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2008 J. Phys.: Condens. Matter 20 425214

(http://iopscience.iop.org/0953-8984/20/42/425214)

IOP Publishing Journal of Physics: Condensed Matter

J. Phys.: Condens. Matter **20** (2008) 425214 (6pp) doi:10.1088/0953-8984/20/42/425214

Bound magnetic polarons with extended spin distortions on frustrated lattices

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Received 21 May 2008, in final form 15 August 2008
Published 25 September 2008
Online at stacks.iop.org/JPhysCM/20/425214

Abstract

The structure of magnetic polarons in doped two-dimensional antiferromagnets on square and triangular lattices is analyzed. We study the case when a conduction electron is bound by a nonmagnetic donor impurity and forms a ferromagnetic core of the size about the electron localization length (bound magnetic polaron). The exchange interactions between nearest and next-nearest neighbors are taken into account. The crystal is assumed to have a uniaxial magnetic anisotropy. It is found that the magnetic polaron can produce rather extended spin distortions of the antiferromagnetic background around the core. In a wide range of distances r from the core, these distortions decay as $1/r^2$ and $1/r$ for square and triangular lattices, respectively. The characteristic size of this 'coat' decreases when the contribution of the next-nearest-neighbor interactions increases. It is shown that the 'coated' magnetic polaron may be favorable in energy in comparison to the usually considered polaron having the ferromagnetic core without extended spin distortions. We also discuss briefly the shape and the structure of standard unbound (or free) magnetic polarons on square and triangular lattices.

1. Introduction

The formation and structure of small ferromagnetic (FM) metallic droplets (magnetic polarons or ferrons) in an antiferromagnetic (AFM) insulating matrix was discussed beginning from the late 1960s [1, 2] (see [3, 4] for reviews). The simplest case of such objects is a well-defined magnetic polaron with exponentially decreasing tails of magnetic distortions around it. In this case, the intermediate region where the canting angle ν (the angle between nearest-neighbor local spins) changes from 0 (FM domain) to π (AFM domain) is of the order of the interatomic distance d and the radius of the magnetic polaron is a well-defined quantity [5, 6].

However, in the seminal paper of de Gennes on double exchange, the possibility of a slow decay of the AFM order distortions (dipole-like decay of distortions) was discussed [7]. An attempt to get such a type of 'coated' magnetic polarons was made for a one-dimensional (1D) AFM chain in [8–10]. In these papers, it was shown that the characteristic length of the distorted spin surroundings is much larger than the size of the trapping region. In [11], this 1D model was extended to the two-dimensional (2D) case and it was found that the spin distortions decay as $1/r^2$ on a square lattice.

In the present paper, we generalize the model considered in [11] to the case of frustrated lattices. We consider two types of 2D frustrated lattices of antiferromagnetically coupled local spins $\mathbf{S_n}$, namely the square lattice with nearest-neighbor (NN) and next-nearest-neighbor (NNN) or diagonal interactions and the triangular lattice.

Since a lot of magnetic oxides including manganites and cobaltites have layered magnetic structures, and a 2D structure is simply a limiting case of the layered system, our results could be applicable to real magnetic materials.

This paper is organized as follows. In section 2, we introduce the model Hamiltonian and the magnetic configuration of local spins in the absence of conduction

electrons. In section 3, we find the wavefunction and the energy of a conduction electron bound by a donor impurity. In section 4, we calculate the magnetic structure of a 'coated' magnetic polaron. In section 5, we find the energy of a 'coated' magnetic polaron and compare it with the energy of a 'bare' one (a ferromagnetic core without extended spin distortions). In section 6, we discuss the case of unbound magnetic polarons on square and triangular lattices. Finally, in section 7, we summarize our work.

2. Model Hamiltonian

In our model, we treat local spins as classical vectors. We assume that the crystal has uniaxial magnetic anisotropy. Nonmagnetic donor impurities are located in the centers of some unit cells of the lattice. It is assumed that the concentration of dopants is small enough, and therefore we can consider an isolated impurity and restrict ourselves to a single-electron problem. We consider an electron which is bound at a donor impurity by the Coulomb attractive potential. The Coulomb potential V is assumed to be strong in comparison to the other relevant interactions. Namely

$$V \sim J_{\mathrm{H}} \gg t \gg J > J^{'} \gg K, \tag{1}$$

where J_{H} is the Hund's rule coupling, t is the electron hopping integral, J and $J^{'}$ are the NN and NNN AFM exchange interactions, respectively, and K is a constant of the magnetic anisotropy. For this range of parameters, the radius of the electron localization is of the order of d. Below we will measure the distance in units of the lattice constant d, assuming $d = 1$.

We represent classical spins in the form $\mathbf{S_n} = S\mathbf{e_n}$, where $\mathbf{e_n}$ is a unit vector, describing the direction of $\mathbf{S_n}$. The model Hamiltonian can be written as

$$\hat{H} = \hat{H}_{\mathrm{el}} + \hat{H}_{\mathrm{m}}, \tag{2}$$

where

$$\hat{H}_{\mathrm{el}} = -t \sum_{\langle \mathbf{nm}\rangle\sigma} \hat{a}^{\dagger}_{\mathbf{n}\sigma}\hat{a}_{\mathbf{m}\sigma} - \frac{1}{2}J_{\mathrm{H}} \sum_{\mathbf{n}\sigma\sigma'} \hat{a}^{\dagger}_{\mathbf{n}\sigma}(\mathbf{e_n}\boldsymbol{\sigma})_{\sigma\sigma'}\hat{a}_{\mathbf{n}\sigma'} - V\sum_{\mathbf{n}\sigma}\frac{\hat{a}^{\dagger}_{\mathbf{n}\sigma}\hat{a}_{\mathbf{n}\sigma}}{|\mathbf{n}-\mathbf{n}_0|}, \tag{3}$$

$$\hat{H}_{\mathrm{m}} = J\sum_{\langle \mathbf{nm}\rangle} \mathbf{e_n}\mathbf{e_m} + J^{'}\sum_{\langle\langle \mathbf{nm}\rangle\rangle} \mathbf{e_n}\mathbf{e_m} + \hat{H}_K. \tag{4}$$

In these equations, $\hat{a}^{\dagger}_{\mathbf{n}\sigma}$, $\hat{a}_{\mathbf{n}\sigma}$ are the creation and annihilation operators for a conduction electron with spin projection σ at the site $\mathbf{n}$, $\boldsymbol{\sigma}$ are the Pauli matrices, and symbols $\langle\cdots\rangle$ and $\langle\langle\cdots\rangle\rangle$ denote the summation over nearest neighbors and next-nearest neighbors, respectively. The first two terms in $\hat{H}_{\mathrm{el}}$ describe the kinetic energy of the conduction electrons, and the Hund's rule coupling between the conduction electrons and the localized spins, respectively. The last term in $\hat{H}_{\mathrm{el}}$ describes the Coulomb interaction between electrons and the impurity ion located in the center of the unit cell. The first and second terms in $\hat{H}_{\mathrm{m}}$ are the AFM exchange between local spins. The last term is the magnetic anisotropy energy (we will give an explicit expression for this term below). Note that, in contrast to a standard notation, the Hund's rule coupling constant J_{H} already includes the factor S and, similarly, exchange integrals J and J' include the factor S^2.

Let us consider $\hat{H}_{\mathrm{m}}$ without an anisotropy term. This is the so-called 2D J–$J^{'}$ model. In the classical limit, the minimum energy configuration of this model on a square lattice has the conventional Néel order (with two sublattices) for $J^{'}/J < 1/2$ [12]. The minimum energy configuration of the 2D J–$J^{'}$ model on a triangular lattice corresponds to three sublattices with spins in sublattices 2 and 3 rotated by $\pm 120°$ with respect to sublattice 1 (the Yafet–Kittel order) for $J^{'}/J < 1/6$. We consider the Néel order on a square lattice and the Yafet–Kittel order on a triangular lattice. Note that, in the range of parameters under study (J, $J' \ll K$), the anisotropy term does not change the proposed ground state magnetic configuration and only breaks the rotational symmetry of the $\hat{H}_{\mathrm{m}}$ Hamiltonian.

3. Energy of conduction electron

Conduction electrons, appearing at doping, change the antiferromagnetic order of local spins around them. In order to find the magnetic structure at $n \neq 0$, we need to diagonalize first the electronic Hamiltonian $\hat{H}_{\mathrm{el}}$. As was mentioned above, at small doping $n \ll 1$, one can consider a single-electron problem. In this section, we find the energy of the conduction electron both on square and triangular lattices.

We assume that all local spins lie in the xy plane, that is

$$\mathbf{S_n} = S\{\cos\phi_{\mathbf{n}}, \sin\phi_{\mathbf{n}}, 0\}, \qquad (-\pi < \phi_{\mathbf{n}} \leqslant \pi). \tag{5}$$

Note that we treat local spins as classical vectors. In such a treatment for the two-dimensional case, there is not much difference between the Heisenberg model with the usual 3D spins and the xy model. In the limit of strong Hund's rule coupling, $J_{\mathrm{H}} \to \infty$, the spin of the conduction electron at site $\mathbf{n}$ should be parallel to $\mathbf{S_n}$. In this case, the wavefunction of the conduction electron can be written as

$$|\Phi\rangle = \frac{1}{\sqrt{2}}\sum_{\mathbf{n}} \Psi_{\mathbf{n}}\left(\hat{a}^{\dagger}_{\mathbf{n}\uparrow} + \exp(-\mathrm{i}\phi_{\mathbf{n}})\hat{a}^{\dagger}_{\mathbf{n}\downarrow}\right)|0\rangle, \qquad \sum_{\mathbf{n}}|\Psi_{\mathbf{n}}|^2 = 1, \tag{6}$$

where $|0\rangle$ is the vacuum state. The energy of the conduction electron in the state $|\Phi\rangle$ is then

$$E_{\mathrm{el}}[\Phi] = \langle\Phi|\hat{H}_{\mathrm{el}}|\Phi\rangle = -t\sum_{\langle \mathbf{nm}\rangle}\left[T_{\mathbf{nm}}\Psi^{*}_{\mathbf{n}}\Psi_{\mathbf{m}} + T^{*}_{\mathbf{nm}}\Psi_{\mathbf{n}}\Psi^{*}_{\mathbf{m}}\right] - \frac{1}{2}J_{\mathrm{H}} - V\sum_{\mathbf{n}}\frac{|\Psi_{\mathbf{n}}|^2}{|\mathbf{n}-\mathbf{n}_0|}, \tag{7}$$

where

$$T_{\mathbf{nm}} = \frac{1}{2}\left[1 + \exp\left(\mathrm{i}(\phi_{\mathbf{n}} - \phi_{\mathbf{m}})\right)\right] = \cos\frac{\nu_{\mathbf{nm}}}{2}\exp(\mathrm{i}\omega_{\mathbf{nm}}), \qquad \nu_{\mathbf{nm}} = \phi_{\mathbf{n}} - \phi_{\mathbf{m}}, \qquad \omega_{\mathbf{nm}} = \frac{\nu_{\mathbf{nm}}}{2}. \tag{8}$$

Here, $\nu_{\mathbf{mn}}$ is the angle between local spins $\mathbf{S_m}$ and $\mathbf{S_n}$ (canting angle), and $\omega_{\mathbf{mn}}$ is the Berry phase [13, 14]. Note that we consider here a planar configuration of local spins, so all angles in equation (8) are within the xy plane.

The ground state electron energy at given angles $\phi_{\mathbf{n}}$ is found by minimization of equation (7) with respect to $\Psi_{\mathbf{n}}$. In the limit of strong electron–impurity coupling, $V \to \infty$, we can assume that $\Psi_{\mathbf{n}}$ are nonzero only at sites nearest to the impurity ($\mathbf{n}_j$, $j = 1, \ldots, 4$ for a square lattice, $j = 1, \ldots, 3$ for a triangular lattice). In this case, we obtain an analytical expression for the electron energy:

$$E_{\mathrm{el}}(\phi_i) = -\frac{1}{2}J_{\mathrm{H}} - \frac{V}{a} - t\varepsilon(c_{ij}), \tag{9}$$

where

$$\varepsilon(c_{ij}) = \frac{1}{\sqrt{2}}\Big[c_{12}^2 + c_{23}^2 + c_{34}^2 + c_{41}^2 + \Big[[(c_{12} - c_{34})^2 + (c_{23} + c_{41})^2] \times [(c_{12} + c_{34})^2 + (c_{23} - c_{41})^2]\Big]^{1/2}\Big]^{1/2}, \qquad a = \frac{1}{\sqrt{2}} \tag{10}$$

for a square lattice, and

$$\varepsilon(c_{ij}) = g(c_{ij}) + \frac{c_{12}^2 + c_{23}^2 + c_{31}^2}{3g(c_{ij})},$$
$$g(c_{ij}) = \Big[c_{12}c_{23}c_{31} + \frac{1}{3\sqrt{3}}|(c_{12}^2 + c_{23}^2 + c_{31}^2)^3 - 27c_{12}^2c_{23}^2c_{31}^2|^{1/2}\Big]^{1/3}, \qquad a = \frac{1}{\sqrt{3}} \tag{11}$$

for a triangular lattice. In these equations, $\phi_i = \phi_{\mathbf{n}_i}$, $c_{ij} = \cos[(\phi_i - \phi_j)/2]$ and a is the distance (in units of lattice constant d) between the impurity ion and the site nearest to the impurity.

The electron energy E_{el} has a minimum when all spins $\mathbf{S}_{\mathbf{n}_j}$ are parallel to each other. So, we have a bound magnetic polaron state, which can be described by a ferromagnetic core of radius a embedded into the antiferromagnetic matrix.

4. Magnetic structure

Now, we consider the magnetic structure in the system of local spins with one bound electron. It can be done by minimization of the total energy

$$E = E_{\mathrm{el}}(\phi_i) + E_{\mathrm{m}},$$
$$E_{\mathrm{m}} = J\sum_{\langle\mathbf{nm}\rangle}\cos(\phi_{\mathbf{n}} - \phi_{\mathbf{m}}) + J'\sum_{\langle\langle\mathbf{nm}\rangle\rangle}\cos(\phi_{\mathbf{n}} - \phi_{\mathbf{m}}) + H_K(\phi_{\mathbf{n}}) \tag{12}$$

with respect to angles $\phi_{\mathbf{n}}$, but it is convenient to make first the following transformation. In the absence of a magnetic polaron, the square lattice consists of two magnetic sublattices with antiparallel magnetizations. In one sublattice, we perform the transformation of angles $\phi_{\mathbf{n}} \to \pi + \phi_{\mathbf{n}}$. As a result, an AFM order becomes an FM one, and vice versa. Such a transformation allows us to work with a continuously changing orientation of spins outside the ferron core. A triangular lattice consists of three magnetic sublattices with magnetizations rotated with respect to each other by an angle $2\pi/3$. In two of them, we perform the transformation of the angles $\phi_{\mathbf{n}} \to \phi_{\mathbf{n}} \pm 2\pi/3$.

In expression (12), $H_K(\phi_{\mathbf{n}})$ is an anisotropy term. We assume that, after the transformation of angles, the magnetic anisotropy term has the same form both for square and triangular lattices:

$$H_K(\phi_{\mathbf{n}}) = K\sum_{\mathbf{n}}\sin^2\phi_{\mathbf{n}}, \tag{13}$$

where K effectively contains a factor S^2, in contrast to the standard notation. For a square lattice, embedded into equation (13) describes the usual uniaxial magnetic anisotropy with the x axis being an easy axis, whereas for a triangular lattice, this kind of anisotropy favors the alignment of spin along one of the sides of the triangular unit cell in each sublattice.

From the symmetry considerations, it is clear that angles ϕ_i for local spins inside the magnetic polaron are related to each other by some relationships. In the case of a magnetic polaron with extended spin distortions, these relationships are the following:

$$\phi_1 = \phi_3 = \phi_0, \qquad \phi_2 = \phi_4 = -\phi_0, \qquad 0 < \phi_0 \leqslant \pi/2 \tag{14}$$

for a square lattice and

$$\phi_1 = 0, \qquad \phi_2 = -\phi_3 = \phi_0, \qquad 0 < \phi_0 \leqslant 2\pi/3 \tag{15}$$

for a triangular lattice.

We find the magnetic structure by minimization of the total energy (12), for a triangular lattice numerically (similar calculations for a square lattice without a J' term were carried out in [11]). In order to get analytical estimations concerning the behavior of spin distortions, we also perform calculations of the magnetic structure in the continuum approximation. Namely, angles $\phi_{\mathbf{n}}$ are treated as the values of the continuous function $\phi(\mathbf{r})$ at points $\mathbf{r} = \mathbf{n} - \mathbf{n}_0$. This approximation is valid when canting angles do not change significantly between two neighboring sites. Expanding $\phi(\mathbf{r})$ on the nearest-neighbor sites in a Taylor series up to second order in the intersite distance and changing in (12) the summation by integration over $\mathbf{r}$ outside the magnetic polaron core, we find an approximate expression for the magnetic energy $E_{\mathrm{m}} = E_{\mathrm{m}}^1 + E_{\mathrm{m}}^2$:

$$E_{\mathrm{m}}^1 = 8J\left(1 + \frac{\kappa_0}{4}\right)\sin^2\phi_0 \tag{16}$$

for square lattice,

$$E_{\mathrm{m}}^1 = J\left(\frac{1}{2} - 4\cos^2\left(\frac{\pi}{3} - \frac{\phi_0}{2}\right) + 8\cos^4\left(\frac{\pi}{3} - \frac{\phi_0}{2}\right) + \frac{3\kappa_0}{4}\sin^2\phi_0\right) \tag{17}$$

for a triangular lattice, and

$$E_{\mathrm{m}}^2 = \alpha J\left(1 - \frac{\eta}{\eta_{\mathrm{c}}}\right)\int_{|\mathbf{r}|\geqslant a} \mathrm{d}^2r\big[(\nabla\phi)^2 + \kappa\phi^2\big], \tag{18}$$

where $\eta = J'/J$, $\kappa_0 = K/(\alpha J)$, $\kappa = \kappa_0/(1-\eta/\eta_c)$, and $\eta_c = 1/2$, $\alpha = 1/2$ ($\eta_c = 1/6$, $\alpha = 3/8$) for a square (triangular) lattice. We assume that the state without magnetic polarons has zero energy. The term E^1_m comes from the summation over spins in the magnetic polaron core. In E^2_m we use an approximation $\sin^2\phi_{\mathbf{n}} \approx \phi^2_{\mathbf{n}}$ in the anisotropy term.

Minimizing the energy E^2_m with respect to an angle $\phi(\mathbf{r})$, we obtain

$$\Delta\phi - \kappa\phi = 0. \tag{19}$$

Equation (19) should be solved with the boundary conditions at infinity:

$$\phi(\mathbf{r}) \to 0, \qquad \mathbf{r} \to \infty, \tag{20}$$

and with some boundary conditions at the surface of the magnetic polaron.

We model the magnetic polaron by a circle of radius a and choose $\phi(\mathbf{r})$ using the Dirichlet boundary conditions $\phi(\mathbf{r})|_{r=a} = \widetilde{\phi}(\zeta)$, where we introduce polar coordinates (r, ζ) in the xy plane. The function $\widetilde{\varphi}(\zeta)$ can be found in the following way. On a square lattice, $\widetilde{\varphi}(\zeta)$ should satisfy the symmetry conditions (14) at points $\zeta_j = \pi(2j-1)/4$:

$$\widetilde{\phi}(\zeta_j) = \phi_j, \qquad j = 1, 2, 3, 4. \tag{21}$$

On a triangular lattice, $\widetilde{\varphi}(\zeta)$ should satisfy the symmetry conditions (15) at points $\zeta_j = 2\pi(j-1)/3$:

$$\widetilde{\phi}(\zeta_j) = \phi_j, \qquad j = 1, 2, 3. \tag{22}$$

Since the function $\widetilde{\phi}(\zeta)$ is a periodic one, it can be expanded in a Fourier series:

$$\widetilde{\phi}(\zeta) = \sum_{m=0}^{\infty}[a_m \cos(m\zeta) + b_m \sin(m\zeta)]. \tag{23}$$

Keeping the minimal number of terms in these series needed to satisfy the boundary conditions (21) or (22), we obtain

$$\widetilde{\phi}(\zeta) = \phi_0 \sin 2\zeta \tag{24}$$

for a square lattice and

$$\widetilde{\phi}(\zeta) = \frac{2\phi_0}{\sqrt{3}} \sin\zeta \tag{25}$$

for a triangular lattice.

The solution to equation (19) is

$$\phi(\mathbf{r}) = \phi_0 \frac{K_2(r/R_*)}{K_2(a/R_*)} \sin 2\zeta \tag{26}$$

for a square lattice and

$$\phi(\mathbf{r}) = \frac{2\phi_0}{\sqrt{3}} \frac{K_1(r/R_*)}{K_1(a/R_*)} \sin\zeta \tag{27}$$

for a triangular lattice, where $K_1(x)$ and $K_2(x)$ are the Macdonald functions of the first and second order, respectively.

The characteristic decay length of the spin distortions around the ferromagnetic core is $R_* = 1/\sqrt{\kappa}$:

$$R_* = R_0\sqrt{1 - \frac{\eta}{\eta_c}}, \tag{28}$$

where $R_0 = 1/\sqrt{\kappa_0} \sim \sqrt{J/K} \gg 1$ is the decay length of the distortions in the absence of the NNN interaction. We see that R_* decreases with the growth of $\eta = J'/J$, the ratio between the NNN and NN coupling constants. Note that the continuum approximation fails at $R_* \sim 1$, when η is closed to η_c. In the limit $\eta \to \eta_c$, the decay length of distortions becomes less than the lattice constant and the 'coat' disappears.

Within the range $r < R_*$, $\phi(\mathbf{r})$ behaves as a^2/r^2 for a square lattice and as a/r for a triangular lattice, whereas at large distances, it decreases exponentially $\phi(\mathbf{r}) \propto \exp(-r/R_*)$. Let us note that, in the case of low anisotropy ($K \ll J$), the distance, where the function $\phi(\mathbf{r})$ has a power-law behavior, can be large enough (in agreement with the argument of de Gennes [7]). Let us recall that a rather weak uniaxial anisotropy leads to the competition between the energy loss due to the alignment of spins perpendicular to the anisotropy axis and the energy gain due to a slower decay of distortions.

5. Energy of magnetic polaron

Let us calculate the energy of the 'coated' magnetic polaron, E^{coated}_f, in the continuous approximation. Substituting solutions (26) and (27) in equation (18) and performing the integration, we find

$$E^2_m = \pi J\phi_0^2\left(1 - \frac{\eta}{\eta_c}\right)\left[1 + \frac{a\sqrt{\kappa}K_s(a\sqrt{\kappa})}{2K_{s+1}(a\sqrt{\kappa})}\right], \tag{29}$$

where $s = 1$ ($s = 0$) for a square (triangular) lattice. We remind ourselves that the total magnetic energy $E_m = E^1_m + E^2_m$, where E^1_m is given by equations (16) and (17) for different lattices.

Substituting the symmetry relations (14) and (15) for angles ϕ_i into expression (9) for electron energy, we express the energy of a conduction electron E_{el} via the angle ϕ_0:

$$E_{el} = -2t \sin\phi_0 \tag{30}$$

for a square lattice and

$$E_{el} = -t\varepsilon(y), \qquad y = \cos\left(\frac{\pi}{3} - \frac{\phi_0}{2}\right),$$
$$\varepsilon(y) = g(y) + \frac{2y^2 + (2y^2-1)^2}{3g(y)},$$
$$g(y) = \left[y^2(2y^2-1) + \frac{1}{3\sqrt{3}}\left|1 - 3y^2 - 6y^4 + 8y^6\right|\right]^{1/3} \tag{31}$$

for a triangular lattice.

The energy of a 'coated' magnetic polaron is $E^{\text{coated}}_f = E_{el}(\phi^*_0) + E_m(\phi^*_0)$, where the angle ϕ^*_0 is found by minimization of E^{coated}_f. Note that this angle differs from $\pi/2$ (on a square lattice) or $2\pi/3$ (on a triangular lattice) at any finite t/J, and $\phi^*_0 \to \pi/2$ ($\phi^*_0 \to 2\pi/3$) at $t/J \to \infty$, that is, canting angles inside the magnetic polaron core are nonzero. This means that the 'coated' magnetic polaron has a magnetization lower than its saturation value. It follows from (29) that the energy of the 'coated' magnetic polaron

increases with the growth of the constant K of magnetic anisotropy.

In addition to a 'coated' magnetic polaron, there is another solution to the set of equations $\partial(E_{\rm el}(\phi_i) + E_{\rm m}(\{\phi_{\mathbf{n}}\}))/\partial\phi_{\mathbf{n}} = 0$, describing the magnetic polaron without spin distortions ('bare' magnetic polaron). The angles $\phi_{\mathbf{n}}$ for the local spins (after the transformation described above), corresponding to this solution, are the following:

$$\phi_{\mathbf{n}} = 0, \qquad \mathbf{n} \neq \mathbf{n}_j, \qquad \phi_{\mathbf{n}_1} = \phi_{\mathbf{n}_3} = 0, \qquad \phi_{\mathbf{n}_2} = \phi_{\mathbf{n}_4} = \pi \tag{32}$$

for a square lattice and

$$\phi_{\mathbf{n}} = 0, \qquad \mathbf{n} \neq \mathbf{n}_j, \qquad \phi_{\mathbf{n}_1} = \pi, \qquad \phi_{\mathbf{n}_2} = -\phi_{\mathbf{n}_3} = -\phi_0^{'}, \qquad 0 < \phi_0^{'} \leqslant \pi/3 \tag{33}$$

for a triangular lattice. The energy of a 'bare' magnetic polaron is

$$E_f^{\rm bare} = -2t + 16\left(1 - \tfrac{3}{4}\eta\right) J \tag{34}$$

for a square lattice and

$$E_f^{\rm bare} = -t\varepsilon\left(\sin\left(\frac{\phi_0^{'}}{2} + \frac{\pi}{3}\right)\right) - 10\eta\left(2 - \cos\phi_0^{'}\right) J + \frac{3\kappa_0}{4} J \sin^2\phi_0^{'} + \left[\frac{19}{2} - 2\sin\left(\phi_0^{'} + \frac{\pi}{6}\right) - 4\cos\left(\phi_0^{'} + \frac{\pi}{3}\right) - \cos\left(2\phi_0^{'} + \frac{\pi}{3}\right)\right] J \tag{35}$$

for a triangular lattice, where the function $\varepsilon(y)$ is given by equation (31) and the angle $\phi_0^{'}$ is found by minimization of $E_f^{\rm bare}$.

Note that expressions (34) and (35) are derived by exact minimization of the total energy. If we compare the energies of 'bare' and 'coated' magnetic polarons using formulae of the continuous approximation for $E_f^{\rm coated}$, we obtain for a triangular lattice that, even for $K = 0$, $\Delta E = E_f^{\rm coated} - E_f^{\rm bare} > 0$ (for a square lattice we have in this case $\Delta E < 0$). The numerical analysis shows, however, that $\Delta E < 0$ (we consider a cluster containing 40×40 sites, and the further increase of the number of sites does not change the obtained results). For example, at $t = 50J$ and $J^{'} = K = 0$, the numerical calculations give $\Delta E/J = -1.2$. Thus, formulae for $E_f^{\rm coated}$ of the continuous approximation overestimate significantly the magnetic polaron energy. A main error comes from the region near the magnetic polaron. On the other hand, the analysis shows that these formulas properly describe the dependence of $E_f^{\rm coated}$ on the model parameters. Thus, at relatively small values of K/J, the 'coated' magnetic polaron is more favorable in energy than the 'bare' one, both for square and triangular lattices.

6. Free and bound magnetic polarons

Let us notice again that in the previous sections we considered 'coated' and 'bare' magnetic polarons bound by nonmagnetic donor impurities. Effectively, we were dealing with an insulator (the Mott limit) with a small density of the charge carriers $n \ll 1/R_*^2$, where the 'coats' of bound polarons do not overlap. In this limit, we find that the 'coated' state of the bound magnetic polaron with nontrivial magnetic structure of slowly decaying spin distortions at intermediate distances $a < r < R_*$ and non-saturated small FM core for $r < a$ is more favorable in energy. Note that, for the typical anisotropy energies $K/J \sim 10^{-2}$, we have $R_* = (J/2K)^{1/2} \simeq 7$ ($J^{'} = 0$) in units of the lattice constant d. At the same time, $a \sim 1$.

Let us now consider the model without impurity ions ($V = 0$). Here and further on in this section, n denotes the density of conduction electrons. Even without interaction with impurities the charge carriers can become self-trapped (a conduction electron forms the well of FM-ordered local spins and becomes bound by it), giving rise to magnetic polarons. Let us refer to such polarons as unbound or free. It is interesting to compare the size and the structure of free and bound ('coated') magnetic polarons for square and triangular lattices. In [15], it was shown that the radius of a free magnetic polaron on a square lattice is

$$R_{\rm pol} = \left(\frac{j_{0,1}^2 t}{4\pi J}\right)^{1/4}, \tag{36}$$

where $j_{0,1}$ is the first zero of the Bessel function, $J_0(j_{0,1}) = 0$. This result is obtained by the standard minimization procedure (see [15] for details). The most favorable shape of the magnetic polaron is a circle with an area $\Omega = \pi R_{\rm pol}^2$. To be more specific, in order to find $R_{\rm pol}$ from the Ψ function of the electron inside the magnetic polaron with rigid boundary conditions $\Psi(r = R_{\rm pol}) = 0$ in the 2D circular geometry, we have to find the energy of the deepest bound state (counting from the bottom of the potential well) in the well with the depth $W/2$ ($W = 2zt$, where z is the number of nearest neighbors) and the width $r = R_{\rm pol}$ (where r is the polar coordinates in 2D) [15]. The corresponding Schrödinger equation is

$\hat{H}\Psi = E\Psi$, where

$$\hat{H} = -t\Delta_r = -t\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right). \tag{37}$$

As a result, $E_{\rm kin} = t(j_{0,1}/R_{\rm pol})^2$. We also take into account the loss in the Heisenberg exchange energy, which for the circular shape of the magnetic polaron yields

$$E_{\rm mag} = \pi J z R_{\rm pol}^2. \tag{38}$$

After that, we minimize the total energy $E_{\rm tot} = E_{\rm kin} + E_{\rm mag}$ with respect to $R_{\rm pol}$ and arrive at the result (36).

In the same manner, we can get the radius and the most favorable shape of a free magnetic polaron on the triangular lattice in the case of the planar spin configurations. It is again a circle with a radius

$$R_{\rm pol} = \left(\frac{j_{0,1}^2 t}{3\pi J}\right)^{1/4}. \tag{39}$$

Note that the difference for the Schrödinger equation on a triangular lattice from equation (37) is a factor 3/4 at $t\Delta_r$.

This difference is just a difference in effective masses for the two lattices. Hence, the volumes (areas) of free magnetic polarons on square and triangular lattices in 2D differ only by a numerical factor $\frac{\Omega_{\rm square}}{\Omega_{\rm triang}} = \sqrt{\frac{3}{4}}$. For the values typical of manganites, $\frac{t}{J} \sim 100$, we have $R_{\rm pol} \sim 3$ for free polarons both on square and triangular lattices. Hence, the typical sizes (extensions) of free and bound polarons are of the same order of magnitude: $R_* \simeq (5–7)$ for the bound polaron and $R_{\rm pol} \simeq (2–3)$ for the free polaron. However, their structures are quite different. Note that a free polaron has a saturated FM core of the size of $R_{\rm pol}$ and very rapidly (exponentially) decaying spin distortions outside of it (see [8]).

It is interesting to follow more closely how the free and bound magnetic polarons become more similar when we decrease the value of the Coulomb interaction energy V (or enhance the density of impurity ions). Preliminary estimates show that the bound magnetic polarons with the structure, considered in this paper, exist for $V > V_{\rm c} \sim 2t$. For $V < V_{\rm c}$, the FM core of the bound magnetic polaron starts to grow and could reach the typical values of the core of the free magnetic polaron, so the free and bound magnetic polarons are very similar in this case. Note that in real manganites $V \sim V_{\rm c}$.

It is possible, also, to estimate the typical Mott limit value of the critical charge carrier density (corresponding to non-overlapping polarons) $n_{\rm c}$ for manganites: $n_{\rm c} \sim 1/R_*^2$ in 2D. So, $n_{\rm c} \simeq (0.5–1)\%$ if $R_* \simeq (5–7)$.

7. Conclusions

We considered the structure of bound magnetic polarons in 2D antiferromagnets with square and triangular lattices. We found that the magnetic distortions created by a magnetic polaron decay as $1/r^2$ and $1/r$ on square and triangular lattices, respectively. On a triangular lattice, the magnetic distortions decay more slowly (as $1/r$) due to the strong geometrical frustration. On the other hand, the additional frustration coming from the NNN exchange interaction decreases the characteristic decay length of the spin distortions R_* around the ferromagnetic core. At not too large a magnetic anisotropy constant, the difference in energies of 'coated' and 'bare' magnetic polarons, ΔE, is negative and the 'coated' magnetic polaron is more favorable than the 'bare' one.

Note that on a triangular lattice the value of $\eta = J'/J$, when the transformation of magnetic configuration takes place, is about $0.77\eta_{\rm c}$. However, the long-range spin distortions exist when $R_* \sim \sqrt{(1-\eta/\eta_c)J/K} \gg 1$, and the difference between $\eta_{\rm c}$ and $0.77\eta_{\rm c}$ does not lead to the qualitative difference in the behavior of spin distortions.

Our results were obtained in the limit of strong electron–impurity coupling, $V \to \infty$. In this case, the wavefunction $\Psi_{\mathbf{n}}$ of the conduction electron is nonzero only at the sites nearest to the impurity, and one can calculate the electron energy $E_{\rm el}$ exactly. At finite V, the wavefunction extends over larger distances and we should calculate the magnetic structure simultaneously with $\Psi_{\mathbf{n}}$. As we already mentioned, even at $V = 0$, the magnetic polaron is a stable object in a wide range of parameters of the model. This (unbound or free) magnetic polaron exists due to the trapping of a charge carrier in the potential well of ferromagnetically oriented local spins.

The structure of 'coated' magnetic polarons can be more complicated on kagomé lattices or for the lattices with more complicated types of magnetic interactions (self-trapped magnetic polarons in the case of anisotropic exchange integrals were investigated in [15]).

Acknowledgments

The work was supported by the European project CoMePhS (contract NNP4-CT-2005-517039), the International Science and Technology Center, grant G1335, the Russian Foundation for Basic Research, project 08-02-00212, and the Russian Science Support Foundation.

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