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On the theory of nucleation in cylindrical magnetic nanoparticles

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1 Introduction

The magnetic properties of nanometric systems, such as metallic granular systems, dots and cylinders, have been investigated during several years; and the behavior of them are interesting for both fundamental and applied point of view. Two particular interesting topics are the study of the equilibrium magnetic states and the magnetization reversal mechanism in these nanosized objects. These features are strongly determined by the interplay among exchange, magnetic anisotropy and dipolar interactions, and such interactions depend on the geometry of the considered object [1]. Hence, the study of the nucleation of magnetic nanoparticles taken into account the geometry is really important and in order.

The goal of the present work is to find an explicit form of the magnetic energy, which allows describing the nucleation phenomenon in a particle of cylindrical shape, taking into account the surface anisotropy effect. We find an analytical solution for corresponding nonlinear differential equation of the nucleation phenomena for this kind of object. The paper is arranged in the following way: In Section 2 the theoretical model is developed and the phase transition of the system is calculated. The conclusions are presented in Section 3.

2 Theoretical model

In order to make a description of the magnetic distribution of a magnetized body we need to take into account its geometrical characteristics, in particular when the diameter of a magnetic cylinder is smaller than the typical domain wall size, i.e. of the order or less than 10^2 nm, we have a single-domain structure [2]; in such case, the wire can be represented as simple a monodomain and the Brown theory for the nucleation problem [3] is applicable. Therefore, for a local extreme of the total energy, $E(\boldsymbol{r})$, we use the variational principle:

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$$\delta \int_{V(S)} d^3r\, E(\boldsymbol{r}) = 0 \tag{1}$$

Where δ indicates the functional variation, the integration spreads in all the volume of the magnetic body. So, if the explicit structure of $E(\boldsymbol{r})$ is known, the equation (1) provides, generally, a differential equation to solve; in a classical magnetic system it is usually standard to find a set of nonlinear differential equations and, in only few cases, it is possible to find analytical solutions [4].

In the present work we focus on the magnetization field distribution of magnetic nanoparticles with cylindrical shape without external field. This problem was addressed by Brown [3] and Aharoni *et al.* [5] only in the linearized and numerical point of view respectively, by analyzing the equilibrium state. First, when only the exchange term is taken into account and using the azimuthal symmetry, the energy can be written as:

$$E_{ex}(\rho) = \frac{A}{2}\left[(\theta'(\rho))^2 + \rho^{-2}\sin^2(\theta(\rho))\right] \tag{2}$$

Where $\theta(\rho)$ is the angle between the magnetization field vector and the cylinder axis, θ is chosen to lie in the interval $\pi \ge \theta \ge \pi/2$; A is the exchange constant in the continuum Heisenberg theory and ρ is the relative radial cylinder coordinate, defined as $\rho = r/r_w$, being r_w the wire radius, so $0 < \rho < 1$. The equation (1) with the function (2) produces the following nonlinear equation:

$$\theta''(\rho) + \rho^{-1}\theta'(\rho) - \rho^{-2}\cos(\theta(\rho))\sin(\theta(\rho)) = 0\,, \tag{3}$$

the exact solution of equation (3) with the boundary condition $\theta(\rho = 0^+) = \pi$ and $\theta(\rho = 1) = \pi/2$ can be cast as:

$$\tan(\theta/2) = \rho^{-1} \tag{4}$$

We note that, similar types of nonlinear differential equations, with their exact analytical solutions are presented in reference [6].

Next, let us analyze the magnetization distribution in a single thin amorphous cylindrical nanoparticle, this is done by adding an anisotropy term; using the azimuthal symmetry the energy in this case can be modeled as:

$$E_{ex-an}(\rho, a) = \frac{A}{2}\left[(\theta'(\rho))^2 + (a/\rho)^2\sin^2(\theta(\rho))\right], \tag{5}$$

where a^2 is an anisotropy coefficient (which has normalized surface units) such that $a = 1$ represents the previous case with no anisotropy. Therefore, using equation (1) with the function (2) provides the following differential equation:

$$\theta''(\rho) + \rho^{-1}\theta'(\rho) - (a/\rho)^2\cos(\theta(\rho))\sin(\theta(\rho)) = 0\ . \tag{6}$$

Since equation (6) for $a = 1$ reduces to the equation (3), an extension of the solution (4) with the same boundary condition, i.e. the exact solution of the equation (6) , is given by:

$$\tan(\theta/2) = \rho^{-a} \tag{7}$$

We can easily recognize that the form of this expression (7) has a soliton structure. Figure 1(a) shows the 3D behavior of θ as function of parameters a, ρ; we note that, when a, ρ increases the function θ strongly decreases, increases, respectively. Figure 1(b) shows implicit plots for $\tan(\theta/2)$ as function of θ for different values of a, we remark that from this figure it is clear the soliton structure, and when a increase the form of the curve is expanded toward to extremes.

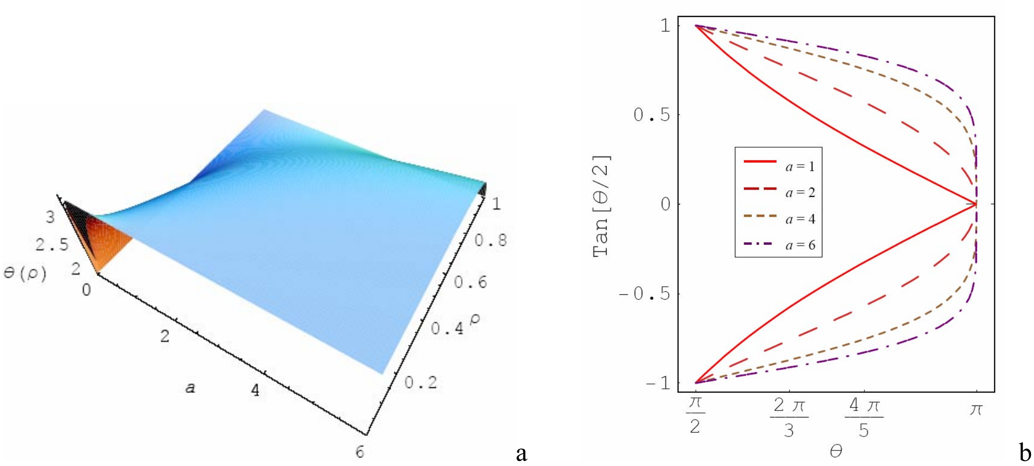

Fig. 1 (a) 3D behavior of θ as function of a and ρ. (b) Implicit plot for $\tan(\theta/2)$ as function of θ for different values of a.

Obviously, once $\theta = \theta(\rho)$ has been obtained, we can calculate any average quantity. In addition let us comment a few about other application of equation (7), it can be used for analyze the magnetic properties of a single glass-coated magnetic microwires with positive magneto-elastic constant when the Brown theory of is applicable [7], in this problem the boundary conditions are: $\theta(\rho = 0) = \pi$ and $\theta(\rho = 1) = \pi/2$, and the most important result is that the remanent magnetization field vector has a finite value for null external magnetic field. Let us comment some features of this model; first, it is recognized that in an ensemble of noninteracting nanoparticles all of them have not exactly the same characteristic due inherently to the grow process; therefore, the anisotropy constant is not the same in all particles of the ensemble; consequently, for taking into account this experimental feature in some models of nucleation, it will be necessary to introduce some distribution of anisotropy constants which can be deduced from the particular experiment to analyze.

Now we look at the structure of the energy. In analogy with classical mechanics we can write the energy (5) in the following way:

$$E = T + W \quad , \tag{8}$$

where T corresponds to the energy determined by equation (2) and W can be seen as the potential energy, or the effect of the anisotropy, and it is determined by the following expression:

$$W(\rho) = \frac{A}{2}\left(a^2 - 1\right)\rho^{-2}\sin^2\left(\theta(\rho)\right) \tag{9}$$

Therefore using the solution (7) in the equation (8) we obtain a functional form the total energy:

$$E = 4Aa^2\left[\rho^{a-1}/\left(1+\rho^{2a}\right)\right]^2 . \tag{10}$$

We note that, in the specific case of absence of anisotropy, $a^2 = 1$, the surface energy of the cylinder, i.e. at $\rho = 1$, goes to A. In a case when $a^2 > 1$, the energy on the surface of the cylinder goes to Aa^2 for $\rho = 1$ and so it is possible to consider the parameter Aa^2 as superficial energy. The energy at the center of the cylinder is not zero if $a^2 = 1$, and equal to zero if $a^2 > 1$.
Figure 2 shows the energy as function of ρ and a and the corresponding density plot, Fig. 2(b). We note from these frames two maxima in the total free energy. It is known that, a characteristic minimum in the

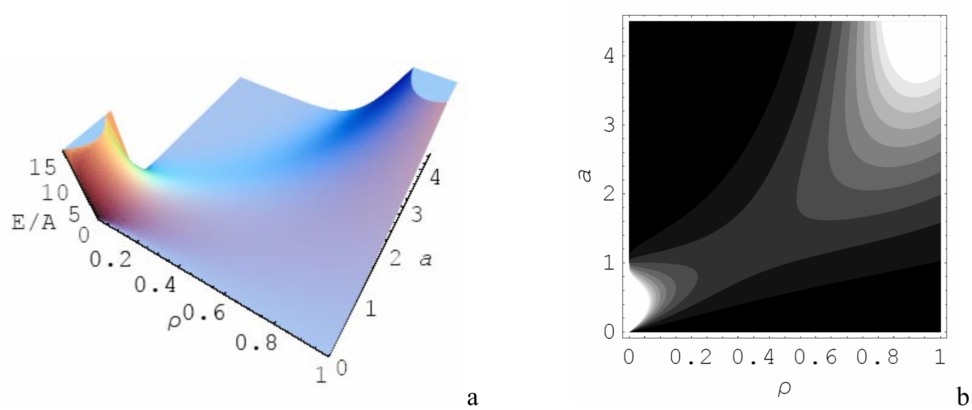

Fig. 2 (a) 3D behavior of *E/A* as function of *a* and ρ. (b) Density plot for *E/A* as function of ρ and *a*.

free energy may correspond to a phase transition. Such transition produces a change of distribution of magnetization. This elementary model showed that, in this case becomes difficult to separate in the thermodynamic function, the volumetric and superficial contributions. Criterion is the existence of enough large parameter a^2.

3 Conclusions

In this work the problem of a single cylindrical nanoparticle is analyzed in detail, taken into account the exchange energy and surface anisotropy energy. We find an analytical solution of the corresponding nucleation nonlinear problem and the exact structure of the total energy in term of the strength parameter.

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References

[1] P. Landeros, J. Escrig, D. Altbir, D. Laroze, J. d'Albuquerque e Castro, and P. Vargas, Phys. Rev. B **71**, 094435 (2005).
[2] S. A. Baranov (unpublished).
[3] W.F. Brown, Micromagnetism (Nauka, Moscow, 1974) (in Russian).
[4] A. Aharoni, Introduction of the Theory of Ferromagnetism (Clarendon Press, Oxford, 1996).
[5] A. Aharoni and S. Shtrikman, Phys. Rev. **109**, 1522 (1958).
[6] G. Woo, J. Math. Phys **18**, 1264 (1977).
[7] S. A. Baranov, D. Laroze, P. Vargas, and M. Vazquez, Physica B **372**, 320 (2006).

