Bridging the gap between discrete and continuous magnetic models in the scaling approach

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(Received 29 December 2014; revised manuscript received 20 March 2015; published 15 April 2015)

The scaling technique, often used to study magnetic properties of nanostructures, is based on a reduction in the geometrical lengths of the system via a scaling factor $x$ and a scaling exponent $\eta$ [Phys. Rev. Lett. 88, 237202 (2002)]. At the same time, to keep competition among the energy terms involved, the exchange constant $J$ is reduced throughout the system in accordance with the scaling factor $x$. Different values for the scaling exponent $\eta$ have been used in several studies, and the discussion of whether there is just one or several values is resolved here. In this study we revise the scaling method and propose a different approach than the above. In this generalized approach, the scaling scheme is applied to the energy term as a whole, instead of only to the exchange coupling $J$. We apply this proposed methodology to typical iron cylindrical samples and find that the application of the scaling technique to systems in the mesoscopic range does not depend on the selection of the value of a scaling exponent. We show that this generalized approach gives the same results when it is applied under both discrete and continuous frameworks, and, therefore, it represents a solution for this pending issue.

DOI: 10.1103/PhysRevB.91.134418

PACS number(s): 75.75.—c, 75.60.—d, 75.10.—b

I. INTRODUCTION

Within the exciting field of study of matter at the very small scale, besides the remarkable efforts in the experimental work, great attention has been devoted to the theoretical and computational frameworks in order to better understand the new observed features and phenomena. Along with the myriad of experimental results revealing the effects of several factors, such as geometry, size, internal structure, external interactions, etc., on the magnetic properties of nanometric systems, there has been an increasing amount of models and theoretical approaches proposed for the study of the relationships among the different physical factors and the exhibited behaviors that allow the wide extent of current technological applications. With the advent of growing computational facilities, the numerical simulations of micromagnetics [1] have been developed. This methodology is based on the continuous approximation to solve a Landau-Lifshitz-type equation [2–4]. On the other hand, the discrete scheme currently known as the fast Monte Carlo method [5–7], is also being extensively employed. In this last method, the difficulty of studying systems formed by about $10^7$ spins within reasonable amounts of time with the current computers is circumvented by scaling down the size of the system and the exchange interaction $J$ by using a factor $x$ ($x < 1$). In their original work, d’Albuquerque et al. showed that, for systems characterized by lateral dimensions $D$ (diameter) and $H$ (height), the magnetic phase diagram can be obtained from that of a smaller system with dimensions $D'$ and $H'$ by implementing the scaling relations $D' = x^2 D$, $H' = x^\theta H$, and $J' = x J$ [8]. Here, $\eta$ represents a positive scaling exponent, and $x$ is the scaling factor. In other words, the phase diagram for the actual sample $(D, H)$ can be obtained from the small system $(D', H')$ by scaling the axes up by a factor of $(1/x)^{\eta}$. This scheme has been successfully employed to study several kinds of magnetic systems, such as nanowires [7,9,10], magnetic nanodots [11], nanotubes [12–14], nanorings [15,16], truncated conical nanoparticles [17], and elliptical nanoparticles [16]. A strong consensus is observed among the various experimental results [11] and micromagnetic calculations [6] as well.

So far, due to the wide applicability of the methodology, the value of the scaling exponent $\eta$ has been a source of debate. In particular, an analytical work states that $\eta$ must be greater than 0.55 [18], whereas other researchers claim that the value could not be any other than 0.5 [16]. Furthermore, from the micromagnetics viewpoint, $\eta$ values that differ from 0.5 are not accepted. This fact lays in the functional form of the exchange length $l_{ex} = \sqrt{2A/(\mu_0 M_S^2)}$, where $A$ is the stiffness constant, which is proportional to $J$, $\mu_0$ is the vacuum permeability, and $M_S$ is the saturation magnetization. The argument is that, whenever $J$ scales linearly with the scaling factor $x$, $l_{ex}$ should scale as $l_{ex}' = x^{0.5} l_{ex}$; i.e., $\eta = 1/2$. These last facts clearly offer a point of discussion which must be solved and completely understood in order to get a clear view of the problems that arise in the application of the scaling approach from these two perspectives, continuous and discrete.

Consequently, in this study we address the scaling technique from a fundamental point of view and show that there is a more general form of the scaling scheme [6,8]. Within this more fundamental conception of the scaling approach we show, in the next section, that the parameters $\eta$ and $x$ can be considered as mere mathematical artifacts, and thus the above-mentioned physical discussions and discrepancies are not fundamental.

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II. MODELS AND RESULTS

We consider typical samples of cylindrical shape. The interest is to identify the magnetic states of the true sample for the different set of values \((D, H)\), which can be a ferro-in-plane (Fi), a ferro-out-of-plane (Fo), and a vortex state (V). Within each cylinder the magnetic structure is mainly determined by the competition between the exchange interaction among neighboring atoms and the long-range dipolar interaction (which is responsible for the shape anisotropy) \([11]\).

As a starting point, we will begin with static simulations in the discrete approach in which we compute energies for the different magnetic states for a wide range of system sizes. Then, for a rigorous comparison, we will consider some sizes in the continuous case in order to show similarities. We will also discuss comparisons with previous results from both the experimental and the simulation viewpoints and will present conclusions. Since dipolar interactions are taken into account, the number of different sizes that will be considered is limited by the available computational resources.

A. Discrete model

Let us first consider the discrete approach. Here, since the simulations require samples with a specific crystalline structure, we take advantage of the many experimental data on granular Fe systems and consider typical Fe cylindrical samples (growth along the [110] direction) in which magnetic moments (\(\vec{\mu}_i\)) occupy the sites of a bcc lattice. Therefore, we use: \(\vec{\mu}_i = \mu\text{Fe} = 2.2\mu_B\), the lattice parameter \(a_0 = 2.86\ \text{Å} [19]\), and \(J = J\text{Fe} = 43\ \text{meV}\), which reproduces the ordering temperature for the bulk case \((T_C = 1043\ \text{K}) [19]\).

Thus, total energy \(E_{\text{tot}}\) for a single nanocylinder with \(N\) magnetic moments in a given configuration \(\{\vec{\mu}_i\}\) is given by \(E_{\text{tot}} = E_{\text{ex}} + E_{\text{dip}}\), where

\[
E_{\text{ex}} = -\frac{1}{2} \sum_{\langle i,j \rangle} J_{i,j} \hat{\mu}_i \cdot \hat{\mu}_j \tag{1}
\]

is the exchange energy, computed in the nearest-neighbor approximation and

\[
E_{\text{dip}} = \frac{1}{2} \sum_{i \neq j} \frac{\vec{\mu}_i \cdot \vec{\mu}_j - 3(\vec{\mu}_i \cdot \hat{n}_{ij})(\vec{\mu}_j \cdot \hat{n}_{ij})}{r_{ij}^3} \tag{2}
\]

is the dipolar energy. Here, \(\vec{\mu}_k\) represents the unit vector along the direction of the magnetic moment \(\vec{\mu}_k\), \(r_{ij}\) is the distance between \(\vec{\mu}_i\) and \(\vec{\mu}_j\), and \(\hat{n}_{ij}\) is the unit vector along the direction that connects the two magnetic moments: \(\hat{n}_{ij} = \hat{r}_{ij}/r_{ij}\).

Originally the scaling technique proposes a scaling down of the exchange constant \((J' = \kappa J)\) with \(\kappa < 1\) with the aim of preserving the competition between exchange and dipolar energies at least size of the sample since the corresponding new scale of the system decreases through the factor \(\kappa^3\). However, there is not a fundamental reason to think that this scaling scheme should be applied particularly to \(J\). Instead, in a more fundamental conception, a scaling on the energy (not on \(J\)) must be considered, through a \(\lambda\) parameter, that is

\[
E'_{\text{tot}} = \lambda E_{\text{ex}'} + E_{\text{dip}}, \tag{3}
\]

where scaled terms are identified as primed quantities. Here, \(\lambda\) stands for several different effects that are produced whenever a scaling of dimensions is applied in order to produce a scaled system; these effects include changes in the number of particles, i.e., limits of the sums in Eq. (1), changes in the spin values of the atoms of the systems, and/or changes in the intensity of the interaction between atoms. This aspect represents a remarkable conceptual difference with respect to the original scaling scheme where a change is implied only in the \(J\) value during the scaling down process.

Thus, in this general conception, the key is to find the relationship between scaling parameters \(x\) (which acts on the linear dimensions of the sample) and \(\lambda\) (which acts on the exchange term as a whole) in order to obtain the equivalent magnetic states in both the true and the scaled systems. To do this, we consider a relationship of the form \(\lambda = x^\beta\) and look for the \(\beta\) parameter. Let us consider ideal magnetic states. Let the cylinder axis be the \(z\) axis, then, the Fo state will be defined by \(\mu_{i,z} = (0,0,1) \forall i\), and its energy will be represented by \(E_{\text{Fo}}\). Let the Fi state be given by the arrangement of spins along the \(x\) axis \(\mu_{i,x} = (1,0,0) \forall i\) with energy \(E_{\text{Fi}}\). Thus, the transition line must follow \(E_{\text{Fo}} = E_{\text{Fi}}\), which, after considering Eqs. (1)–(3) on the Fo and Fi states, gives

\[
\begin{align*}
\frac{\lambda^2}{2} \sum_{\langle i,j \rangle} J \mu_{i,x} \mu_{j,x} + \sum_{i<j} \frac{\vec{\mu}_{i,x} \cdot \vec{\mu}_{j,x} - 3(\vec{\mu}_{i,x} \cdot \hat{n}_{ij})(\vec{\mu}_{j,x} \cdot \hat{n}_{ij})}{r_{ij}^3} \\
= -\frac{\lambda^2}{2} \sum_{\langle i,j \rangle} J \mu_{i,z} \mu_{j,z} + \sum_{i<j} \frac{\vec{\mu}_{i,z} \cdot \vec{\mu}_{j,z} - 3(\vec{\mu}_{i,z} \cdot \hat{n}_{ij})(\vec{\mu}_{j,z} \cdot \hat{n}_{ij})}{r_{ij}^3} \\
- \frac{\lambda}{2} \sum_{\langle i,j \rangle} J + \sum_{i<j} \frac{1}{r_{ij}^3} - 3 \sum_{i<j} \frac{x_{ij}}{r_{ij}^3} \\
= -\frac{\lambda}{2} \sum_{\langle i,j \rangle} J + \sum_{i<j} \frac{1}{r_{ij}^3} - 3 \sum_{i<j} \frac{x_{ij}}{r_{ij}^3}
\end{align*}
\]

these conditions lead to the following relation between the \(x_{ij}\) and the \(z_{ij}\) coordinates,

\[
\sum_{i<j} \frac{x_{ij}^2}{r_{ij}^3} = \sum_{i<j} \frac{z_{ij}^2}{r_{ij}^3}. \tag{4}
\]

A similar relationship is obtained if the Fi states along the \(y\) axis are considered in which \(y_{ij}^2\) appears instead of \(x_{ij}^2\) in Eq. (4).

Furthermore, whenever an alternative approach using a scaling up of the dipolar energy according to the relation,

\[
E'_{\text{tot}} = E_{\text{ex}} + \kappa E_{\text{dip}} \quad (\kappa > 1) \tag{5}
\]

is considered, the same result of Eq. (4) is obtained. Both of these routes, Eqs. (3) and (5), lead to the same result.

It is worth highlighting that the transition line that separates the Fi and Fo states satisfies the following conditions: (i) It does not depend on any scaling choice since the scaling factor \(\lambda (\kappa)\) has been eliminated in the process; (ii) it does not depend on the term to which the scaling is applied, either \(E_{\text{ex}}\) or \(E_{\text{dip}}\); and (iii) its slope does depend just on the crystalline structure of the material being studied. Besides, the triple point (which
suggests a power dependence between $x$ and $\eta$ which allows us to explore the size dependence of the exchange stiffness parameter for a given sample. Within this more general scaling formulation, parameters to the methodology as presented in its original framework, implicitly use $x$ and $\eta$ as employed in the original works regarding the value of the exchange length and the exchange stiffness parameter for a given system can be studied with different scaling values ($\eta = 0.5, 0.55, 0.57, \text{etc.}$) provided the mentioned $\beta/\eta$ ratio remains unaltered. A second point to highlight is that the second term on the right-hand side of Eq. (6) gives, through the relationship schematized in Fig. 1, the exact location of the triple point ($D_t, H_t$) for the true sample.

Interestingly, in the scaling process, it is not necessary to know or select any values of parameters $x$ and $\eta$. Indeed, according to this fundamental conceptual view of the scaling approach (in which the scaling is not over $J$ but on the energy term as a whole), if the scaling relation is considered for the triple point ($H'_{t} = x^\delta H_t$), it is enough to choose a desired triple point, any triple point one wants for representing a true system, and the scaling can be performed by applying the following simple relationships:

$$H' = \left( \frac{H'_{t}}{H_{t}} \right) H; \quad D' = \left( \frac{H'_{t}}{H_{t}} \right) D. \quad (7)$$

Thus, the scaling factor $x^\eta$, as employed in the original formulation of the scaling approach, indeed represents the ratio between the height [or diameter since Eq. (7)] can also be written in terms of $D'$ and $D$, i.e., $x^\eta = D'/D_t$ of a selected scaled system and the true one at the triple point, and therefore both parameters $x$ and $\eta$ appear now to be mathematical parameters to the methodology as presented in its original form. Therefore, within this more general scaling formulation, $\eta$ could always be chosen to have the value 0.5 in order to fulfill the relationship between the exchange length and the exchange stiffness parameter for a given sample.

This is one of the interesting findings of this study; it solves the previously mentioned discrepancies among different works regarding the value of the $\eta$ parameter, which have been related as a complete or incomplete similarity of the samples in an interesting work by Zhang et al. [16]. In particular, for published works (which, in the context of the present framework, implicitly use $\beta = 1.00$) reporting $\eta = 0.56$ the $\beta$ value would go to $\beta = 1.008$, whereas for those with $\eta = 0.57$ a value $\beta = 1.026$ would be obtained. Since these $\beta$ values are identical within numerical accuracy, its use would give results very similar to those already reported. However, the deviations from the value $\beta = 1.00$, although small, are important since they account for the effect of scaling on the other parameters involved in the exchange energy (different from $J$), such as magnetic moment magnitudes, number of particles in these samples, etc.

Additionally, to give a more complete view, by appealing to the information of the triple point, the functional form of the scaling factor on the energy can be written as

$$\lambda = x^\beta \quad (as \text{ was previously mentioned}). \quad By \text{ taking into account this last relationship and the scaling equation for the height at the triple point } H'_{t} = x^\delta H_t, \text{ we obtain}$$

$$\log_{10} \lambda = \frac{\beta}{\eta} \log_{10} H'_{t} - \frac{\beta}{\eta} \log_{10} H_t. \quad (6)$$

FIG. 1. (Color online) $H$ vs $D$ diagram for several dots (no scaling implemented). This line separates the Fi (below) and Fo (above) magnetic states. The linear fit (solid line) is included yielding $H = 0.908(2)D$.

separates the states Fo, Fi, and V moves along the line depicted by Eq. (4) when the system is scaled down (see Fig. 1).

Figure 1 shows numerical results obtained from several cylinders ($D, H$) for which the energies corresponding to configurations Fi and Fo have been tested [20]. The linear fit in this case gives $H = (0.908 \pm 0.002)D$. This result is in accordance with the one obtained by continuum analytical models [18].

As stated above, the triple point of any scaled system must be on this line [Eq. (4), Fig. 1]. Then, in order to look for a relationship among the involved parameters, we take these cylinders as the scaled samples ($D', H'$) of a huge true sample ($D, H$). Clearly, samples ($D', H'$) come from certain scaling choices $x^\delta; D' = x^\delta D, H' = x^\beta H$; note that no $\eta$ value has been imposed so far. We impose that these structures be the triple point by changing $\lambda$ in such a way that the V configuration has the same energy as that of the Fo and Fi states.

With this, we find the set ($D'_t, H'_t, \lambda$) for the triple points, which allows us to explore the size dependence of $\lambda$ by drawing $\lambda$ vs $H'_t$ in a log-log plot as shown in Fig. 2.

The linear behavior obtained between these two quantities suggests a power dependence between $x$ and $\lambda$ of the form

$$\lambda = x^\beta \quad (as \text{ was previously mentioned}). \quad By \text{ taking into account this last relationship and the scaling equation for the height at the triple point } H'_{t} = x^\delta H_t, \text{ we obtain}$$

$$\log_{10} \lambda = \frac{\beta}{\eta} \log_{10} H'_{t} - \frac{\beta}{\eta} \log_{10} H_t. \quad (6)$$

The first remarkable result is the constraint which exists between $\beta$ and $\eta$, i.e., $\delta = \beta/\eta = 1.80 \pm 0.02$ (see Fig. 2). This is to say, there is not just one valid scaling scheme, i.e., a given system can be studied with different scaling values ($\eta = 0.5, 0.55, 0.57, \text{etc.}$) provided the mentioned $\beta/\eta$ ratio remains unaltered. A second point to highlight is that the second term on the right-hand side of Eq. (6) gives, through the relationship schematized in Fig. 1, the exact location of the triple point ($D_t, H_t$) for the true sample.

Interestingly, in the scaling process, it is not necessary to know or select any values of parameters $x$ and $\eta$. Indeed, according to this fundamental conceptual view of the scaling approach (in which the scaling is not over $J$ but on the energy term as a whole), if the scaling relation is considered for the triple point ($H'_{t} = x^\delta H_t$), it is enough to choose a desired triple point, any triple point one wants for representing a true system, and the scaling can be performed by applying the following simple relationships:

$$H' = \left( \frac{H'_{t}}{H_{t}} \right) H; \quad D' = \left( \frac{H'_{t}}{H_{t}} \right) D. \quad (7)$$

Thus, the scaling factor $x^\eta$, as employed in the original formulation of the scaling approach, indeed represents the ratio between the height [or diameter since Eq. (7)] can also be written in terms of $D'$ and $D$, i.e., $x^\eta = D'/D_t$ of a selected scaled system and the true one at the triple point, and therefore both parameters $x$ and $\eta$ appear now to be mathematical parameters to the methodology as presented in its original form. Therefore, within this more general scaling formulation, $\eta$ could always be chosen to have the value 0.5 in order to fulfill the relationship between the exchange length and the exchange stiffness parameter for a given sample.

This is one of the interesting findings of this study; it solves the previously mentioned discrepancies among different works regarding the value of the $\eta$ parameter, which have been related as a complete or incomplete similarity of the samples in an interesting work by Zhang et al. [16]. In particular, for published works (which, in the context of the present framework, implicitly use $\beta = 1.00$) reporting $\eta = 0.56$ the $\beta$ value would go to $\beta = 1.008$, whereas for those with $\eta = 0.57$ a value $\beta = 1.026$ would be obtained. Since these $\beta$ values are identical within numerical accuracy, its use would give results very similar to those already reported. However, the deviations from the value $\beta = 1.00$, although small, are important since they account for the effect of scaling on the other parameters involved in the exchange energy (different from $J$), such as magnetic moment magnitudes, number of particles in these samples, etc.

Additionally, to give a more complete view, by appealing to the information of the triple point, the functional form of the scaling factor on the energy can be written as

$$\lambda = \left( \frac{H'_{t}}{H_{t}} \right)^{\delta} = \left( \frac{H'_{t}}{H_{t}} \right)^{1.80} \quad (8)$$

FIG. 2. (Color online) Log-log diagram showing the relationship between $\lambda$ and scaled $H$ for several dots. The solid line stands for the linear fit: $\log_{10} \lambda = 1.80(3) \log_{10} H'_{t} - 2.87(2)$. 

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where \( \delta = 1.80 \) is the value for Fe-based systems. With this, the complete magnetic phase diagram can be obtained.

To evidence the validity of the generalized scaling scheme discussed, Fig. 3 shows the phase diagram for four different values of \( \lambda \) (see the inset) as well as their corresponding collapse in just one coincident phase diagram when the scaling up process is carried out towards the true sample (main frame).

As can be inferred from Eqs. (3) and (5), the scheme is equally successful and valid when applied to the exchange energy or to the dipolar energy. Indeed, the important facts are as follows: (i) that the scaling scheme should be applied on the energies and (ii) that the requirement is to keep unaltered the balance among them. With this, the scaling is completely defined when the user selects the triple point for a certain system, through Eqs. (7) and (8). In other words, scaling on \( J \) or \( l_{c} \) is not essential, and the discussion about the value of \( \eta \) is meaningless because it can always be chosen as 0.5 provided that \( \beta/\eta \) is a constant value for a given magnetic system.

To sum up, from the practical viewpoint, with this more fundamental perspective the scaling process consists of: (i) Computationally determining samples \( (D, H) \) so as to draw a graph similar to the one presented in Fig. 1. These samples will be taken as triple points of scaled systems (since for them the condition \( E_{F0} = E_{Fi} \) is fulfilled). (ii) Obtaining, computationally and for a small number (4 or 5) of the very small samples, the set of values \( (H', \lambda) \). This is performed by equating the energy of the vortex state with those of the in plane and out of plane \( E_{Fo} = E_{Fi} = E_{Fv} \) by varying \( \lambda \). With this the \( \lambda \) vs \( H' \) figure is obtained. (iii) Obtaining the linear fit for the log-log \( \lambda \) vs \( H' \) diagram (Fig. 2). With this the parameters of the scaling [Eqs. (7) and (8)] are obtained, and the complete magnetic phase diagram can be computed.

### B. Continuous model

Here, with the aim of comparing discrete and continuous cases by using the analytical description presented in Ref. [18], we take the continuous model and follow the same procedure already used in the discrete model, i.e., applying the \( \lambda \) factor to the complete energy term \( (E_{ex} \ or \ E_{dip}) \). In the continuous approach the distribution of magnetic moments is sketched through a continuous function \( \tilde{M}(\tilde{r}) \) describing the magnetization density. This function in the ferromagnetic states \( Fi \) and \( Fo \) has the forms \( M_{0}\hat{e}_{z} \) and \( M_{0}\hat{e}_{\phi} \), respectively; here \( \hat{e}_{z} \) and \( \hat{e}_{\phi} \) are the unit vectors along the axis and the basis of the cylinder, respectively. The assumed form of the magnetization density for a perfect vortex state is \( \tilde{M}(\tilde{r}) = M_{z}(\rho)\hat{e}_{z} + M_{\phi}(\rho)\hat{e}_{\phi} \), where \( \hat{e}_{z} \) and \( \hat{e}_{\phi} \) represent the unit vectors in cylindrical coordinates and \( M_{z} \) and \( M_{\phi} \) satisfy \( M_{z}^{2} + M_{\phi}^{2} = M_{0}^{2} \) [18]. With this model we can proceed to evaluate energy terms for each configuration in order to compute the magnetic phase diagram. The dipolar energy can be computed through the expression [3],

\[
E_{dip} = \frac{\mu_{0}}{2V} \int \tilde{M}(\tilde{r}) \cdot (\nabla U) dV, \tag{9}
\]

where \( U(\tilde{r}) \) is the magnetostatic potential and a term independent of the configuration has been dismissed.

Hereafter we describe the procedure in dimensionless quantities, which are indicated by the symbol \( ^{\ast} \) on them. In particular, with the aim of completing the description independent of the material, length dimensions are expressed in terms of the exchange length \( l_{c} \) (i.e., \( D = D/l_{c} \)). From Eq. (9), the energy expressions for the ferromagnetic configurations in dimensionless form can be written for \( Fi \) and \( Fo \) states as

\[
\tilde{E}_{dip}^{(Fi)} = N_{Fi} \left\{ \frac{1}{4} z_{F1} \left[ \left( 1 - \frac{1}{2} \frac{1}{2} \right) \left( \frac{\tilde{D}}{H} \right)^{2} \right] - \frac{\tilde{D}}{3\pi H} \right\}, \tag{10}
\]

and

\[
\tilde{E}_{dip}^{(Fo)} = N_{Fo} \left\{ \frac{1}{2} \left[ 1 - 2z_{F1} \left[ \left( 1 - \frac{1}{2} \frac{1}{2} \right) \left( \frac{\tilde{D}}{H} \right)^{2} \right] + \frac{4\tilde{D}}{3\pi H} \right] \right\}, \tag{11}
\]

where \( N_{a} \) represents the demagnetizing factors, given in \textit{Système International} units [21], which depend on the ratio of the dimensionless lengths \( D/H \). In these last equations, \( z_{F1}(a,b,c,d) \) is a hypergeometric function.

For the vortex case, taking into account the expressions for the magnetostatic potential and for the top and bottom bases of the cylinder [18], the dipolar term can be written as

\[
\tilde{E}_{dip}^{(V)} = \frac{\pi}{M_{0}^{2}V} \int_{0}^{\infty} \left( \int_{0}^{\tilde{D}/2} \rho J_{0}(\kappa\rho) M_{z}(\rho) d\rho \right)^{2} (1-e^{-\tilde{m}_{z}r}) d\kappa, \tag{12}
\]

where \( J_{0}(x) \) is the order zero cylindrical Bessel function. On the other hand, for this vortex case, the exchange energy can be obtained as

\[
\tilde{E}_{ex}^{(V)} = \frac{8\lambda A}{\mu_{0}M_{0}^{2}D^{2}} \int_{0}^{\tilde{D}/2} \left( \frac{(\partial m_{z}/\partial \rho)^{2}}{1-m_{z}^{2}+\frac{m_{z}^{2}}{\rho^{2}}} \right) \rho d\rho, \tag{13}
\]

where \( m_{z}(\tilde{r}) = M_{z}(\hat{\rho})/M_{0} \) and \( A = JcS^{2}/a \) for a cubic system with \( c \) as the number of atoms within a unit cell of size \( a \). To describe the vortex core of the cylinder we use the expression \( m_{z}(\hat{\rho}) = (1 - (\hat{\rho}/\hat{\rho}_{c})^{2})^{n} \) for \( \hat{\rho} \leq \hat{\rho}_{c} \) and \( m_{z}(\hat{\rho}) = 0 \) otherwise [18]. Here, \( \hat{\rho}_{c} \leq \tilde{D}/2 \), and \( n \) is a non-negative constant. With this form for the \( m_{z}(\hat{\rho}) \) function the dipolar...
and exchange energies for the V state can be computed from Eqs. (12) and (13) and expressed as

$$E_{ex}^{(V)} = \frac{4\rho_c^3}{H D^2} \left[ \alpha_n - \frac{\tilde{\rho}_c}{4H} \beta_n F \left(n, \frac{\tilde{\rho}_c}{H} \right) \right], \quad (14)$$

where

$$\alpha_n = \frac{2n-1}{\Gamma(\frac{3}{2} + n)} \Gamma(\frac{3}{2} + 2n), \quad \beta_n = \frac{1}{(1+n)^2},$$

$$F \left(n, \frac{\tilde{\rho}_c}{H} \right) = _3F_2 \left[ \frac{1}{2}, -\frac{3}{2} + n, n + 2, 2n + 3, -\frac{4\tilde{\rho}_c^2}{H^2} \right],$$

here, $_3F_2$ is the generalized hypergeometric function. The exchange energy is expressed by

$$\tilde{E}_{ex} = \frac{4\tilde{\rho}_c^3}{D^2} \left( \ln \frac{\tilde{D}}{2\tilde{\rho}_c} + \gamma_n \right), \quad (15)$$

where

$$\gamma_n = \frac{1}{2} Q[2n] - n Q[-1/2n]$$

and

$$Q[z] = \sum_{i=1}^{\infty} \left( \frac{1}{i} - \frac{1}{i+z} \right).$$

As a first point, by equating the energy of the Fi and Fo states [Eqs. (10) and (11)] we can find the line for the triple points, which adopts the form $H = 0.9065D$. This result is in complete agreement with the one obtained for the discrete case (Fig. 1), which reads as $H = 0.908(2)D$. By following the same procedure described in the previous section we can obtain a relationship between $\lambda$ and $H'$ and obtain Fig. 4. The graph follows the same functional form of Eq. (6). In this case, from the fitting process, the corresponding value $\delta = 1.768 \pm 0.003$ is obtained. This result is in agreement within the uncertainties with the result from discrete treatment. With these values we proceed to obtain the phase diagram for several scaling selections ($H'_c/H_c$). The inset of Fig. 5 shows the phase diagrams computed by the continuous model for some selected scaling values. From these scaled diagrams, by scaling up to obtain the phase diagram in true dimensions [Eq. (7)], the collapsed phase diagram is obtained (mainframe of Fig. 5). It is worth highlighting that, in the cases of both scaled and true lengths, a similar behavior is obtained for both the continuous and the discrete schemes.

Finally, as an additional proof for this generalized methodology, we have carried out some comparisons with simulations and experimental results.

Figure 6 shows a comparison among a hysteresis loop for the dot with $D = 65$ and $H = 20$ nm obtained through our generalized methodology and the previously published results from both experiments and simulations [11,22]. In our calculation, $10^4$ Monte Carlo steps for equilibration, $10^4$ more for computation, and at least five seeds were taken into account for the obtention of the average physical quantities. For this case the hysteresis loop shape appears narrowed, i.e., a reduced coercivity is observed near zero magnetization. This already known effect has been attributed to the apparition of a vortex state in the magnetization reversal process as has been reported from magneto-optical Kerr effect measurements as well as

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from micromagnetic and Monte Carlo simulations [11,22,23]; this is also the case in our results. On the other hand, for the sizes considered here it is known that the domain-wall width and dot sizes are of the same order of magnitude, so there is no formation of multidomain states in the samples, and the magnetic behavior strongly depends on size. In particular, a nonmonotonic behavior of coercivity as function of size is observed. In order to study this size dependence, a parameter (Δ), which illustrates the effect of size on the hysteresis loop shape, has been proposed by Mejía-López et al. [11] and Roshchin et al. [22]. This Δ is defined as the ratio of the hysteresis loop widths (W) at zero magnetization (M = 0) and at half the saturation magnetization (M S), i.e., at M = 0.5M S. This is to say, Δ = W(M = 0)/W(M = 0.5M S). In Fig. 7 we show a comparison with the size dependence of Δ for some selected dot sizes. The complex behavior observed has already been studied in detail [11,22], and the features associated with it have been fairly well reproduced by our model. In particular, the minimum observed at D = 65 nm is ascribed to the presence of a vortex state in the inversion process. This vortex has been observed for all considered seeds in our simulation. For diameters below 60 nm, inversion takes place through a coherent mechanism. For diameters between 60 and 65 nm some seeds present coherent rotation and some others inversion through a vortex. And, finally, for diameters beyond 65 nm inversion for some seeds occurs through a vortex whereas for others through a S state, which increases coercivity and, consequently, Δ. In this comparison the experimental setup involves an ensemble of noninteracting dots, and each seed of our simulation stands for a dot of that ensemble. It is worth pointing out that very good qualitative agreement is obtained in the comparison.

The very good agreement observed between the two schemes used in this study as well as with previous experimental and simulation results suggests the reliability of the fundamental conceptual viewpoint we have proposed here to apply within the scaling technique. In this alternative, which is a more fundamental conception, the importance relies on parameter δ instead of on the values of parameters x and η. In this sense, the longstanding discussion on the values of parameter η is solved.

III. CONCLUSIONS

To sum up, we have revisited the fundamental aspects of the scaling technique and proved the existence of general relations in the scaling of the exchange energy and the scaling when applied to the dipolar energy in order to find magnetic configurations of nanometric samples.

In particular, we consider a generalized scaling approach, describe it in detail, apply it to both discrete and continuous cases, and find equal results under the uncertainty, which suggests that the proposed generalized scheme is valid. We find that the application of the scaling technique does not depend on the value of a scaling exponent. Instead, the scaling factor can be expressed as the ratio between the heights (or diameters) of the true and scaled samples at the triple point, which are values obtainable from the process itself, not imposed from outside. With this we offer a solution to the discrepancies reported in the values of the scaling exponents [16,18], an issue which was previously considered to be pending. These results are of interest to the theoretical and computational study of the magnetic properties of structures in the nanometric range where experiments cannot yet help to have an atomistic view of the involved phenomena.

ACKNOWLEDGMENTS

This work was supported by several projects: the bilateral Project COLCIENCIAS-CONICYT 2014-2016, the FONDECYT Grants No. 1130672 and No. 1130950, Postdoctorado Grant No. 3150525, Financiamiento basal para centros científicos y tecnológicos de excelencia Grant No. FB 0807, the “Estrategia de Sostenibilidad 2014-2015” at the Universidad de Antioquia, and the Universidad de San Buenaventura Grants No. 9511501-01 and 9511501-02. J.M.-Z. acknowledges the Universidad de Antioquia for the “Dedicación Exclusiva” program and Project No. IN3068CE.

[20] Since we are working with discrete systems, in general, it is not possible to find a size \((D,H)\) for which the relation \(E_{Fi} - E_{Fo} = 0\) holds exactly. In practice, to obtain Fig. 1, we do for every diameter \(D\) is to compute the energy difference \((\Delta E = E_{Fo} - E_{Fi})\) for several \(H\) values. This progressive increase in \(H\) is discrete since it is made by adding a new atomic shell in the sample height. Then, whenever a change in the sign of \(\Delta E\) takes place, the two \(H\) values closest to the \(E_{Fi} = E_{Fo}\) relationship have been found. In order to perform the process as accurately as possible, a linear interpolation between these values is computed, and the resultant \(H\) is taken into account to draw Figs. 1–3.