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Abstract

We analyse the possibility of nanoscale phase separation manifesting itself in the formation of ferromagnetic (FM) polarons (FM droplets) in the general situation of doped anisotropic three- and two-dimensional antiferromagnets. In these cases, we calculate the shape of the most energetically favourable droplets. We show that the binding energy and the volume of a FM droplet in the three-dimensional (3D) case depend upon only two universal parameters $\bar{J} = (J_x + J_y + J_z)S^2$ and $t_{\text{eff}} = (t_x t_y t_z)^{1/3}$, where $\bar{J}$ and t_{eff} are effective antiferromagnetic (AFM) exchange and hopping integrals, respectively. In the two-dimensional (2D) case these parameters have the form $\bar{J} = (J_x + J_y)S^2$ and $t_{\text{eff}} = (t_x t_y)^{1/2}$. The most favourable shape of a ferromagnetic droplet corresponds to an ellipse in the 2D case and to an ellipsoid in the 3D case.

1. Introduction

The problem of electronic phase separation with the formation of ferromagnetic (FM) or paramagnetic (PM) spin polarons (magnetic droplets or ferrons) due to the self-trapping of charge carriers in an antiferromagnetic (AFM) matrix has become very popular, especially in studies of high-T_c superconductors and systems with the colossal magnetoresistance (such as LaMnO$_3$ manganites doped by Ca). For isotropic materials, the size and shape of FM droplets was evaluated in several papers, starting with the seminal work of Nagaev [1] (for more details see [2]). The characteristic size of a FM droplet turns out to be of the order of 15–20 Å and its optimum shape in isotropic three-dimensional (3D) manganites is a spherical. Later on, Kagan and Kugel [3] analysed the case of layered manganites (like(La, Ca)$_{n+1}$Mn$_n$O$_{3n+1}$) and demonstrated that the droplets with the lowest energy have an ellipsoidal shape. The FM droplets of cylindrical shape considered first by Nagaev [5] for this class of manganites

correspond to a higher energy. Currently, the phase separation in anisotropic materials is also being addressed in connection with low-dimensional organic compounds [6] and quasi-one-dimensional magnets such as $BaCoO_3$ [7, 8]. Magnetic polarons in doped one-dimensional (1D) AFM magnetic chains were recently considered in [9–11]. In these papers, the possibility of rather long-range magnetic distortions around the polaron was demonstrated.

Another possibility for a strongly anisotropic situation arises when we take into account the interplay between the microscopic phase separation and charge ordering (stripe formation), include Jahn–Teller-type effects (orbital degrees of freedom), or consider stable crystallographic distortions. In these cases, the quasi-1D zig-zag or ladder structures are often observed in the corresponding systems [12, 13].

In this paper we present calculations concerning the shape and size of FM droplets in anisotropic two-dimensional (2D) or 3D cases when, generally speaking, the electron hopping integrals t_x, t_y and t_z along x, y and z directions, as well as the AFM exchange integrals J_x, J_y and J_z are different. We find that, by analogy with the situation in layered manganites [3], the most favourable shape of a FM droplet is ellipsoidal. Moreover, the binding energy and the effective volume of the droplet are expressed only in terms of universal averaged parameters $\bar{J} = (J_x + J_y + J_z)S^2$ and $t_{eff} = (t_x t_y t_z)^{1/3}$. These results are interesting, in particular in relation to the neutron scattering experiments, giving an indication of the existence of FM clusters with different shapes in perovskite and layered manganites [14–16]. Additional evidence concerning nanoscale inhomogeneities in layered manganites comes from scanning tunnelling microscopy with atomic-scale resolution [17].

Our paper is organized as follows. First, we consider the purely 2D situation and find the most favourable shape for a 2D ferron comparing the energies of elliptical and rectangular droplets in the general anisotropic 2D case: $t_x \neq t_y$ and $J_x \neq J_y$. We find that in two dimensions the minimum energy corresponds to an elliptical shape. Then we include the third dimension (J_z and t_z) and compare the energies of the cylinder and ellipse in the case when both of them have the optimum elliptical shape of the 2D cross-sections. We find again that the minimum energy in the 3D case corresponds to an ellipsoidal shape for FM droplets. At the end of the paper we provide some discussions and conclusions.

2. The shape of FM droplets in the anisotropic 2D case

Let us first consider the anisotropic 2D case. In this case, there are two different electron hopping integrals, $t_x \neq t_y$, and two different constants of the AFM exchange interaction, $J_x \neq J_y$. To some extent, this case has a lot of similarities with the two-leg ladder systems rather popular nowadays (see, for example, [18] and references therein).

Throughout this paper, we consider the Kondo-lattice model with the Hamiltonian

$$\hat{H} = J_H \sum_i \mathbf{S}_i \boldsymbol{\sigma}_i + \sum_{\langle ij \rangle_\alpha} J_\alpha \mathbf{S}_i \mathbf{S}_j + \sum_{\langle ij \rangle_\alpha} t_\alpha c_i^\dagger c_j, \tag{1}$$

where $c_i^\dagger$ and c_i are electron creation and annihilation operators at site i, $\alpha = \{x, y\}$ for a square lattice in 2D, $\langle ij \rangle_\alpha$ denote the neighbouring sites in the lattice along the α direction, $\boldsymbol{\sigma}_i = \frac{1}{2} c_i^\dagger \boldsymbol{\sigma} c_i$ is the spin of a conduction electron ($\boldsymbol{\sigma}$ is the Pauli matrix), $\mathbf{S}_i$ is a local spin, J_α are AFM exchange integrals, t_α are the hopping integrals for conduction electrons and the parameter J_H corresponds to the Hund's rule coupling between a local spin $\mathbf{S}$ and a spin of a conduction electron.

We work in the double-exchange limit, which implies that $J_H \gg \{t_x, t_y\} \gg \{J_x, J_y\}$. In this case, the ground state of the system is unstable toward the nanoscale phase separation [1–3] with the formation of FM polarons inside the AFM matrix. Let us now evaluate the total energy of the phase-separated state for different shapes of ferrons possible in the 2D case.

2.1. A rectangular ferron

Let us first consider a rectangular FM droplet (ferron) located at the square lattice with the intersite distance a. Its characteristic sizes along the x- and y-axes are L_x and L_y, respectively. The dimensionless volume Ω of such a ferron can be defined as $\Omega = L_x L_y / a^2$. The kinetic energy of charge carriers (electrons or holes) within the FM droplet is

$$E_{\text{kin}} = -2t_x n - 2t_y n + \varepsilon_0 n, \tag{2}$$

where n is the concentration of charge carriers and ε_0 is a binding energy corresponding to the first (the lowest) level in the rectangular potential well. The latter can be found by solving the corresponding Schrödinger equation (see [3])

$$\hat{H}_{\text{kin}} \Psi(x, y) = \varepsilon_0 \Psi(x, y), \tag{3}$$

where

$$\hat{H}_{\text{kin}} = -a^2 \left(t_x \frac{\partial^2}{\partial x^2} + t_y \frac{\partial^2}{\partial y^2} \right). \tag{4}$$

In the present paper, we consider a well-defined ferron (without an extended tail of magnetic distortions). Such a situation is characteristic for almost all models of ferrons (see the discussion in [4] and references therein); however, it was shown recently that ferrons with more extended spin distortions can also exist [9, 10, 19], but this problem requires special consideration. For ferron with sharp boundaries, the corresponding boundary conditions have the form

$$\Psi(x = L_x, y) = \Psi(x, y = L_y) = 0. \tag{5}$$

Hence,

$$\Psi(x, y) = \sin \frac{\pi x}{L_x} \sin \frac{\pi y}{L_y} \tag{6}$$

and

$$\varepsilon_0 = t_x \left(\frac{\pi a}{L_x} \right)^2 + t_y \left(\frac{\pi a}{L_y} \right)^2. \tag{7}$$

Now, we can proceed to the evaluation of the potential energy given by the terms related to the AFM exchange interaction. In the domains with ferromagnetic order (ferrons), the AFM exchange leads to the positive contribution to the total energy

$$E_{\text{pot1}} = 2(J_x + J_y)S^2 n \frac{L_x L_y}{a^2}. \tag{8}$$

For the AFM regions which are free of ferrons the corresponding contribution to the energy can be written as

$$E_{\text{pot2}} = -2(J_x + J_y)S^2 \left(1 - n \frac{L_x L_y}{a^2} \right). \tag{9}$$

Hence, the total potential energy yields

$$E_{\text{pot}} = -2(J_x + J_y)S^2 + 4(J_x + J_y)S^2 n \frac{L_x L_y}{a^2}. \tag{10}$$

Note that since a lattice site interacts with the sites along all axes we always have the sum of exchange integrals in the expressions for the magnetic energy. As a result, the total energy related to the formation of FM droplets has the form

$$E_{\text{tot}} = -2[t_x n + t_y n + (J_x + J_y)S^2]$$
$$+ n \left[t_x \left(\frac{\pi a}{L_x} \right)^2 + t_y \left(\frac{\pi a}{L_y} \right)^2 \right] + 4(J_x + J_y)S^2 n \frac{L_x L_y}{a^2}. \tag{11}$$

The minimization of energy (11) with respect to L_x and L_y gives

$$
\begin{aligned}
\frac{\partial E_{\text{tot}}}{\partial L_x} &= -2nt_x \frac{\pi^2 a^2}{L_x^3} + 4(J_x + J_y)nS^2 \frac{L_y}{a^2} = 0, \\
\frac{\partial E_{\text{tot}}}{\partial L_y} &= -2nt_y \frac{\pi^2 a^2}{L_y^3} + 4(J_x + J_y)nS^2 \frac{L_x}{a^2} = 0.
\end{aligned}
\tag{12}
$$

A solution to equations (12) reads

$$
\begin{aligned}
t_x \pi^2 &= 2\frac{L_y L_x^3}{a^4}(J_x + J_y)S^2, \\
t_y \pi^2 &= 2\frac{L_x L_y^3}{a^4}(J_x + J_y)S^2.
\end{aligned}
\tag{13}
$$

Multiplying both equations (13) by each other, we find

$$
\left(\frac{L_y L_x}{a^2}\right)^4 = \frac{\pi^4 t_x t_y}{4(J_x + J_y)^2 S^4}.
\tag{14}
$$

Now, introducing notation

$$
t_{\text{eff}} = (t_x t_y)^{1/2}, \qquad \bar{J} = (J_x + J_y)S^2,
\tag{15}
$$

we find

$$
\left(\frac{L_y L_x}{a^2}\right)^4 = \Omega^4 = \frac{\pi^4 t_{\text{eff}}^2}{4\bar{J}^2}.
$$

Thus, the dimensionless volume (area) Ω of a 2D ferron can be written as

$$
\Omega = \frac{\pi}{\sqrt{2}}\left(\frac{t_{\text{eff}}}{\bar{J}}\right)^{1/2}.
\tag{16}
$$

We get quite a remarkable relationship expressing the volume of a 2D ferron in terms of the $t_{\text{eff}}/\bar{J}$ ratio.

The ratio of sizes for this rectangular ferron can be easily found from equations (12)

$$
\frac{L_x}{L_y} = \sqrt{\frac{t_x}{t_y}}.
\tag{17}
$$

Note that this ratio is independent of exchange integrals J_x and J_y, since the magnetic energy depends only on their sum.

Correspondingly, the minimized total energy (11) takes the form

$$
E_{\text{tot}} = -2(t_x n + t_y n + \bar{J}) + 4\pi\sqrt{2}n(t_{\text{eff}}\bar{J})^{1/2}.
\tag{18}
$$

Introducing the energy of a FM polaron by the relationship

$$
E_{\text{pol}} = E_{\text{tot}} + 2(t_x n + t_y n + \bar{J}),
\tag{19}
$$

we get finally

$$
E_{\text{pol}} = 8n\Omega\bar{J} = 4\pi\sqrt{2}n(t_{\text{eff}}\bar{J})^{1/2}.
\tag{20}
$$

It is again worth noting that the energy of the FM polaron in 2D depends only upon the product of t_{eff} and $\bar{J}$.

2.2. An elliptical ferron

Now, we can consider the energy a two-dimensional FM polaron having the shape of an ellipse. For the same characteristic sizes (principal axes) of the ferron, its volume in the case of an ellipse is $\Omega = \pi L_x L_y / a^2$. The corresponding kinetic energy is again given by equations (2)–(4). To solve the Schrödinger equation in this geometry, we should transform an ellipse to a circle. This could be done, for example, by dilatation along the y-axis: $y = \tilde{y}\sqrt{t_y/t_x}$. Then, we have

$$\hat{H}_{\text{kin}} = -a^2 t_x \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial \tilde{y}^2} \right) = -a^2 t_x \Delta_{\tilde{R}}, \tag{21}$$

where $\tilde{R}^2 = x^2 + \tilde{y}^2$ and $\Delta_{\tilde{R}} = \frac{\partial^2}{\partial \tilde{R}^2} + \frac{1}{\tilde{R}} \frac{\partial}{\partial \tilde{R}}$ is the radial part of the Laplacian operator in 2D. Thus, the ellipse $x^2/L_x^2 + y^2/L_y^2 = 1$ in the 'old' x, y coordinates transforms to the $x^2 + \tilde{y}^2 = \tilde{R}_{\text{max}}^2$ circle in the 'new' $x, \tilde{y}$ coordinates. From the equation for the circle in terms of 'new' coordinates $x, \tilde{y}$, it is clear that $\tilde{R}_{\text{max}} = L_x$. Hence, we have

$$L_x = L_y \sqrt{\frac{t_x}{t_y}} = \tilde{R}_{\text{max}}, \tag{22}$$

and the ferron volume in the initial ('old') coordinates reads

$$\Omega = \pi \frac{L_x L_y}{a^2} = \pi \frac{L_x^2}{a^2} \sqrt{\frac{t_y}{t_x}}. \tag{23}$$

In this case, a solution to the Schrödinger equation (3) has the form $\Psi = J_0(k\tilde{R})$, where J_0 is the Bessel function of zeroth order. The boundary condition $J_0(k\tilde{R}_{\text{max}}) = 0$ yields $k\tilde{R}_{\text{max}} = j_{0,1} = 2.404 \approx 3\pi/4$, where $j_{0,1}$ is the first zero of function J_0. This means that

$$\varepsilon_0 = t_x a^2 k^2 = t_x \left(\frac{j_{0,1} a}{\tilde{R}_{\text{max}}} \right)^2 = t_x \left(\frac{j_{0,1} a}{L_x} \right)^2. \tag{24}$$

Then, we have

$$E_{\text{tot}} = -2[t_x n + t_y n + (J_x + J_y)S^2] + E_{\text{pol}}, \tag{25}$$

where

$$E_{\text{pol}} = n \left(\frac{j_{0,1} a}{L_x} \right)^2 t_x + 4(J_x + J_y)S^2 n \frac{\pi L_x^2}{a^2} \sqrt{\frac{t_y}{t_x}}. \tag{26}$$

The minimization of polaron energy (26) with respect to L_x gives

$$\frac{\partial E_{\text{pol}}}{\partial L_x} = -2n t_x \frac{j_{0,1}^2 a^2}{L_x^3} + 8(J_x + J_y)S^2 n \frac{\pi L_x}{a^2} \sqrt{\frac{t_y}{t_x}} = 0. \tag{27}$$

Thus, we have (see equations (23) and (27))

$$\Omega^2 = \pi^2 \frac{L_x^4}{a^4} \frac{t_y}{t_x} = \frac{\pi j_{0,1}^2 t_x}{4(J_x + J_y)S^2} \sqrt{\frac{t_y}{t_x}}. \tag{28}$$

Introducing again t_{eff} and $\bar{J}$ defined by equation (15), we find

$$\Omega = \frac{j_{0,1}\sqrt{\pi}}{2} \left(\frac{t_{\text{eff}}}{\bar{J}} \right)^{1/2}. \tag{29}$$

So, the ferron volume is again expressed as a function of the universal ratio $t_{\text{eff}}/\bar{J}$. Comparing expressions (16) and (29) for the volumes of rectangular and elliptical ferrons, we find

$$\frac{\Omega_{\text{ellipse}}}{\Omega_{\text{rectangle}}} = \frac{j_{0,1}}{\sqrt{2\pi}} \simeq 0.96 < 1. \tag{30}$$

This means that the elliptical ferron is a more compact object (i.e. it has a smaller volume) in comparison to the rectangular ferron. Accordingly, the energy of an elliptical magnetic polaron can be written in the following form

$$E_{\text{pol}} = 8n\Omega \bar{J} = 4nj_{0,1}\sqrt{\pi}(t_{\text{eff}}\bar{J})^{1/2}. \tag{31}$$

We can see again that the ferron energy depends only upon the product of t_{eff} and $\bar{J}$. Finally, we can compare the ferron energies for the cases of rectangular and elliptical shapes using equations (20) and (31)

$$\frac{E_{\text{pol}}^{\text{ellipse}}}{E_{\text{pol}}^{\text{rectangle}}} = \frac{j_{0,1}}{\sqrt{2\pi}} = \frac{\Omega_{\text{ellipse}}}{\Omega_{\text{rectangle}}} \simeq 0.96 < 1. \tag{32}$$

We see that the ratio of energies turns out to be identical to the ratio of the volumes. Thus, an elliptical shape for the ferron is more favourable in energy than a rectangular shape. First of all, this is caused by the more compact structure of the elliptical ferron. Also, as emphasized in [3], an elliptical ferron in 2D has a close similarity to the one-electron spectrum characteristic of the empty square lattice: $\varepsilon_p = p_x^2/2m_x + p_y^2/2m_y$, where $m_x/2 = t_x a^2$ and $m_y/2 = t_y a^2$. Concluding this section, we can say that an elliptical shape is the shape most favourable in energy for a FM droplet in doped anisotropic antiferromagnets with a 2D square lattice.

3. The shape of FM droplets in the anisotropic 3D case

Now we can include the third dimension (which means the inclusion of J_z and t_z) and consider the shape of a FM droplet in a doped anisotropic antiferromagnet with a 3D cubic lattice. Of course (having in mind the results of the previous section), we have to consider FM droplets with a 2D cross-section as being most favourable in energy. In other words, we consider 3D droplets having the shape of an ellipse in the x, y plane. Then the problem effectively reduces to the comparison of the energies and the volumes of a cylinder and of an ellipsoid both having an elliptical cross-section with dimensions $L_x = L_y\sqrt{\frac{t_x}{t_y}}$ (see equation (22)).

3.1. FM droplets of cylindrical shape

First, let us consider 3D FM droplets with a cylindrical shape. The volume of such a droplet can be written as

$$\Omega = \pi \frac{L_x L_y L_z}{a^3} = \pi \frac{L_x^2}{a^2}\sqrt{\frac{t_y}{t_x}}\frac{L_z}{a}. \tag{33}$$

In this case, the total energy has the form

$$E_{\text{tot}} = -2[t_x n + t_y n + t_z n + (J_x + J_y + J_z)S^2]$$
$$+ 4(J_x + J_y + J_z)S^2\Omega n + t_x n\left(\frac{j_{0,1}a}{L_x}\right)^2 + t_z n\left(\frac{\pi a}{L_z}\right)^2. \tag{34}$$

The polaron energy

$$E_{\text{pol}} = E_{\text{tot}} + 2[t_x n + t_y n + t_z n + (J_x + J_y + J_z)S^2] \tag{35}$$

is given by the expression

$$E_{\text{pol}} = t_x n\left(\frac{j_{0,1}a}{L_x}\right)^2 + t_z n\left(\frac{\pi a}{L_z}\right)^2 + 4(J_x + J_y + J_z)S^2 n\pi\frac{L_x^2}{a^2}\sqrt{\frac{t_y}{t_x}}\frac{L_z}{a}. \tag{36}$$

The minimization of polaron energy (36) with respect to L_x and L_z yields

$$\frac{\partial E_{\text{pol}}}{\partial L_x} = -2t_x n \frac{j_{0,1}^2 a^2}{L_x^3} + 8\bar{J}n\pi \frac{L_x}{a^2} \frac{L_z}{a} \sqrt{\frac{t_y}{t_x}} = 0,$$
$$\frac{\partial E_{\text{pol}}}{\partial L_z} = -2t_z n \frac{\pi^2 a^2}{L_z^3} + 4\bar{J}n\pi \frac{L_x^2}{a^3} \sqrt{\frac{t_y}{t_x}} = 0, \tag{37}$$

where we introduced the effective exchange integral for the 3D case

$$\bar{J} = (J_x + J_y + J_z)S^2. \tag{38}$$

From equations (37), we get

$$\frac{j_{0,1}^2 t_x}{4\pi \bar{J}} = \frac{L_x^4 L_z}{a^5} \sqrt{\frac{t_y}{t_x}},$$
$$\frac{\pi t_z}{2\bar{J}} = \frac{L_x^2 L_z^3}{a^5} \sqrt{\frac{t_y}{t_x}}. \tag{39}$$

Squaring the second equation in (39) and dividing the result by the first equation, we exclude L_x and obtain the following expression for L_z:

$$L_z = a \left(\frac{\pi^3}{j_{0,1}^2 \bar{J}} \frac{t_z^2}{\sqrt{t_x t_y}} \right)^{1/5}. \tag{40}$$

Substituting equation (40) into the first equation in (39), we get

$$\frac{j_{0,1}^2 t_x}{4\pi \bar{J}} = \frac{L_x^4}{a^4} \sqrt{\frac{t_y}{t_x}} \left(\frac{\pi^3}{j_{0,1}^2 \bar{J}} \frac{t_z^2}{\sqrt{t_x t_y}} \right)^{1/5}. \tag{41}$$

Hence, we have

$$L_x = \frac{a}{\sqrt{2}} \left(\frac{j_{0,1}^3}{\pi^2 \bar{J}} \frac{t_x^2}{\sqrt{t_y t_z}} \right)^{1/5}. \tag{42}$$

Using equations (40) and (42), we find the volume Ω_{cyl} of the cylindrical ferron

$$\Omega_{\text{cyl}} = \pi \frac{L_x^2 L_z}{a^3} \sqrt{\frac{t_y}{t_x}} = \frac{(\pi j_{0,1})^{4/5}}{2} \left(\frac{t_x t_y t_z}{\bar{J}^3} \right)^{1/5}. \tag{43}$$

Introducing the effective hopping integral for the 3D case

$$t_{\text{eff}} = (t_x t_y t_z)^{1/3}, \tag{44}$$

we can rewrite equation (43) as

$$\Omega_{\text{cyl}} = \frac{(\pi j_{0,1})^{4/5}}{2} \left(\frac{t_{\text{eff}}}{\bar{J}} \right)^{3/5}. \tag{45}$$

Similar to the 2D case, we see that the ferron volume in 3D is also a function of $t_{\text{eff}}/\bar{J}$ ratio, where the effective parameters are given by equations (38) and (44).

Substituting expressions (40), (42), and (45) for L_z, L_x, and Ω_{cyl}, respectively, into the energy of a FM polaron (36), we get

$$E_{\text{pol}} = 10n\bar{J}\Omega = 5n(\pi j_{0,1})^{4/5}(t_{\text{eff}}^3 \bar{J}^2)^{1/5}. \tag{46}$$

We see that the polaron energy in the 3D case again depends on the universal parameters t_{eff} and $\bar{J}$, but the specific form of this dependence is slightly different: $(t_{\text{eff}}^3 \bar{J}^2)^{1/5}$ in 3D as compared to $(t_{\text{eff}}\bar{J})^{1/2}$ in 2D.

3.2. FM droplets of ellipsoidal shape

Here, we calculate the volume and the energy of an FM droplet having an ellipsoidal shape. The volume of the ellipsoidal droplet in the 3D case is

$$\Omega_{\text{ell}} = \frac{4}{3}\pi \frac{L_x L_y L_z}{a^3}. \tag{47}$$

In this case, the total energy of the system has the form

$$E_{\text{tot}} = -2[t_x n + t_y n + t_z n + (J_x + J_y + J_z)S^2] + \varepsilon_0 n + 4(J_x + J_y + J_z)S^2 \Omega n. \tag{48}$$

Hence the energy of the ellipsoidal FM polaron can be written as

$$E_{\text{pol}} = \varepsilon_0 n + 4\bar{J}\Omega n, \tag{49}$$

where we again introduce $\bar{J}$ defined by equation (38).

As in the previous cases, the energy ε_0 can be found by solving the corresponding Schrödinger equation

$$\hat{H}_{\text{kin}}\Psi(x, y, z) = \varepsilon_0 \Psi(x, y, z), \tag{50}$$

where

$$\hat{H}_{\text{kin}} = -a^2\left(t_x \frac{\partial^2}{\partial x^2} + t_y \frac{\partial^2}{\partial y^2} + t_z \frac{\partial^2}{\partial z^2}\right). \tag{51}$$

Using the dilatation along the y- and z-axes: $\tilde{y} = y\sqrt{t_y/t_x}$ and $\tilde{z} = z\sqrt{t_z/t_x}$, we get

$$\hat{H}_{\text{kin}} = -t_x a^2 \Delta_{\tilde{R}} \tag{52}$$

in the 'new' coordinates x, $\tilde{y}$, and $\tilde{z}$. Here, we have $\tilde{R}^2 = x^2 + \tilde{y}^2 + \tilde{z}^2$ and $\Delta_{\tilde{R}} = \frac{\partial^2}{\partial \tilde{R}^2} + 2\frac{1}{\tilde{R}}\frac{\partial}{\partial \tilde{R}}$ is the radial part of the Laplacian operator in 3D.

In these coordinates, a droplet is confined within a sphere of the radius $\tilde{R}_{\text{max}} = L_x$. Accordingly, we have

$$L_y\sqrt{t_x/t_y} = L_z\sqrt{t_x/t_z} = L_x = \tilde{R}_{\text{max}} \tag{53}$$

and the droplet volume expressed in terms of initial ('old') coordinates reads

$$\Omega_{\text{ell}} = \frac{4}{3}\pi \frac{L_x L_y L_z}{a^3} = \frac{4}{3}\pi \left(\frac{L_x}{a}\right)^3 \frac{(t_y t_z)^{1/2}}{t_x}. \tag{54}$$

A solution to the Schrödinger equation (50) has the form

$$\Psi(k\tilde{R}) = \frac{\sin(k\tilde{R})}{(k\tilde{R})}. \tag{55}$$

The boundary condition $\Psi(k\tilde{R}_{\text{max}}) = 0$ yields $k\tilde{R}_{\text{max}} = \pi$. Hence, we find

$$\varepsilon_0 = t_x a^2 k^2 = t_x a^2 \frac{\pi^2}{\tilde{R}_{\text{max}}^2} = t_x a^2 \frac{\pi^2}{L_x^2} \tag{56}$$

and the energy of ellipsoidal FM polaron becomes

$$E_{\text{pol}} = t_x \frac{\pi^2 a^2}{L_x^2}n + 4\bar{J}n\frac{4}{3}\pi \left(\frac{L_x}{a}\right)^3 \frac{\sqrt{t_y t_z}}{t_x}. \tag{57}$$

The minimization of polaron energy (49) with respect to L_x yields

$$\frac{\partial E_{\text{pol}}}{\partial L_x} = -2t_x \frac{\pi^2 a^2}{L_x^3}n + 16\bar{J}\pi n \left(\frac{L_x}{a}\right)^2 \frac{1}{a}\frac{\sqrt{t_y t_z}}{t_x} = 0. \tag{58}$$

As a result, we get the expression for L_x

$$L_x = a \left(\frac{\pi}{8} \frac{t_x^2}{\bar{J} \sqrt{t_y t_z}} \right)^{1/5}. \tag{59}$$

Substituting equation (59) to (54), we find the volume of an ellipsoidal droplet

$$\Omega_{\mathrm{ell}} = \frac{\pi^{8/5} 2^{1/5}}{3} \left(\frac{t_{\mathrm{eff}}}{\bar{J}} \right)^{3/5}, \tag{60}$$

where t_{eff} is again given by equation (44). We see that the volume of the ellipsoidal droplet is also determined by the dimensionless universal ratio $t_{\mathrm{eff}}/\bar{J}$. Dividing equation (54) by equation (45), we obtain the ratio of the volumes for ellipsoidal and cylindrical droplets

$$\frac{\Omega_{\mathrm{ell}}}{\Omega_{\mathrm{cyl}}} = \frac{4}{3} \left(\frac{\pi}{2 j_{0,1}} \right)^{4/5} \simeq 0.95 < 1. \tag{61}$$

We see that the ellipsoidal FM droplet is a more compact object (with a smaller volume) than the cylindrical one.

Substituting expression (59) for L_x into the polaron energy (57), we find

$$E_{\mathrm{pol}} = 10n \bar{J} \Omega_{\mathrm{ell}} = 10n \frac{\pi^{8/5} 2^{1/5}}{3} (t_{\mathrm{eff}}^3 \bar{J}^2)^{1/5}. \tag{62}$$

Hence the ratio of the energies corresponding to two different shapes of ferrons is again identically equal to the ratio of their volumes

$$\frac{E_{\mathrm{pol}}^{\mathrm{ell}}}{E_{\mathrm{pol}}^{\mathrm{cyl}}} = \frac{\Omega_{\mathrm{ell}}}{\Omega_{\mathrm{cyl}}} = \frac{4}{3} \left(\frac{\pi}{2 j_{0,1}} \right)^{4/5} \simeq 0.95 < 1. \tag{63}$$

Thus, in the 3D case, the ellipsoidal droplet has the lowest energy in agreement with the results of [3].

4. Conclusions and discussion

We considered the formation and the shape of droplets in the most general cases of doped anisotropic 2D and 3D antiferromagnets with arbitrary values of the electron hopping integrals t_α and the AFM exchange integrals J_α. We found that in the anisotropic 2D case (when $\alpha = \{x, y\}$ and $t_x \neq t_y$, $J_x \neq J_y$), the most energetically favourable shape of FM droplets is an ellipse. In the anisotropic 3D case (when $\alpha = \{x, y, z\}$ and we include into consideration the third dimension with t_z and J_z), the most energetically favourable shape of FM droplets is an ellipsoid. Moreover, the binding energy and volume of FM droplets depend in both 2D and 3D upon only two universal parameters t_{eff} and $\bar{J}$. In the 2D case these parameters are $t_{\mathrm{eff}} = (t_x t_y)^{1/2}$ and $\bar{J} = (J_x + J_y)S^2$, whereas in the 3D case the corresponding expressions have the form $t_{\mathrm{eff}} = (t_x t_y t_z)^{1/3}$ and $\bar{J} = (J_x + J_y + J_z)S^2$.

Note that in the present paper we have considered only the case of 'free' ferrons, which are not strongly localized at donor impurities. The study of strongly localized ferrons bound to impurities, especially their shape and the form of the cloud of magnetic distortions related to them (similar to those described in [10] and [19]) will be the subject of a separate publication.

Note also that the situation would be more complicated for FM droplets on frustrated triangular or kagome lattices. This is a case, for example, in an interesting quasi-1D magnetic material $BaCoO_3$, where the chains of Co^{4+} ions form a triangular lattice [7, 8].

Acknowledgments

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