Magnetic polarons in doped 1D antiferromagnetic chain

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The structure of magnetic polarons (ferrons) is studied for an 1D antiferromagnetic chain doped by non-magnetic donor impurities. The conduction electrons are assumed to be bound by the impurities. Such a chain can be described as a set of ferrons at the antiferromagnetic background. We found that two types of ferrons can exist in the system. The ground state of the chain corresponds to the ferrons with the sizes of the order of the localization length of the electron near the impurity. The ferrons of the second type produce a more extended distortion of spins in the chain. They are stable within a finite domain of the system parameters and can be treated as excitations above the ground state. The ferrons in the excited states can appear in pairs only. The energy of the excited states decreases with the growth in density of impurities. This can be interpreted as a manifestation of an attractive interaction between ferrons.

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I. INTRODUCTION

It is now commonly accepted that the tendency toward phase separation is of fundamental importance for the physics of manganites and related compounds. The self-trapping of charge carriers is the most widely discussed type of phase separation, first predicted in the seminal paper of Nagaeva. In such phase-separated states, charge carriers are confined within small ferromagnetic metallic droplets (magnetic polarons or ferrons) located in an insulating antiferromagnetic matrix. It is usually assumed that the region of the perturbed spins around a ferron is rather narrow that is confirmed by numerical calculations for some models. However, as first pointed out by De Gennes, the distortion of the magnetic order around a magnetic defect (e.g. a ferron) may decay slowly with the distance. The possible existence of ferrons with such extended spin distortions was analyzed for one-dimensional (1D) antiferromagnetic chain in Refs. These calculations performed for an isolated impurity show that the characteristic length of the distorted spin surrounding can be much larger than the size of the trapping region.

The problem arises what kind of ferrons should be expected at different values of the parameters of the system. To study this problem, we consider in this paper 1D antiferromagnetic chain doped with non-magnetic donor impurities of finite density. We find that there are two possible magnetic structures: one characterized by extended spin distortions and another one with a narrow distorted region. For the relationship between parameters characteristic of manganites, the ground state for a regular distribution of impurities corresponds to the ferrons without extended spin distortions. The ferrons with extended spin distortions can appear as excited metastable states. We found that due to the overlapping of extended spin distortions, an attractive interaction among these ferrons arises in the system. This interaction could favor a phase-separation process, that would lead the system to an inhomogeneous state with clusters of ferrons, as observed in the experiment.

II. THE MODEL

In this section, we find the magnetic structure of the ground state of an 1D antiferromagnetic chain doped by non-magnetic donor impurities. We consider an one-dimensional chain of antiferromagnetically coupled local spins, the y-axis being the axis of the chain. We do not considered here specific effects related to one-dimensionality and start from the antiferromagnetic structure characteristic of the mean-field approximation. Non-magnetic impurities occupy the sites of the chain at half-integer positions. The conduction electrons are assumed to be in a bound state of the impurity electrostatic potential. It is also assumed, for simplicity, that the wave function of the conduction electron extends only over the two neighbouring magnetic ions near an impurity. Further on, we assume that for a given density of conduction electrons $n$, the impurities are periodically distributed along the chain, and $L = 1/n > 2$ being the distance between neighboring impurities (in units of the lattice constant). We consider the following Hamiltonian of the system

$$H = H_{el} + J' \sum_{g} \mathbf{S}_g \cdot \mathbf{S}_{g+1} - K' \sum_{g} (\mathbf{S}_g^z)^2,$$  \hspace{1cm} (1)
where

\[ H_{el} = -t \sum_{i,\sigma} \left( a_{iL,\sigma} a_{iL+1,\sigma} + a_{iL+1,\sigma} a_{iL,\sigma} \right) - \]
\[ -\frac{A}{2} \sum_{i,\sigma,\sigma'} \left\{ a_{iL,\sigma}^+ \left( \vec{\sigma} \vec{S}_{iL} \right)_{\sigma,\sigma'} a_{iL,\sigma'} + \right. \]
\[ + a_{iL+1,\sigma}^+ \left( \vec{\sigma} \vec{S}_{iL+1} \right)_{\sigma,\sigma'} a_{iL+1,\sigma'} \} \]  \hspace{1cm} (2)

In Eqs. (1) and (2), \( \vec{S}_g \) is the spin of the magnetic ion located at site \( g \), treated as classical vector, symbols \( a_{iL,\sigma}^+ \), \( a_{iL,\sigma} \) denote the creation and annihilation operators for the conduction electron with spin \( \sigma \) at site \( g \), and \( \vec{\sigma} \) are Pauli matrices. The second and third terms in Eq. (1) are the antiferromagnetic exchange between local spins and the magnetic anisotropy energy, respectively. The two terms in \( H_{el} \) describe the kinetic energy of the conduction electrons bounded by the impurities, which are located between sites with \( g = iL \) and \( g = iL + 1 \) (\( i \) is an integer), and the Hund-rule coupling between the conduction electrons and the localized spins. Parameters \( A \), \( t \), \( J \), and \( K' \) of Hamiltonian (1) are considered to be positive and the \( x \) axis is the easy axis. The energy of Coulomb interaction between the conduction electron and the impurity is an additive constant and, for this reason, omitted in the calculation.

Hamiltonian (1) is applicable for the description both of wide-band and double-exchange (like manganites) magnetic semiconductors. The hierarchy of parameters in wide-band case is \( t \gg AS > J' \) while for the double-exchange case we have \( AS \gg t > J' \). In both cases \( K' \) is assumed to be the smallest parameter, which corresponds in the most cases the experimental situation.

It is well known that due to the Hund-rule coupling \( A \) Hamiltonian (2) favors the deviations from the ideal antiferromagnetic arrangement of spins. These deviations are the most pronounced for the sites neighboring to impurities. This can be illustrated by the diagonalization of Hamiltonian (1), which can be easily performed. As a result, we have that the lowest eigenvalue of \( H_{el} \) corresponding to the ground state and the low-lying excitations can be written as

\[ E_{el} = -\frac{1}{2} \sum_i \sqrt{A^2S^2 + 4t^2 + 4AS \cos \left( \frac{\nu_i}{2} \right)} \]  \hspace{1cm} (3)

where \( \nu_i \) is the angle between vectors \( \vec{S}_{iL} \) and \( \vec{S}_{iL+1} \). We can see that the lowest value of energy \( E_{el} \) corresponds to the parallel orientation of spins nearest to the impurity. So, we get a “seed” ferron centered at the impurity.

To the first approximation, both wide-band and double-exchange cases can be treated in the same manner. At \( t \ll AS \), the first-order term in \( E_{el} \) with respect to \( t/AS \) has the form

\[ E_{el} \approx -\frac{AS}{2}N_{imp} - t \sum_i \cos \left( \frac{\nu_i}{2} \right) \]  \hspace{1cm} (4)

where \( N_{imp} \) is the number of impurities. In the case \( t \gg AS \), the similar expression can be obtained by interchanging \( t \leftrightarrow AS/2 \). Further on, we discuss the double exchange case (4), however, the results for the wide-band case can be obtained by the aforementioned change of the parameters.

Let us consider now the configuration of the local spins corresponding to the ground state. Due to the rotational symmetry of the Hamiltonian (1) with respect to the easy axis, all local spins in the ground state should lie in a plane containing the easy axis. The deviations of any local spin from this plane results in the growth of the energy of the system. We assume without loss of generality that it is the \( xz \) plane.

The direction of a local spin \( \vec{S}_g \) in the \( xz \) plane can be characterized by angle \( \theta_g \) with respect to \( z \) axis (see Fig. 1). Then, the spins located between any two neighboring impurities can be represented as \( \vec{S}_g = S (\pm \sin \theta_g, 0, \cos \theta_g) \), where \( 0 \leq \theta_g \leq \pi \), and \( s = 0 \) or 1. The passing through a ferron changes such a sequence of spins to another one. Since the impurities are periodically arranged along the chain, the magnetic ordering of local spins in the ground state has to be also periodic. There exist several ways to join the solutions at impurities, which preserve the periodicity. The corresponding relationships can be written as \( S_{iL}^{\pm} = \pm S_{iL+1}^{\pm} \). However, only two of them give the energy gain and correspond to the ferron-type solutions. The first one is \( S_{iL}^x = -S_{iL+1}^x, S_{iL}^z = S_{iL+1}^z \). This means that the magnetic moments of ferrons are directed along the \( z \)-axis. In the second case, the magnetic moments of ferrons are directed along the easy axis, and spins close to the \( i \)th impurity satisfy the equality \( S_{iL}^x = S_{iL+1}^x, S_{iL}^z = -S_{iL+1}^z \). The configuration of local spins corresponding to the first case is \( \vec{S}_g = S (\pm (1)^{g-i} \sin \theta_g, 0, \cos \theta_g) \) for all \( g \), and the symmetry condition is \( \theta_g = \theta_{g+1} \). The configuration of local spins corresponding to the second case can be written in the form \( \vec{S}_g = S (\pm (1)^{g-i} \sin \theta_g, 0, \cos \theta_g) \) for \( iL + 1 \leq g \leq (i+1)L \), and the symmetry condition in this case is \( \theta_g = \pi - \theta_{g+1} \). Both configurations are schematically shown in Fig. 1.

In the 1D antiferromagnetic chain under study the
magnetic moments of neighboring ferrons are either parallel or antiparallel for odd and even \( L \), respectively. If \( L \) is odd integer, the periodicity condition is \( \theta_{g+L} = \theta_g \), and the magnetic moments of all ferrons are parallel each other. For even \( L \), the periodicity condition is \( \theta_{g+L} = \pi - \theta_g \) and the magnetic moments of neighboring ferrons are antiparallel.

Taking into account the periodicity of the problem and the aforementioned symmetry conditions, we readily come to the relationships between the canting angles \( \nu_i \) in Eqs. (3) and (4) and the angles \( \theta_{iL}, \theta_{iL+1} \). For any \( L \), these relationships can be written in the following form:

\[
\cos \left( \frac{\nu_i}{2} \right) = \left| \cos \left( \frac{\theta_{iL} + \theta_{iL+1}}{2} \right) \right|,
\]

where plus (minus) sign corresponds to the first (second) configuration.

Now let us find the form of magnetic ordering for local spins and the energy of the system corresponding to each configuration. Substituting the expressions for \( \vec{S}_g \) and Eq. (5) for canting angles \( \nu_i \), into the Eqs. (3) and (4), we obtain the energy of the system in the following form:

\[
E = J \sum_{g \neq iL} \cos (\theta_g + \theta_{g+1}) - K \sum_g \sin^2 \theta_g + \sum_i \left( J \cos (\theta_{iL} + \theta_{iL+1}) - 2F \left| \cos \left( \frac{\theta_{iL} + \theta_{iL+1}}{2} \right) \right| \right), \tag{6}
\]

where we use the notation \( J = J'S^2, \ K = K'S^2, \) and \( F = t/2 \) in the case \( t \ll AS \), or \( F = AS/4 \) for \( t \gg AS \). The plus (minus) sign in Eq. (6) corresponds to the first (second) configuration of local spins. The constant term in (6) is omitted here.

To find the spin structure of the ground state, one has to minimize the energy (6) with respect to the angles \( \theta_g \). A set of nonlinear equations is obtained

\[
\begin{align*}
J \sin (\theta_g + \theta_{g+1}) + J \sin (\theta_{g-1} + \theta_g) + K \sin (2\theta_g) = 0 \\
J \sin (\theta_{iL+1} + \theta_{iL+2}) \pm J \sin (\theta_{iL} + \theta_{iL+1}) + K \sin (2\theta_{iL+1}) = 2F \frac{\partial}{\partial \theta_{iL+1}} \cos \left( \frac{\nu_i}{2} \right) \quad g \neq iL + 1, (i + 1) L \\
J \sin (\theta_{i+1} L) + J \sin (\theta_{i+1} L - 1 + \theta_{i+1} L) + K \sin (2\theta_{i+1} L) = 2F \frac{\partial}{\partial \theta_{i+1} L} \cos \left( \frac{\nu_{i+1}}{2} \right)
\end{align*}
\]

Using the periodicity conditions \( \theta_{iL} = \theta_{i+1} L \), \( \theta_{i+1} L = \theta_{i+1} L + 1 \) for odd \( L \), or \( \theta_{iL} = \pi - \theta_{i+1} L \), \( \theta_{i+1} L = \pi - \theta_{i+1} L + 1 \) for even \( L \), the number of equations in system (7) becomes equal to \( L \). After this, the system of equations is solved numerically at different values of \( F/J \) and \( K/J \) assuming that \( K/J \ll F/J \). As a result, we obtain the magnetic structure of the system of local spins with donor impurities. This structure is discussed in the next section.

### III. RESULTS

The numerical analysis of the solutions of Eqs. (7) demonstrates that two types of ferrons schematically shown in Fig. 1 can exist in the system under study. For relatively large \( F/J \gtrsim 1.5 \) the ground state corresponds to the ferrons of the second type (see right panel in Fig. 1). For \( F/J \gtrsim 2 \), we have a classical ferron configuration, namely, ideal ferromagnetic ordering inside the localization region of the doped electron (two lattice constants in our case) and ideal antiferromagnetism outside this region. The solution corresponding to the first configuration of the local spins (see left panel in Fig. 1) is characterized by a long-range deviation from the ideal antiferromagnetic ordering and can be considered as an excitation above the ground state. This spin structure is illustrated in Fig. 2 where we plot the directions of local spins between two impurities for \( n = 1/21 \).

For smaller \( F/J \), the ground state of the system corresponds to the first type of ferrons. However, in this limit the difference between the two types of ferrons is not so drastic. Both types of ferrons create a distortion of antiferromagnetic ordering outside the electron localization region. Moreover, the characteristic size of the distorted region is larger for the ferrons of the second type. Therefore, we come to the conclusion that for any value of the ratio \( F/J \) the ground state of the system corresponds to the ferrons with smaller radius of spin distortions.

Let us consider in more detail the case \( F/J > 2 \) (typical of manganites). Let us refer the ferrons with and without extended spin distortions as “coated” and “bare”, respectively. The system of “bare” ferrons forms the ground state, whereas, the system of “coated” ferrons can form a metastable state. In Figs. 3 and 4, we show the energy of the “coated” ferron and the angle of the local spin in the trapping region, \( \theta_0 \) as functions of the inverse impurity density, \( 1/n \). The ferron energy \( E_{\text{pol}} \) is defined as the difference between energies of the system with and without doped electrons divided by the number of impurities, that is, \( E_{\text{pol}} = E/N_{\text{imp}} + L(J + K) \). The energy of the “bare” ferron does not depend on the density of impurities (up to \( 1/n = 1/2 \)) and equals to \( E_{\text{pol}} = -2(F - J) \).
FIG. 2: Magnetic ordering for the first configuration of local spins between two non-magnetic impurities (dots) for \( n = 1/21 \). This structure is repeated between any two non-magnetic impurities of the chain. It can be seen that in the region occupied by the conduction electrons (the first and the last magnetic sites), we have almost ferromagnetic ordering, while in the remaining part of the chain, there exists a distorted antiferromagnetic ordering. The parameters of the Hamiltonian are \( F = 3, K = 2.5 \times 10^{-2} \) (both in \( J \) units).

FIG. 3: Energy of “coated” ferron versus the inverse density of impurities \( L = 1/n \). The values of parameters are \( F = 3, K = 2.5 \times 10^{-2} \) (in \( J \) units). The energy of a “bare” ferron equals to \( E_{\text{pol}} = -2(F - J) = -4 \). At \( L \leq L_{\text{cr}} = 1/n_{\text{cr}} = 12 \) (vertical line), the “coated” ferrons become unstable (see figures and text below).

In Fig. 3 we plot the energy of the “coated” ferron as a function of the canting angle \( \nu_0 \) at different impurity densities. At small densities the minimum of the ferron energy corresponds to nonzero value of \( \nu_0 \), whereas at the densities exceeding some critical value \( n_{\text{cr}} \) the ferron energy has a minimum at \( \nu_0 = 0 \).

The numerical analysis of Eqs. shows that for impurity densities higher or equal than some critical density \( n_{\text{cr}} \), the angle \( \theta_0 \) (which is one-half of the canting angle \( \nu_0 \)) for the “coated” ferrons is equal to zero (see Fig. 4).

Moreover, all spins in the chain become perpendicular to the easy axis. Thus, at \( n \geq n_{\text{cr}} \), the periodic structure of “coated” ferrons becomes unstable. Indeed, such ferrons become structurally identical to “bare” ferrons but have higher energy. Any rotation of this spin structure toward the easy axis leads to the monotonic decrease of its energy. In other words, at small densities each “coated” ferron creates a long-range spin distortion of the antiferromagnetic background around it. This long-range spin...
distortion stabilizes the “coated” ferrons. The radius of extended spin distortion created by a single “coated” fer-
ron can be estimated as \( r_0 \approx 1/2n_{cr} \). When the density increases, the distortions created by neighboring ferrons
start to overlap, the corresponding energy barrier lowers, and disappears at \( n = n_{cr} \).

The critical density increases with \( K \) since any devi-
ation of the spins from the easy axis become less favor-
able with the growth of anisotropy energy. The value of \( n = n_{cr} \) decreases with the increase of ratio \( F/J \) since
the smaller canting angles become more favorable with the growth of the electron kinetic energy \( t \) compared with
the exchange integral \( J' \). Note that for small values of
\( F/J \ll 1 \) both types of ferrons remain stable up to the
density \( n = 1/2 \).

Let us consider now the low density limit \( n \to 0 \).
As can be seen from Figs. 8 and 9 the ferron en-
ergy and angle \( \theta_0 \) are practically density independent
at \( n \ll n_{cr} \). Therefore, in zero approximation, we can
consider “coated” ferrons as isolated objects. The nu-
merical analysis shows that the difference between ener-
gies of “coated” and “bare” ferrons \( \Delta E \), weakly depends
on the ratio \( F/J \). Following Ref. 8 it can be shown in
continuous approximation that \( \Delta E \approx \sqrt{8KJ} \), which
is confirmed by computational results. Since the ground
state of the system corresponds to “bare” ferrons, the
ferrons with extended spin distortions can be considered
as elementary excitations with the energy \( \Delta E \). Note,
that these excitations can appear only in pairs since a
creation of a single “coated” ferron strongly disturbs the
ground state and costs the energy at least of the order
of \( J \). It is easy to see that to create a pair of neighbor-
ring “coated” ferrons, one needs to overcome the energy
barrier of the order of \( K/n \) (because it is necessary to
change the orientation of all spins between two ferrons
with respect to easy axis). So, at low densities, this pair
can be considered as a metastable state.

The energy of a ferron in excited state \( \Delta E \) is propor-
tional to the square root of \( K \) and, for the case \( K \ll J \),
it can be rather small in comparison with \( J \). There-
fore, even at low temperatures \( T \ll T_N \sim J \), one can
expect to have a relatively large number of ferrons in
excited state. Using conventional formulas for thermal
averages and having in mind that “coated” ferrons arise
in pairs, we have for the averaged density \( n_1 \) of excited
ferrons \( \langle n_1 \rangle_T = n/(1 + \exp(\Delta E/kT)) \). This approach is
valid only when the density of impurities is less than \( n_{cr} \),
otherwise the ferrons could not be considered as weakly
interacting particles. However, within the order of mag-
nitude the estimates for \( \langle n_1 \rangle_T \) and \( \Delta E \) are valid up to
\( n \approx 2n_{cr} \). Then, at \( n > 2n_{cr} \) the excitations under discus-
sion become unstable if the temperature exceeds a certain
critical value \( kT_{cr} \approx \Delta E/\ln(n/n_{cr} - 1) \). At \( T > T_{cr} \) the
density of “coated” ferrons exceeds \( n_{cr} \).

The “coated” ferrons can be treated as isolated objects
only in the limit of \( n \to 0 \). At finite \( n \), it is necessary to
take into account the density dependence of the fer-
non energy. Since the energy of the “coated” ferrons de-
creases with the growth of their density, the interaction
between them is attractive. This interaction arises due
to the overlapping of the spin distortions of neighboring
ferrons and its characteristic length far exceeds the
lattice constant. Although the calculation presented in
Fig. 8 is valid only for a periodic distribution of the im-
purities, it is natural to expect that the similar attractive
interaction should take place for random distribution of
“coated” ferrons. The detailed calculation of an attrac-
tive interaction between ferrons in a general case is the
subject of further research. We just note here that this
attractive interaction can be, in principle, the possible
mechanism for formation of a long-range phase-separated
state involving large clusters of ferrons.

**IV. CONCLUSION**

We studied the magnetic structure for 1D antiferro-
magnetic chain doped by homogeneously distributed non-
magnetic donor impurities. The ground state of the sys-
tem corresponds to a set of ferrons with characteristic
size of the order of the localization length of electrons
near the impurity. The elementary excitations in the
system are ferrons with extended long-range spin distor-
tions. These excitations can be unstable for some range
of parameters of the system, in particular, at sufficiently
high impurity density. An attractive interaction exists
between ferrons in excited state due to the overlapping
of the extended spin distortions of neighboring ferrons.
This attractive interaction can lead to a phase-separated
state with large clusters of ferrons.

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1. E.L. Nagaev, Phys. Reports 346, 387 (2001).
2. E. Dagotto, T. Hotta, and A. Moreo, Phys. Reports 344, 1
   (2001).
3. M.Y. Kagan and K.I. Kugel, Usp. Fiz. Nauk. 171, 577
   (2001) [Physics - Uspekhi 44, 553 (2001)].
4. E.L. Nagaev, Pis'ma v ZhETF 6 484 (1967) [JETP Lett. 6,
   18 (1967)].
5. S. Pathak and S. Satpathy, Phys. Rev. B 63, 214413 (2001).
6 M.Yu. Kagan, A.V. Klaptsov, I.V. Brodsky, K.I. Kugel, A.O. Sboychakov, and A.L. Rakhmanov, J. Phys. A 36, 9155 (2003).
7 P.G. de Gennes, Phys. Rev. 118, 13 (1960).
8 E.L. Nagaev, JETP Lett. 74, 431 (2001).
9 J. Castro, I. González, and D. Baldomir, cond-mat/0210279