

## Fast Monte Carlo method for magnetic nanoparticles

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We present a fast and reliable method for investigating the magnetic properties of nanostructures. It combines the standard Monte Carlo and scaling techniques to allow results for such systems to be obtained by carrying out calculations for much smaller systems. The method is illustrated by applying it to the well-known problem of determining the single-domain limit of a cubic magnetic particle with an easy axis parallel to one of the cube directions. Results are in good agreement with those of micromagnetic calculations.

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In the last decades, the study of the magnetic properties of nanostructures has become one of the most active areas of research in condensed matter physics.<sup>1</sup> Such systems exhibit rather interesting properties, often distinct from those of bulky materials, which result from the combination of several factors such as finite size and quantum interference effects, as well as competition between the interactions (exchange, dipolar, and anisotropy) which the magnetic moments within the structures are subjected to. Magnetic nanostructures are regarded as having great potential for technological applications, which include the production of magnetic sensors, nanoactuators, and high-density recording media.

Progress in the field of nanomagnetism has been boosted by advances in the techniques of material preparation and characterization which took place in recent years. As an example, new developments in this area have made possible the preparation of regular arrays of magnetic particles of different shapes and sizes,<sup>2-4</sup> which might make possible the production of magnetic storage devices with the record storage density of 1 Tbit/in.<sup>2</sup> (Ref. 5). Regarding magnetic nanoparticles, interest has been focused on the determination of their internal magnetic structure, which is of fundamental importance for practical applications. On experimental grounds, magnetic force microscopy and magnetization measurements have been used to investigate the arrangement of the magnetic moments within the particles.<sup>4,6</sup> One of the key points in such studies is the determination of the so-called single-domain limit, which corresponds to the size limit beyond which particles of ferromagnetic materials may exhibit complex internal magnetic structures, often with rather reduced total magnetization. However, one of the main difficulties one faces in such studies results from the fact that in many cases the internal magnetic configuration of the nanoparticle is not readily identifiable from the experimental data.

From the theoretical point of view, the determination of the internal magnetic structure of nanoparticles is by no means a simple task. Particles in the size range currently produced may have over  $10^7$  magnetic moments, which are subjected to both short-ranged (exchange and anisotropy) and long-ranged (dipolar) interactions. As a consequence, with present standard computational facilities, the determination of the low-temperature magnetic configuration of such

particles based on the investigation of the behavior of their individual magnetic moments, using, for instance, the Monte Carlo technique, becomes prohibitively time-consuming. Therefore, one has to resort to approximations in order to deal with these systems theoretically.

One possibility is to operate on a larger scale by regarding the particle as being composed of small units, which are nevertheless large enough to allow a continuous approximation for their magnetization. This is the basis of the micromagnetism approach, which has been largely used to determine internal structures such as domain walls in magnetic materials. Clearly, the larger the number of units one considers, the better the description of the system. Such a number, however, is limited by the available computational power.

In this communication we present an alternative approach for the study of magnetic nanostructures, which is based on what we call the fast Monte Carlo method. It combines the standard Monte Carlo and scaling techniques to allow the magnetic properties of nanostructures to be obtained from results of calculations for much smaller systems, consisting of no more than few hundreds of magnetic moments. In what follows we illustrate the method by applying it to the well-known problem of determining the single-domain limit of a cubic magnetic particle with an easy axis parallel to one of the cube directions. We recall that such a system may exhibit two distinct internal magnetic configurations, which are called flower and vortex states. The first one is basically a modified single-domain state in which the magnetic moments in the center of the cube are essentially aligned along the easy axis, whereas the direction of those close to the cube surfaces deviate from such an alignment. In the second state, the magnetic moments curl around one axis, crossing the cube center and parallel to the easy direction. The single-domain limit corresponds to the size  $L$  of the cube for which the flower and vortex states have equal energies. This problem has been suggested by NIST's Micromagnetic Modeling Activity Group<sup>7</sup> ( $\mu$ MAG) as a standard problem for testing micromagnetic approaches to magnetic nanosystems. The limit is expected to be around  $L \approx 8l_{ex}$ , where  $l_{ex}$  is the exchange length given by  $(A/E_m)^{1/2}$ . Here  $A$  is the exchange stiffness constant and  $E_m$  is the magnetostatic energy density  $(1/2)\mu_0 M_s^2$ , where  $M_s$  is the saturation magnetization. Mi-

chromagnetic calculations lead to results for  $L/l_{ex}$  which approach values close to 8 as the number of cells or subdivisions of the system increases.<sup>7</sup>

Our method is based on the assumption that a scaling relation exists, which allows the magnetic properties of a system consisting of  $N$  magnetic moments subjected to exchange, dipolar, and anisotropy interactions to be obtained from Monte Carlo calculations for a smaller system with  $N' < N$  moments. In the smaller system, the exchange interaction  $J$  between neighboring moments is reduced, whereas all the other parameters are kept constant. This includes the lattice spacing, which means that in our method the density of magnetic moments does not change upon scaling, differently from what happens in previous approaches.<sup>8</sup> We also claim that if the exchange interaction  $J'$  in the smaller system is equal to  $xJ$ , with  $x < 1$ , then  $N' = x^{-3\eta}N$ , where  $\eta$  is a positive number. The existence of such scaling relations and the possibility of combining them with the Monte Carlo technique to speed up calculations, as well as the procedure for determining the exponent  $\eta$ , are the main results in this communication.

Let us consider a system consisting of  $N$  magnetic moments  $\{\vec{\mu}_i\}$  of equal magnitude  $\mu$  positioned at the sites of a simple cubic lattice, in a cubic arrangement. The size of the cube is  $L = N^{1/3}a_0$ , where  $a_0$  is the lattice parameter. The total energy of such a system is  $E_{tot} = E_{ex} + E_{dip} + E_K$ , where  $E_{ex} = \sum_{\langle i,j \rangle} J_{ij} \vec{\mu}_i \cdot \vec{\mu}_j$ ,  $E_{dip} = \sum_{i>j} \{ \vec{\mu}_i \cdot \vec{\mu}_j - 3(\vec{\mu}_i \cdot \hat{n}_{ij})(\vec{\mu}_j \cdot \hat{n}_{ij}) \} / r_{ij}^3$ , with  $r_{ij}$  the distance between the magnetic moments  $i$  and  $j$ , and  $E_K = -\sum_i U_K \cos^2 \theta_i$  are the exchange, classical dipolar, and uniaxial anisotropy energies, respectively. In the latter,  $U_K$  is the anisotropy constant and  $\theta_i$  is the angle between  $\vec{\mu}_i$  and the  $z$  axis (easy axis). The exchange interaction  $J_{ij}$  is equal to  $J$  when  $\vec{\mu}_i$  and  $\vec{\mu}_j$  are nearest neighbors and zero otherwise. To make contact with the problem defined in Ref. 7, we set  $\mu = 1.6\mu_B$ ,  $J = 2357.44$  kOe/ $\mu_B$ ,  $a_0 = 0.2$  nm, and  $U_K = 1.3492 \times 10^{-3}$  eV/nm<sup>3</sup>. Here  $\mu_B$  is the Bohr magneton. For such set of parameters,  $A = JS^2/a_0 = 1.747 \times 10^{-1}$  eV/nm (the number of atoms per unit cell is 1) and  $l_{ex} = 3.598$  nm. Since  $L$  is expected to be about  $8l_{ex}$  (Ref. 7), it follows that in order to determine the single-domain limit one would have to investigate the magnetic configuration of systems with as many as  $3 \times 10^6$  magnetic moments. However, with the present standard computational facilities, it would be absolutely impossible to find the ground-state (or even the low-temperature) magnetic configuration of such systems by carrying out Monte Carlo calculations. As we show below, the method we propose overcomes such difficulty.

Taking under consideration that the stability of the ferromagnetic (or “flower”) state is strongly dependent on the strength of the exchange interaction  $J$ , one expects that by reducing the value of this parameter the single-domain limit would also be reduced. Thus, the following question could be posed: For which value of the exchange interaction the single-domain limit  $L'_1$  would be equal to, say,  $5a_0$ ? Since a cube of such size would contain just 125 magnetic moments, its magnetic configuration could be determined easily using the Monte Carlo technique. Thus, by carrying out calculations for different values of the exchange interaction, the value  $J'_1$  for which the transition between the flower and

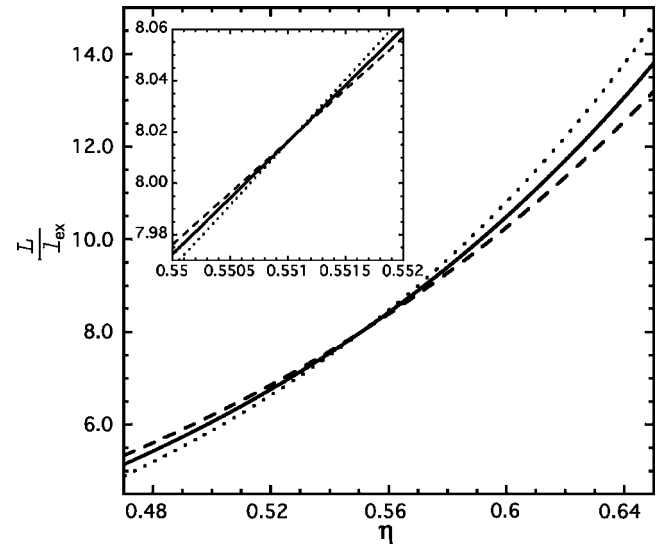


FIG. 1. Dependence of  $L$  (in units of  $l_{ex}$ ) on the exponent  $\eta$  in the scaling relation, for different values of the scaling parameter  $x$ , namely  $x_1 = 2.240 \times 10^{-3}$  (dotted line),  $x_2 = 4.125 \times 10^{-3}$  (solid line), and  $x_3 = 6.509 \times 10^{-3}$  (dashed line). The inset shows a blowup of the figure in the region where the three curves cross each other, corresponding to  $\eta \approx 0.551$  and  $L \approx 8.02l_{ex}$ .

vortex states occurs can be determined. For the values of  $\mu$ ,  $a_0$ , and  $U_K$  given above, we find  $J'_1 = 5.2807$  kOe/ $\mu_B$ . The temperature  $T$  in the Monte Carlo calculations was taken equal to  $10^{-4}$  meV/ $k_B$ . We remark that this is much smaller than mean-field Curie temperature of the bulk material, which is of the order of  $J'_1 S^2 / k_B \approx 400$  K, where  $k_B$  is the Boltzmann constant.

It follows that the scaling factor  $x_1 = J'_1 / J$  of the exchange interaction results in being equal to  $2.240 \times 10^{-3}$ . Our claim is that the value of  $L$  corresponding to the full strength of  $J$  is related to  $L'_1$  according to equation  $L = L'_1 / x_1^\eta$ , where the exponent  $\eta$  has not been determined yet.

We emphasize that the choice of the value  $L'_1 = 5a_0$  was arbitrary, so we could as well have considered other values for the single-domain limit. For instance, for  $L'_2 = 7a_0$  (corresponding to 343 magnetic moments) Monte Carlo calculations give  $J'_2 = 9.7244$  kOe/ $\mu_B$  and, consequently,  $x_2 = 4.125 \times 10^{-3}$ , whereas for  $L'_3 = 9a_0$  (729 magnetic moments) they give  $J'_3 = 15.3446$  kOe/ $\mu_B$  and  $x_3 = 6.509 \times 10^{-3}$ . However, if the method we are proposing is correct, the final result should not depend on the choice of  $L'$  or, equivalently, on the scaling parameter  $x$ . In other words, the three relations  $L'_1 / x_1^\eta = L'_2 / x_2^\eta = L'_3 / x_3^\eta$  should give the same value for  $L$ , provided the right value of  $\eta$  is used.

In order to verify whether this is the case, we present in Fig. 1 curves of  $L/l_{ex}$  as a function of  $\eta$ , corresponding to  $x_1$  (dotted line),  $x_2$  (solid line), and  $x_3$  (dashed line). We notice that, within numerical accuracy, the three curves cross each other at the same point  $\eta = 0.551$ , the solution of the equation  $L'_1 / x_1^\eta = L'_2 / x_2^\eta = L'_3 / x_3^\eta$ , which represents the sought-after value of the exponent in our scaling relation. In addition, the single-domain limit turns out to be  $L = 8.02l_{ex}$ , which is in perfect agreement with what had been expected.

We remark that the scaling relations we have obtained had

already been introduced in the study of magnetic nanoparticles to investigate the relative stability of idealized and fixed internal magnetic configurations of cylinders<sup>9</sup> and cones.<sup>10</sup> In those works, the exponent in the scaling relations was determined numerically and resulted in being equal to 0.55, to within 1% error. The occurrence of the same scaling relations in different contexts involving magnetic nanoparticles supports the idea that they represent a general property of these systems. It is worth stressing that the possibility of using such scaling relations in conjunction with the Monte Carlo calculations, without imposing any condition on the final equilibrium configuration of the magnetic moments, could not be anticipated from those previous works.

In conclusion, we have demonstrated the existence of scaling relations which when combined with the Monte Carlo technique provides a fast and reliable method for in-

vestigating the magnetic properties of nanostructures. The method has been introduced and tested by applying it to the solution of a well-defined problem. It represents a useful tool for studying magnetic nanostructures and might be applicable to other systems, provided appropriate scalable variables are identified.

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