \) is the corresponding probability amplitude. We use the variational method of solving the eigenproblem. We treat \( \Psi \) as the trial function, which is normalized by the condition:

\[
\sum_i |\varphi(i)|^2 = 1.
\]

For \( \Psi \) given by Eq. (2) the diagonalization of the kinetic and exchange terms of Hamiltonian (1) can be done separately.

\[
H' = \langle \Psi | H | \Psi \rangle = T + H_x.
\]

The kinetic energy, \( T \), does not depend on the spin state \( X_S \) and can be easily evaluated from the probability amplitude of the carrier \( \varphi(i) \):

\[
T = z |t_1| - 2 |t_1| \sum_{<i,j>} \varphi(i) \varphi(j),
\]

if only the hopping to the nearest neighbors (NN), \( t_1 \) is considered, and \( z \) is the number of NN. The term \( z |t_1| \) has been added to have zero kinetic energy for fully delocalized states. Calculations of the exchange energy need diagonalization of the spin Hamiltonian:

\[
H_x = 2J_{dd} \sum_{<i,j>} S_i S_j + \sum_i j_{pd}(i) S_i S_i.
\]

Here \( s \) is the spin operator of the carrier spin and the \( p-d \) exchange integrals are given by

\[
j_{pd}(i) = J_{pd} |\varphi(i)|^2.
\]

We use Lanczos method of diagonalization of the spin Hamiltonian (7). Diagonalization of matrices for AF cluster with \( N \leq 20 \) is possible with the PC computer. For larger clusters the calculation time increases rapidly.

A detailed study of quantum coupling between spins within the polaron in an AF medium is the main goal of the paper. We focus our analysis on the gain \( E_{ex} \) of the spin exchange energy. \( E_{ex} \) is the difference between the energy of the ground state of the unperturbed AF \( E_{dd} \)
formed. Their energy is given by:

$$E_{\text{ex}} = E_{dd}^0 - (E_{dd} + E_{pd}).$$  

(9)

In this way, we analyze the zero temperature case only. We found that for a weak $p-d$ exchange the gain $E_{\text{ex}}$ is a half of the $p-d$ coupling energy, $E_{\text{ex}} = -E_{pd}/2$.

The Hamiltonian includes neither effects of external magnetic field nor any other terms which could lead to the symmetry breaking and to the formation of Neel sublattices. As a consequence, the mean values of the magnetic moments of each spin of this system are exactly equal zero. Because of this, we describe the spin structure of the antiferromagnetic polarons (AFP) and the mechanism of the magnetic polaron formation by means of correlators between spins of AF $\langle S_s S_s \rangle$ and between the AF spin and that of an additional hole $\langle sS_i \rangle$:

$$\langle sS_i \rangle = (X_S sS_i | X_S).$$  

(10)

The assumption that the wave function can be described by Eq. 2 is simplified. In general, the total wave function is a linear combination of wave functions given by Eq. 2. In particular, because polarons localized on two Neel sublattices are equivalent, at least the combination of the pair of such states should be considered. This problem is discussed in section IIIG.

Hamiltonian (1) does not contain a phonon term. In general, the coupling of the carrier to the lattice polarization and the exchange interactions act together to form the polaron. The phonon term is treated in Section 5 within the simplest possible approach. It is calculated from the Fröhlich interaction with optical phonons. It is known that in the range of parameters typical for high-$T_c$ superconductors small phonon polarons are formed. Their energy is given by:

$$E_{\text{ph}} \approx \frac{qD\epsilon^2}{\pi \kappa},$$  

(11)

where $qD = \left(\frac{2\pi \hbar}{v_F}\right)^{1/3}$ is the Debye momentum, $\frac{1}{\kappa} = \frac{1}{\varepsilon} - \frac{1}{\varepsilon_0}$; $\varepsilon, \varepsilon_0$ are dynamic and static dielectric constants respectively, and $e$ is the electron charge.

III. SPIN STRUCTURE OF MAGNETIC POLARONS

We examine various types of trial functions $\varphi$. Depending on the size and shape of the carrier distribution, $|\varphi|^2$ (Fig. 1), as well as on the value of exchange constants (Fig. 2) various types of magnetic polarons with very different spin structures can be found.

A. Large AFP. Its size $r'_p$ is much greater than the lattice constant $a_0$ and the antiferromagnetic correlation range $\xi$. Thus, it can be described within the theory of the linear response. For very large polarons the local magnetization $M(r)$ becomes proportional to the local carrier density.

B. Medium AFP. Its size $r'_p$ is comparable or smaller than $\xi$, but bigger than 0.5$a_0$ (see Fig. 1). The induced polarization is of staggered character, and the carrier interacts with few local spins of different orientation.

C. Small AFP It is localized within a single elementary cell. For very strong $p-d$ coupling it corresponds to the Zhang-Rice polaron.

D. Ferron. It forms when the $p-d$ exchange is strong enough to break AF bonds and to induce a local magnetic moment.

E. Comb like AFP It is the case when the carrier is distributed on one Neel sublattice only. The staggered polarization is the dominant response of the AF medium.

The clear difference between AFP of different sizes.
function $\phi$ which describes the ratio of different magnetic polarons as a function of $J'_{pd}$. $E_{ex}$ for a small AFP were obtained for a 1D chain with PBC (open circles) and for a 2D $4 \times 4$ square with PBC (filled circles). $E_{ex}$ for a trial function evenly distributed on all AF spins are shown by open and filled squares for a 1D chain with PBC and 2D $4 \times 4$ with PBC respectively. Results for a trial function distributed on two neighbor AF spins and a 1D spin, was used to calculate almost all curves. The curve plotted by triangles, however, was calculated using another trial function, and it represents the formation of a comb-like AFP. It will be discussed in part III E.

The calculations were performed for weak $p$-$d$ coupling for 1D and 2D AF clusters. The number of AF bonds has been assumed to be twice as big for 2D as for a 1D cluster, where the number of ligands is two times smaller. To compare the results for 1D and 2D clusters we introduce the following quantity, $J'_{pd} = J_{pd}/(2zJ_{dd})$, which describes the ratio of $p$-$d$ to $d$-$d$ coupling normalized by the number of AF bonds, $2z$. Ratio of the $p$-$d$ to the $d$-$d$ exchange energies defined this way is the same for 1D and 2D AF clusters. Moreover, $J'_{pd} \ll 1$ describes the range of weak $p$-$d$ coupling, while $J'_{pd} > 1$ that of strong $p$-$d$ coupling, independent of the dimension of the AF cluster. $J'_{pd}$ is set 1/4 in Fig. 1. Here the small AFP corresponds to $r'_p < 0.4a_o$, medium to $0.4a_o < r'_p < a_o$, and large to $r'_p > a_o$. The dependence of $E_{ex}$ on the chain length is shown in the inset. The linear dependence of the $E_{ex}$ on the inverse AF cluster size $1/N$ makes the extrapolation to an infinite chain possible. The extrapolated values of $E_{ex}$ are shown by full circles in Fig. 1.

The results of calculations for small and medium AFP in the 1D case are reasonable even without extrapolation to infinite clusters. Because of that, we assume that also for the 2D case the energy of small and medium polarons can be found with reasonable accuracy. Unfortunately, because of computational limitations, we can not carry out full extrapolation for large AFP in 2D clusters.

A comparison of numerical results for open chains and chains with PBC shows that the use of PBC does not lead to an improvement of the convergence of numerical results with the cluster size. In part, this is an effect of the normalization condition given by (Eq. 4) and of specific properties of the dangling spins at the cluster border.

### A. Large AFP

The numerical results, with the characteristic dependence of the $E_{ex}$ decreasing as $1/r'_p$ for 1D AF, can be approximated by an analytical solution in which the magnetic susceptibility of AF is described by two phenomenological parameters. The analytical solution gives a better description of large AFP while the comparison with the numerical results allows to explain the physical meaning of the phenomenological parameters.

For simplicity in the analytical approximation, we use an exponential distribution of carrier density, $|\varphi'(r')|^2 = \frac{2}{r'_p} \exp(-|r' - r_0|)/r_p$, where $r_0$ is the center of the density distribution and $r'_p = 2r^2_p$. We assume that the susceptibility in wave vector space can be described by the phenomenological formula introduced in the MMP model: $\chi(q) = \chi_{q_0} \frac{1}{1/(q - q_0) - \xi}$, where $q$ is the wave vector, $q_0 = \pi/a_o$ and corresponds to the staggered magnetization. The phenomenological parameters $\chi_{q_0}$ and $\xi$ describe the staggered magnetic susceptibility and the spin correlation length, respectively. An effective field corresponding to $\varphi(r')$ is $H_{eff}(r') = H_{eff}(a_o) \exp(-|r' - r_0|/r_p)$. Within the model of continuous media, an effective field acting at a point $r'$ results in magnetization $M(r) = \int dr' \chi(r - r')H_{eff}(r')$ at the point $r$. Such an approach takes into account the non-local effects of correlated systems but neglects the atomic structure of AF. For large AFP, i.e. for $r_p \gg \xi$, $M(r)$ takes a simple form:

$$M(r) = \frac{J_{pd}a_o\chi_{q_0}}{16\pi^2 g\mu_B^2 \xi^2 g_0 r_p} \exp\left(-\frac{|r - r_0|}{r_p}\right). \quad (12)$$

[FIG. 2: The exchange energy gain, $E_{ex}$, from formation of different magnetic polarons as a function of $J'_{pd}$. $E_{ex}$ for a small AFP were obtained for a 1D chain with PBC (open circles) and for a 2D $4 \times 4$ square with PBC (filled circles). $E_{ex}$ for a trial function evenly distributed on all AF spins are shown by open and filled squares for a 1D chain with PBC and 2D $4 \times 4$ with PBC respectively. Results for a trial function distributed on two neighbor AF spins and a 1D spin, was used to calculate almost all curves. The curve plotted by triangles, however, was calculated using another trial function, and it represents the formation of a comb-like AFP. It will be discussed in part III E.]

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Thus $M(r)$ induced by a large AFP is smooth and described by the same spatial dependence as the carrier density. In the icon in Fig. 1, the correlators between the carrier spin, $s$ and the consecutive local spins, $S_i$, for a large AFP are presented. They also show that for a large AFP the induced magnetization is smooth and proportional to the carrier density. In that sense the analytical solution is equivalent to the numerical one. $E_{xx} = 1/2E_{pd}$ for a large AFP and it takes a simple form:

$$E_{xx} = \frac{(J_{pd}a_0)^2\chi_{q_0}}{256\pi^2 (g\mu_B)^2 \xi^2 q_0^2 r_p}.$$  \hspace{1cm} (13)

The absolute value of $E_{xx}$ and its dependence on the $d$-$d$ exchange and on the correlation length cannot be analyzed within the discussed phenomenological approach. However, an evaluation of $E_{xx}$ can be done by numerical calculations. If one attributes the correlation length to the cluster size, then the comparison of Eq. (13) with the numerical result, showing that the energy gain is almost independent of the chain length (see inset to Fig. 1), leads to the conclusion that $\chi_{q_0} \propto \xi^2/J_{dd}$ for a large 1D polaron. We found out that the character of the obtained dependencies does not change if a Gaussian trial function was applied.

In the 2D case, the results of numerical integration for large AFP in a 2D system are characterized by a faster decrease of $E_{xx}$ with the polaron size in comparison to the 1D case. The energy scales with $1/r_p^2$ instead of $1/r_p$.

To summarize, the large AFP is characterized by a smooth magnetization of the antiferromagnet, proportional to the carrier density. Because for a 2D polaron $E_{xx}$ and the kinetic energies scale with the inverse square of the polaron size, two scenarios are possible: (i) no polaron can be formed when $T > E_{xx}$, or, in the opposite case, (ii) the minimum of the total energy occurs for the polaron radius tending to zero (see also Fig. 6). In that case, however, it is no longer a large polaron and a different approximation should be considered.

### B. Medium AFP

As it is shown in Fig. 1, with a decrease of $r_p$, $E_{xx}$ does not follow the $1/r_p$ dependence, but for $r_p < a_0$ a sharp increase of $E_{xx}$ is seen. For 1D the increase of $E_{xx}$ ~ 10, as compared to the extrapolated $1/r_p$ dependence, and for 2D is even bigger. The rapid increase of $E_{xx}$ shows that the medium AFP has a tendency to localization. The decrease of $r_p$ is also accompanied by a change of the character of induced magnetization in the AF medium. As it is shown by icons in Fig. 1, numerical calculations predict a smooth magnetization for $r_p > a_0$ but a staggered one for $r_p < a_0$.

For a weak $p$-$d$ coupling, $E_{xx}$ increases with the square of $J_{pd}$ (see filled triangles in Fig. 2). However, calculations show that for $J_{pd} > 1$ a more complex mechanism occurs. The AF bonds broke and a ferromagnetic-like polaron forms. The details are described in part IID.

### C. Small AFP

When the polaron radius becomes comparable to the size of the elementary cell, $E_{xx}$ saturates. The plateau in Fig. 1 corresponds to the case when the polaron is localized in a single elementary cell, i.e. $r_p < a_0$. The numerical results weakly depend on the size of AF cluster and on boundary conditions. The magnetization induced by the small AFP is similar to that of the medium AFP, as it is shown by icons in Fig. 1.

A dependence of the numerically calculated $E_{xx}$ on the normalized ratio $p$-$d$ to $d$-$d$ exchange $J_{pd}$ is shown by circles in Fig. 2. There is no considerable difference between 1D and 2D cases. For a weak $p$-$d$ coupling...
The correlator \(\langle sS_0 \rangle\) between the carrier spin, \(s\), and AF spin on which the carrier is localized, \(S_0\), is shown in Fig. 3a. In the range of weak \(p-d\) couplings, the magnetization of the local spin, as seen by the carrier spin, \(\langle sS_0 \rangle\), increases linearly and saturates for the strong \(J'_{pd}\). This corresponds to quadratic and linear dependence of \(E_{xx}\) versus \(J'_{pd}\), respectively. For a strong \(J'_{pd}\), the correlator \(\langle sS_0 \rangle = -3/4\) that means AF spin is compensated by the spin of a carrier.

The icons in Fig. 3a show the correlators between the carrier spin \(s\) and the consecutive \(d\) spins of AF chain for different \(J'_{pd}\). It is seen that a small polaron induces a staggered magnetization within the AF correlation range, \(\xi\). But the amplitude of \(\langle sS_0 \rangle\) varies with \(J'_{pd}\). The increase of the correlator \(\langle sS_0 \rangle\) is accompanied by a reduction of the correlators between the carrier spin and other \(d\) spins. Also, the correlator of the spin \(S_0\) with neighboring spins \(S_i\), \(\langle S_0S_i \rangle\), decreases with \(J'_{pd}\) increase. The dependence of correlator for NN and the next nearest neighbor (NNN) are shown in Fig. 3c. The correlators are not affected by the presence of a weak polaron, but for stronger \(J'_{pd}\) they decrease as \(1/J'_{pd}\).

The ground state of a system consisting of a carrier with \(s = 1/2\) and an AF cluster of an even number of local spins is a spin doublet, for any \(J'_{pd}\). However, depending on the value of \(J'_{pd}\), the magnetic moment can be transferred from the carrier to the system of local spins. For a non-interacting spin \(s\), or for a very weak \(p-d\) coupling, the carrier spin has a magnetic moment while the total moment of localized spins is zero. In Fig. 3b the \(z\)-component of the carrier spin, \(s_z\), the local spin \(S_0\), and the sum of all local spins \(\sum S_i\) are plotted as a function of \(J'_{pd}\). To distinguish the \(z\)-direction, we put a small magnetic field which does not perturb the spin structure of polaron. With an increase of \(J'_{pd}\), the magnetic moment is transferred from the carrier to the local spins. For a very strong \(p-d\) coupling, the moment of local spins \(\sum S_i\) saturates at value 1/2. At the same time, the moment of carrier spin and of the local spin, vanish. The magnetic moments of the local spins, \(\sum S_i\), are distributed in a staggered way among the whole cluster. In the limit of strong \(p-d\) coupling, \(J'_{pd} \gg 1\) the small polaron is equivalent to the Zhang-Rice (ZR) one. Here the spins, \(s\) and \(S_0\), are compensated and form a local singlet state, not coupled to other local spins, \(S_i\) (see Fig. 3c and the icon in Fig. 3a.). On the other hand, the formation of a central pair of compensated spins is accompanied by a transfer of the magnetic moment to the neighboring local spins and formation of staggered \(M(\mathbf{r})\) around the central cell. Such an effect was described in details, for example in [4].

As it is shown in Fig. 1, \(E_{xx}\) for a weak \(p-d\) coupling decreases with an increase of the polaron size. For big \(J'_{pd}\), however, some new effects occur. As it is shown in Fig. 2, for a weak polaron evenly localized on two \(d\)-spins antiferromagnetically correlated \(E_{xx}\) is smaller by a factor \(\sim 80\) than in the case of a small AFP. With an increase of \(J'_{pd}\), instead of the expected saturation, a faster increase of \(E_{xx}\) for such a polaron occurs.

An even more pronounced effect is seen for a homogeneously distributed carrier density. As it is shown by squares in Fig. 2, \(E_{xx}\) for a weak \(p-d\) coupling is practically zero but sharply increases for \(J'_{pd} \simeq 2\). Moreover, a further increase of \(J'_{pd}\) is accompanied with a step-like increase of \(E_{xx}\). Studies of the spin structure show that this critical behavior is caused by a breakdown of the AF bonds and the formation of a magnetic moment in the antiferromagnetic medium. Such a magnetic polaron is known as ferron, and it was described decades ago [4]. In the whole range of \(J'_{pd}\) values there is no considerable difference between the 1D and 2D cases.

The spin structure of a ferron localized on two local spins is complex. The correlator of the carrier spin \(s\) with the two local AF spins \(S_{p1}, \langle sS_p \rangle\), is negative (for antiferromagnetic \(p-d\) coupling) for the whole range of \(J'_{pd}\). For a weak \(J'_{pd}\), \(\langle sS_p \rangle\) increases linearly, then saturates for very large \(J'_{pd}\) approaching \(-0.5\). The sharper increase of \(E_{xx}\), which is seen for \(J'_{pd} \simeq 2.5\) is caused by a spin-flip of the two local spins, \(S_p\). The systematic increase of \(E_{xx}\) faster than the linear increase, for \(J'_{pd} > 4\) originates neither from the correlation \(\langle sS_p \rangle\) nor from the correlation between two local spins \(\langle S_{p1}S_{p2} \rangle\) but results from a systematic reconstruction of the AF environment of the ferron. The correlation of each of the \(S_p\) with surrounding spins, \(S_i\), gradually decreases. Simultaneously, there appears a reconstruction of \(d-d\) couplings among the surrounding spins.
the carrier, for J step-like behavior of \(|J\rangle\) cases. For \(J = 1/2\) values of \(E_z\) is also characterized by steps occurring for the same spin as a function of \(J_{pd}'\). The data are shown in Fig. 4. The homogeneous distribution of the carrier on the whole AF cluster with PBC is shown by open stars.

More apparent data about the mechanism of the formation of a ferron can be found if one assumes a homogeneous distribution of the carrier on the whole AF cluster with PBC. The data are shown in Fig. 4. The correlator between one of the AF spins and the carrier spin as a function of \(J_{pd}'\) is presented in Fig. 4a. The step-like behavior of \((\langle sS_i\rangle)\) is visible for both 1D and 2D cases. For \(J_{pd}' < 2.5\) correlator \((\langle sS_i\rangle) = 0\) and \(E_x = 0\). For \(J_{pd}' > 2.5\) \(E_x\) increases in accordance with the observed steps of \((\langle sS_i\rangle)\). In Fig. 4b the total magnetic moment of the polaron, \(s_{iz} = \sum_s s_i s_z\), is presented. It is also characterized by steps occurring for the same values of \(J_{pd}'\) as those of \((\langle sS_i\rangle)\) when \(J_{pd}'\) is large. For \(J_{pd}' < 9\) and 2D case the total magnetic moment is equal to 1/2. For \(J_{pd}' < 2.5\) this moment is located at the carrier, for \(J_{pd}' > 2.5\) it is the result of the coupling of the electron spin (\(s_z = 1/2\)) with \(\sum_s s_i s_z = 1\) AF spin. The correlator between two neighbor AF spins \((\langle S_i S_{i+1}\rangle)\) is presented in Fig. 4c. It changes from \(-0.4\) for a pure AF to 0.25 (both spins parallel) with an increase in the strength of \(p-d\) coupling. At the same time, \(s_{iz}\) approaches value 7.5 (all bonds broken). It is worth to note that the step-like behavior of \((\langle S_i S_{i+1}\rangle)\) is not a consequence of breaking of the subsequent bonds, but it is associated with steps of the total magnetic moment of the system.

To summarize, the ferron can form when homogeneous, Curie-Weiss magnetization is induced. Our results complete well the classical model of ferron.

E. Comb-Like AFP

A homogeneous distribution of the carrier on many AF spins makes the \(E_x\) on opposite spins cancel each other out. Thus we introduced a carrier trial function which is distributed on one of the Neel sublattices only as intuitively energetically favorable. The carrier distribution is described as follows:

\[
|\varphi (i)|^2 = f (r_i) \cos^2 \left( \frac{\pi}{2a} r_i \right),
\]

where \(f (r_i)\) is an envelope function, usually Gaussian. We call such a polaron comb-like AFP.

\(E_x\) versus \(J_{pd}'\) for the comb-like polaron with a Gaussian envelope function is presented by triangles in Fig.1. For a small \(r_p'\), the comb-like AFP is equivalent to the small AFP. For a bigger \(r_p'\), the gain \(E_x\) decreases, but it is still much greater than that for large AFP. \(E_x\) for a large comb-like AFP is only three times smaller than that of a small AFP. This stems from a decrease of quantum fluctuations (see part IIIF).
The comb-like AFP induces a staggered magnetization in the AF medium. This is shown in Fig. 5b, where the mean value of the correlator between the carrier spin $s$ and the spins of the AF sublattice on which the polaron is acting $S_A$, $\langle sS_A \rangle$, and the spins of other sublattice $S_B$, $\langle sS_B \rangle$, are presented by circles and squares, respectively. The values of the correlators increase linearly for small $p-d$ coupling, and they saturate when $J_{pd}' > 1$. The saturation value for $\langle sS_B \rangle = 0.25$ and it is independent of the number of spins. The saturation value of $\langle sS_A \rangle > 0.25$ and depends on the number of spins. The difference between the magnetization of the A and B sublattices gives the net magnetic moment of AF.

A part of the magnetic moment which is transferred from the carrier to the AF medium depends on $J_{pd}'$ as it is shown in Fig. 5b. Here the change versus $J_{pd}'$ of $z$-components of the carrier spin, $s_z$, of one of the spins on which the carrier acts, $S_{iz}$, and of the total spin, $\sum_i S_{iz}$, is presented. For small values of $p-d$ coupling a quadratic increase of the moment transferred to AF is observed. $\sum_i S_{iz}$ saturates at a value smaller than 0.5. Simultaneously, the $z$-component of the carrier spin decreases from 0.5 for weak $p-d$ coupling to the saturation value of 0.15 for an AF cluster consisting of 16 spins. However, $s_z + \sum_i S_{iz} = 0.5$ is independent on $J_{pd}'$.

The presence of the comb-like AFP on one of the Neel sublattices breaks the translation symmetry and leads to the formation of two magnetized sublattices. In Fig. 5c the correlators between NN, $\langle S_i S_{i+1} \rangle$, and NNN, $\langle S_i S_{i+2} \rangle$, are presented as a function of $J_{pd}'$. While $\langle S_i S_{i+1} \rangle$ decreases for large $J_{pd}'$, the correlator $\langle S_i S_{i+2} \rangle$ increases. Thus, a comb-like AFP increases the AF correlation radius. In the limit of very large $J_{pd}'$ and not too small sizes of the AF cluster, the comb-like AFP transforms the quantum antiferromagnet into a classical one.

Although $E_{ex}$ for the comb-like AFP is large, the probability of its formation is small because it is characterized by a big kinetic energy. Moreover, the comb-like AFP has a tendency to localize into small AF. This comes from the fact that the kinetic energy is almost the same for both types of polarons (as long as only $t_1$ is taken into account) while $E_{ex}$ due to quantum fluctuations increases three times with localization.

### F. Quantum effects

In this section we summarize the results concerning the formation mechanisms of different magnetic polarons. We pay particular attention to the appearance of quantum effects. In paragraphs A-E, five types of antiferromagnetic polarons were presented. The formation of weak small, medium, and comb-like polarons is associated with the induction of staggered magnetization. In contrast, the formation of a strong ZR polaron is caused by the compensation of the AF spin by the carrier spin. The mechanism of ferron formation is the breaking of AF bonds, which is equivalent to the induction of a homogeneous moment.

Classically, the only possible mechanism of AF polaron formation at zero temperature is the turning of the spins in the direction of the effective field induced by the carrier spin. However, this mechanism does not explain the formation of the remaining polarons. The induction of staggered magnetization is directly associated with the quantum treatment of the AF. In a quantum approach the ground state of AF is a combination of Neel states, hence no sublattice is distinguishable. The simplest measure of AF quantum fluctuations is the difference between the ground and the first excited states, which are both composed of Neel states. In the presence of staggered magnetization the Neel sublattices are distinguishable and the damping of spin fluctuations occurs.

The mechanism of compensation responsible for the formation of the ZR polaron should be also considered in a quantum approach. Classically, the carrier couples the AF spin and such interaction does not destroy the AF order. As we have shown in Fig. 3c, in the quantum treatment of the antiferromagnet the affected AF spin may cease to be correlated with neighbor spins. It means that only the quantum approach allows to model the destruction of antiferromagnetic order which is observed in experiments. Despite the quantum character of the discussed above mechanisms, there are some particular situations where the polarons can be described in the classical limit, but the quantum corrections have to be taken into account. These corrections are the result of scaling of spin fluctuations with the number of spins and seem to be important for the antiferromagnetic sign of $J_{pd}'$. By a systematic analysis of the dependence of $E_{ex}$ on $p-d$ coupling in the range of very large $J_{pd}'$, we have found that $E_{ex} = \sum_i J_{pd}(i)(sS_i)$, where the summation is taken over the $N$ spins $S_i$ within the polaron size (see Fig. 2). The correlator depends on $N$ and is equal to $\langle sS_i \rangle = (0.25 + 1/2N)$. Thus $E_{ex}$ changes from 0.75$J_{pd}'$ for a polaron localized on one spin to 0.25$J_{pd}'$ for a polaron interacting with an infinite number of spins. Hence, it is possible to calculate the energy of strong small polarons as well as ferrons classically, but the appropriate scalar spin multiplication (0.25) has to be replaced by the quantum factor. It approaches the classical value when $N \to \infty$, whereas for $N = 1$ it is three times bigger. The same quantum factor 3 is lost when the ZR polaron is delocalized on one of the Neel sub-
lattices forming the comb-like polaron.

The importance of the sign of the $p$-$d$ coupling is shown in the inset to Fig. 2. Here $E_{ex}$ for a small AFP with either a positive or negative sign of $J'_{pd}$ is presented. Different slopes of $E_{ex}$ for ferro- and antiferromagnetic coupling are observed. It is a consequence of the fact that the carrier and AF spins can not couple ferromagnetically to more than 0.25 while for antiferromagnetic coupling are observed. It is a consequence of the fact that the carrier and AF spins can not couple ferromagnetically to more than 0.25 while for antiferromagnetic coupling (\( s\vec{S} \)) approaches $-0.75. Thus, only for antiferromagnetic coupling the corrections associated with the number of spins in the AF system are important. In the case of ferromagnetic coupling, the classical energy calculations for small polarons and ferrons are correct.

G. Polaron mass

In our approach (see Eq. (2)) we assume a simple decoupling of the carrier kinetic energy and the spin degree of freedom. For all the types of polarons discussed, the minimum energy corresponds to the localization of the maximum of the trial function, $\Psi(\mathbf{r})$, exactly at the position of the local spin $\mathbf{r}_0$. But another equivalent minima correspond to the localization at another equivalent spin positions. For PBC, which simulate the translation symmetry, all minima are exactly equivalent. As the consequence, the linear combination of the simplified solutions is expected to be a better solution of the problem. It shows that the carrier motion and the spin structure are really coupled. To study that problem correctly one should, however, diagonalize $N$ times bigger matrices. Anyway, our simplified approach gives a reasonable picture of the spin structure of a magnetic polaron under assumption of its static nature, but it does not allow to study the real correlation of the carrier motion and spin dynamics and does not bring any solid answer on the problem of the polaron localization. However, a hint about the effective polaron mass and the reduction of the kinetic energy can be found within our simple approach through the analysis of the change of the spin structure which accompanies the transfer of the polaron to the NN. When the decoupling of the motion and spin is assumed (Eq. (2)), the kinetic energy is described by the parameter $t_1$, according to Eq. (6). Here, only the transfer without any spin flip is considered. Our solutions show, however, that the transfer is accompanied with a complex change of the spin structure. The spin structure of the surrounding local spins is very different when the carrier is localized on the first, A, or on the neighboring site, B. A posteriori, we are able to claim that the matrix elements describing the kinetic energy are reduced by a factor resulting from the product of the spin states on the site A and B $\langle X^A_i|X^B_j \rangle$, respectively. In other words, to consider the effects which are omitted due to our assumption (Eq.(2)), one has to reduce the value of the parameter of the kinetic energy. Instead of $t_1$ as effective kinetic energy, $t'_1 = t_1 \langle X^A_i|X^B_j \rangle$ should be used. Our numerical study shows that for weak $p$-$d$ coupling, $J_{pd} \ll J_{dd}$, the factor $\langle X^A_i|X^B_j \rangle$ is close to unity. For $J_{pd} \approx J_{dd}$ the value of $\langle X^A_i|X^B_j \rangle$ decreases, and for $J_{pd} > J_{dd}$ it saturates at the value in the range 0.1 - 0.2, depending on the type of polaron. It shows that the effective mass of polaron dressed by the spin polarization is considerably bigger as compared to free polaron.

IV. PHASE DIAGRAM OF MAGNETIC POLARONS

Until now we have considered the $E_{ex}$ from magnetic polarons formation and we have described the spin structure of various polarons. However, the total energy (exchange, phonon and kinetic one) should be taken into account to specify which type of polaron forms. In this section we consider the formation of a pure magnetic polaron.

In Fig. 6 the total energy (sum of kinetic and exchange energies) as a function of polaron radius $r'$ for $J'_{pd} = 1.875$ and effective masses of $m_e$ (triangles), $2m_e$ (circles), $25m_e$ (squares).
ations of the AF medium (see part IIIF). We found that for $J'_{pd} = 1.875$ magnetic polarons can form only if $m_{eff} > 1.6m_e$, what corresponds to $t_1 = 2J_{dd}$. For weaker $p$-$d$ couplings the small AFP is also the only polaron which can form but its $m_{eff}$ should be much greater.

In Fig. 7 the phase diagram of the formation of different magnetic polarons is shown. The area of parameters $t_1$ and $J'_{pd}$ for which the small AFP forms is marked by a solid line.

![Phase diagram of magnetic polaron formation](image)

**FIG. 7:** Phase diagram of magnetic polaron formation. In the inset $E_{tot}$ as a function of $t_1$ for $J'_{pd} = 4.4$ is shown. In the inset dashed line presents $E_{tot}(t_1)$ for two-spin ferron, the solid line shows $E_{tot}(t_1)$ for small AFP. Vertical lines separate the areas of different polarons formation.

For higher $J'_{pd}$, the small ferrons can also form. In the inset to Fig. 7 the total energies of a small AFP and a small ferron are compared for $J'_{pd} = 4.4$. $E_{ce}$ for a small AFP is higher than for the two spin ferron, and it is constant. The kinetic energy of two-spin ferron (polaron localized on two neighboring spins) is smaller than that of a small AFP and scales linearly with $t_1$. Thus the total energies of both polarons are linear functions of $t_1$ but with different slopes. In particular the boundary between small AFP and two spin ferron for $J'_{pd} = 4.4$ crosses for $t_1 = 5.4J_{dd}$, what is equivalent to $m_{eff} \geq 0.6m_e$. For $t_1$, which is greater than $6.25J_{dd}$ any AFP is not formed. In general, the small AFP forms for $m_{eff} \geq m_e$, while the two-spin ferron appears for $m_{eff} < m_e$.

Similarly, we found the range of parameters for which other types of polarons can also form. In Fig. 7 the ranges where small AFP, two, four-spin ferrons can occur are shaded by solid, dotted and dashed lines, respectively. The appearance of a three-spin ferron is indicated by rectangles. Larger ferrons appear for much stronger $p$-$d$ couplings, and we omit their description because they would exist for nonphysical parameters.

The presented results were calculated for a 2D square with PBC. To estimate the error caused by small size of antiferromagnetic cluster, we investigated also such clusters as: a $4 \times 4$ square without PBC, a $4 \times 4$ parallelogram, and $2 \times N$ systems where $2 \leq N \leq 10$. We found that the energy of polarons with small size depends on the nearest vicinity only. It is weakly dependent on both $N$ and boundary conditions. For different 2D clusters the formation range of subsequent polarons can be shifted about 10%–15%.

The investigation of polaron formation in a wide range of parameters is exceptionally valuable when we want to classify what type of polaron could be formed in different materials. For example, in doped EuTe where $J_{pd} \approx 0.125$ eV and $J_{dd} \approx 2$ meV the $p$-$d$ coupling on one AF bonds $J'_{pd} \approx 8$. At the same time, $t_1 \approx 15J_{dd}$. For such parameters our model predicts the ferrons formation (see Fig. 7) in accord with experiments (see Fig. 6 and references therein).

In high-$T_c$ superconductors which are based on CuO$_2$ layers, the $d$-$d$ exchange coupling ranges from 0.055 eV to 0.085 eV, as determined from the Neel temperature of antiferromagnetic precursors of these materials. $J_{pd} \approx 1$–3 eV was determined from the band structure calculations. Thus, the ratio of $p$-$d$ to $d$-$d$ exchange energies is between 1.5 and 4 for $J_{dd} \approx 0.75$ eV. $m_{eff}$ is much more difficult to determine because the mass observed in experiments (e.g. in ARPES) is determined from phonon and exchange interactions. Since the decorated $m_{eff}$ observed in ARPES experiments is about $4m_e$ and $m_{eff}$ in our model is dressed only by phonons, the $m_{eff}$ which should be considered in the phase diagram is smaller than $4m_e$, which is equivalent to $t_1 > 0.8J_{dd}$.

We conclude on the basis of our phase diagram that for parameters typical for weakly doped high-$T_c$ superconductors mainly the small AFP would form. There may be also some competition between the formation of small AFP and two-spin ferrons provided that the effective mass dressed in phonons is a bit lower than the electron mass. Large AFP have energies of few orders of magnitude lower than those of small AFP and ferrons.

**V. THE CONTRIBUTION OF PHONON AND MAGNETIC POLARON**

Now we will compare the phonon and magnetic contributions to the formation of polarons in weakly doped high-$T_c$ superconductors. We have shown that in the 2D case $E_{ce}$ from the formation of large magnetic polarons is close to zero and that they are unlikely to form (Fig. 6 and Fig. 7). Mott and Alexandrov suggest that in high-$T_c$ superconductors only small phonon polarons
In order to obtain the total energy of magnetic and phonon polaron separately, $E_{\text{tot}}$, we have evaluated the energies for a chosen set of parameters: $m_{\text{eff}} = 2.1 m_e$ and $\kappa = 5$. This mass, according to ARPES experiments and band structure calculations, is reasonable for high-Tc superconductors. $\kappa$ is taken from theory of phonon polarons. In Fig. 8c, we show the values of $E_{\text{tot}}$ for phonon as well as magnetic polarons versus $J'_{pd}$. For the phonon polaron $E_{\text{tot}}$ is constant and equal to 0.15 eV since the phonon as well as kinetic energies are independent of $J'_{pd}$. The phonon polaron dominates in the range of weak $p-d$ couplings. In contrast, the magnetic polaron (circles in Fig. 8c) dominates in the range of strong $J'_{pd}$ where its energy increases linearly with $J'_{pd}$. In the range of $J'_{pd} = 1.5 - 4$, which is typical for weakly doped high-$T_c$ superconductors, the energies of both polarons are comparable or magnetic polaron energy slightly overcomes the energy of phonone. This result agrees well with a very recent paper, which stresses the importance of phonon interactions in high-$T_c$ superconductors.

We conclude that within our model the phonon and magnetic polaron energies are comparable and that both contributions should be included in the total polaron energy in high-$T_c$ superconductors.

**VI. SUMMARY**

Using the spin-fermion model and treating all spins in quantum approach, we found that depending on the material parameters five various types of magnetic polarons in antiferromagnetic medium can be distinguished.

We showed that in the range of parameters typical for weakly doped high-$T_c$ superconductors the contributions of phonon and magnetic interactions to the formation of a polaron are comparable and hybrid magnetic-phonon polarons form.

In weakly doped high-$T_c$ superconductors small magnetic polarons as well as small ferrons can form. Our numerical study allows to find a continuous evolution from Zhang-Rice approach, when $p-d$ coupling is assumed to be much stronger than $d-d$ coupling, via important for high-$T_c$ materials intermediate range, to linear response approach suitable for weak $p-d$ coupling.

The here introduced comb-like polarons cannot form when the band is empty (i.e. in undoped material) because of the cost of high kinetic energy. However, they can play a fundamental role in doped high-$T_c$ materials when the band is partially filled.
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