Dynamical Temperature for Anisotropic Magnetic Nanoparticles

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Abstract. In this work we investigate the dynamic properties of classical magnetic anisotropic nanoparticles in the presence of an applied magnetic field, such that it is perpendicular respect to the easy axes. We calculate the analytical expression of the configurational temperature as function of the control parameters of the system and we find that, the temperature has an oscillatory behavior as a function on time when the direction of the external field is different to the easy axes. In addition, we calculate the energy as a function of the average of the temperature and we recover the equilibrium prediction.

1. Introduction

The development of the magnetic nanostructures has been increased in the last years, due to multiple technological applications and the theoretical studies of these structures, in general, are based in numerical calculations or analytical methods [1]. The simulation of classical spin system is mainly performed by using two different methods [2]: Montecarlo (MC) and Spin Dynamics (SD). MC is a stochastic method very useful to calculate static properties of equilibrium system, but does not work for dynamical properties due to its probabilistic nature. So far, there is no clear prescription to link MC step with real time. On the other hand, in SD one can obtain both static and dynamical properties of the system. This is done by solving the associate dynamic equation; obtaining the spin trajectory in function of time and taking average over the configuration; but the problem of the SD case it that, unlike particle molecular dynamic, there is no prescription to estimate the temperature.

Recently, using the microcanonical ensemble a formulation to measure of the configurational temperature for any Hamiltonian system is presented [3] this method provides an intrinsic link between dynamical systems theory and the statistical mechanics of Hamiltonian systems; and it is formalized, in mathematical point of view, by the same author in reference [4] and finally the author formulated a Microthermodynamic formalism in reference [5]. As a consequence of reference [3] a generalization of the dynamical temperature was presented in reference [6]. The Rugh’s approach was extended for classical spin associated to Nambu’s dynamics, being applied to paramagnetic system and spin chain system [7], after that the same authors applied this method to a planar spin chain [8].

The goal of this article is calculate the configurational temperature of anisotropic nanoparticles in presence of applied magnetic field such that, it has different orientations respect
to the easy axis. We found that, for the paramagnetic case the temperature is a constant and its numerical value only depend of the initial conditions. Moreover, when the external field has a variation respect to the direction of the easy axes the dynamical behavior of the temperature appear oscillations and their increases when the angle between the easy axes and the magnetic field increase. The paper is arranged in the following way: In the Sec. II the theoretical model is presented and the results are discussed. Finally, the conclusions are exposed in Sec.III.

2. Theoretical Model and Results

Let us consider a system of N magnetic nanoparticles and assume that each particle can be represented by a magnetic monodomain. The temporal evolution of this system can be modeled by the Landau-Lifshitz equation and in the dimensional and in absence of damping it can be written as [9]:

$$\frac{d\mathbf{m}_i}{d\tau} = -\mathbf{m}_i \times \mathbf{h}_i$$  \hspace{1cm} (1)

where $\mathbf{m}_i$ an normalized individual magnetic moment with and the corresponding ith normalized effective field, $\mathbf{h}_i$, is given by $\mathbf{h}_i = -\nabla \mathbf{m}_i H$ where $H$ represents the appropriate Hamiltonian for the system. The normalized conditions are given by: and , where is the magnitude of a reference magnetic field and is an effective gyromagnetic ratio. We remark that the structure of Eq. (1) has an intrinsic relationship with the Nambu’s equation governing the dynamics for a triplet of canonical variables with two motion constants; in the case of a single magnetic moment, the triplet of canonical variables is given by and the two motion constants are the energy and the normalization stationary condition [10].

In this work we analyzed the case of anisotropic magnetic nanoparticles; so let us then consider a single-domain magnetic particle with all its atomic moments rotating coherently on a plane in the presence of an external magnetic field. The particle is characterized by a constant value of the magnetization modulus $M = V M_s$, being $V$ the volume of the particle and $M_s$ its saturation magnetization. Well below the Curie temperature of the specific magnetic element, $M_s$ is almost temperature independent. The total energy of this nanoparticle has two contributions: the anisotropy energy, either due to shape, stress or crystalline structure of the particle; and the Zeeman energy, owing to the presence of an external magnetic field, $\mathbf{h}$. Under these conditions the normalized Hamiltonian reads

$$H = \sum_i h_a (\mathbf{m}_i \cdot \hat{n})^2 - (\mathbf{m}_i \cdot \mathbf{h})$$  \hspace{1cm} (2)

where $h_a$ is the normalized anisotropy field defined by the following relationship $h_a = 2KV/(H_0 m)$ being $K$ the anisotropy constant, and $\hat{n}$ is a unitary vector in the direction of the easy axis; easy axis; note that, the constant $K$ can be take positive or negative values depending of the particles shape.

In order to express in the microcanonical ensemble for a magnetic nanosystem the temperature, $T$, we start by expression for entropy $S$ given by $S = \ln(W)$, where $W$ is the volume of phase space with energy $E$ and the Boltzmann’s constant set to unity. Hence, the temperature in the microcanonical ensemble can be expresses as

$$\frac{1}{T} = \frac{d \ln S}{dE}$$  \hspace{1cm} (3)

Using the Nurdin et al approach the Eq. (3) can be expresses by

$$\frac{1}{T} = \frac{\sum_j L_j^2 H \sum_i (L_i H)^2}{\sum_i (L_i H)^2} - \frac{\sum_j (L_j H) \cdot \left[ L_j \sum_i (L_i H)^2 \right]}{(\sum_i (L_i H)^2)^2}$$  \hspace{1cm} (4)
with \( \mathbf{L}_j = \mathbf{m}_j \times \nabla \mathbf{m}_j \). In order to express the Eq. (4) in a close form for the Hamiltonian Eq. (2) we analyze the different terms separately:

\[
\mathbf{L}_i H = 2 \hbar a (\mathbf{m}_i \cdot \hat{n}) (\mathbf{m}_i \times \hat{n}) - \mathbf{m}_i \times \mathbf{h}
\]  

(5)

\[
\mathbf{L}_i^2 H = 2 \hbar a \mathbf{m}_i^2 - 6 \hbar a (\mathbf{m}_i \cdot \hat{n})^2 + 2 (\mathbf{m}_i \cdot \mathbf{h})
\]  

(6)

\[
(\mathbf{L}_i H)^2 = 4 \hbar^2 a^2 m_i^2 (\mathbf{m}_i \cdot \hat{n})^2 + m_i^2 \hbar^2 - 4 \hbar a m_i^2 (\mathbf{m}_i \cdot \hat{n})(\mathbf{h} \cdot \hat{n}) - [2 \hbar a (\mathbf{m}_i \cdot \hat{n})^2 - (\mathbf{m}_i \cdot \mathbf{h})]^2
\]  

(7)

Therefore, replacing equations Eq. (5), Eq. (6) and Eq. (7) in equation Eq. (4) is obtained the analytical expression for the dynamical temperature; however for a larger number of spins the second terms of Eq. (4) is negligible, and the corresponding temperature can be cast in the form:

\[
\frac{1}{T} = \frac{2 \hbar a N m^2 - 6 H - \sum_i \mathbf{m}_i \cdot \mathbf{h}}{\sum_i \mathbf{L}_i^2 H}
\]  

(8)

In addition, the average in time can be calculated as \( T^{-1} = \langle T^{-1} \rangle \). We remark that, in the of superparamagnetical particle the temperature is a constant defined by the initial conditions.

Figure 1. Temporal evolution of energy and temperature. Top: evolution of the energy. Center: evolution of the temperature. Bottom: Amplification of the evolution of the temperature for different windows of time.

In order investigate the dynamical behavior of the temperature we integrate the corresponding nonlinear 1 for the hamiltonian 2 using the fourth-Runge-Kutta method. We assume identical
particles and an intermediate number of them, \( N = 64 \). The fixed parameters are \( h_a = 1 \) and \( \hat{n} = \hat{z} \), and the direction of the magnetic field is xy-plane. The initial conditions for the magnetic moments are selected random for a given fixed energy.

The main results of the magnetic effects are displayed in Figures 1 and 2, where we plot the temperature as function on time, for one fixed energy and different energies, respectively. The first graph in Fig. 1 correspond to the energy versus time and in essentially it is our control of the numerical method, because it is clearly show that it is a constant. In the central graphic and the two insets correspond to the temperature as a function on time. These results show that the temperature is a fluctuating function on time, and the fluctuation is around to average, also the envelope function is the temperature is like a ribbon structure.

The Fig. 2 show the temperature as function on time for different energies. We observe that, the fluctuation increases when the temperature increases too; hence the anisotropy effect is an destabilizing effect in the system. The insect represent the energy as function as the total time average of the temperature and this curve confirm the equilibrium prediction for this system.

3. Conclusions
In the present work, the dynamical properties for anisotropic nanoparticles in an external magnetic field is studied, such that it is perpendicular to the anisotropy axes. We determine the analytically the structure of the configurational temperature as function of control parameters. Using Runge Kutta method we solve the corresponding nonlinear differential equation for 64 nanoparticles with random initial condition and, calculate numerically the time dependence of the configurational temperature. Beside, our results shown that the anisotropy effect destabilized the system.
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