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Phase diagram of uniaxial antiferromagnetic particles: Field perpendicular to the easy axis

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Abstract

We consider a spherical uniaxial antiferromagnetic particle in the presence of an external magnetic field perpendicular to its easy axis. The model is described by a classical Heisenberg Hamiltonian including a single-ion uniaxial anisotropy, where the magnetic moments of the particle are represented by continuous spin vectors. We employ mean-field calculations and Monte Carlo simulations to determine the phase diagram of the system. The phase diagram in the plane field *versus* temperature is obtained for particles with radii ranging from three up to twelve spacing lattice units. We have seen that a particle with more than nine shells behaves as a true thermodynamic system. We find the explicit dependence of the zero temperature critical field and the Néel temperature on the diameter of the particle. At low temperatures, we have also shown that, for particles with three or more shells, the critical field follows a T^2 law, which is in agreement with the predictions of the spin-wave theory, when the field is perpendicular to the easy axis.

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1. Introduction

The phase diagram of anisotropic antiferromagnets when the magnetic field is applied along their easy axis direction presents three distinct phases: antiferromagnetic, spin-flop and paramagnetic phases. The phase boundary between the spin-flop and paramagnetic phases has been the subject of several experimental and theoretical investigations [1–3]. For instance, a well-known result is that for uniaxial antiferromagnets, the critical magnetic field along the easy axis direction behaves asymptotically according to a $T^{3/2}$ law. On the other hand, when the field is perpendicular to the easy axis, the phase diagram is simpler, exhibiting only the antiferromagnetic and paramagnetic phases. For uniaxial antiferromagnetic systems, the critical field follows a T^2 law [4].

Recently, the study of the phase diagram of antiferromagnetic systems was revisited by Zysler et al. [5], where they looked at the magnetic properties of hematite particles. They have shown that the transition field between the antiferromagnetic and spin-flop phases decreases with decreasing particle size according to a $1/D$ dependence (D is the particle diameter). This result was corroborated by us through Monte Carlo simulations for uniaxial antiferromagnetic particles described by a classical Heisenberg Hamiltonian [6].

Antiferromagnetic small particles display many interesting magnetic properties [7–12]. They are due to the uncompensated number of spins in each sublattice at low temperatures as well as to the disorder of the spins at the surface of the antiferromagnetic nanoparticle. Deviations of the atomic moments from a perfect collinearity can explain the enhancement of the magnetization at very low temperatures as the size of the particle is reduced [13,14]. Different choices for the single-ion anisotropy in the core and

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at the surface of the particle lead to distinct reversal mechanisms of the magnetization [15–17]. These reversal mechanisms, which determine the form of hysteresis curve and the magnitude of the coercive field of the particle, depend on the size of the surface as well as on the ratio between the anisotropy parameters in the core and at the surface of the particle.

In this work we consider an uniaxial antiferromagnetic particle in a field perpendicular to its easy axis. The model is described by continuous magnetic moments on a simple cubic lattice. The interaction between nearest-neighbor spins is given by a classical Heisenberg Hamiltonian. We use mean-field approximation and Monte Carlo simulations to obtain the phase diagram of the system in the plane temperature *versus* magnetic field. We determine the phase diagram for particles with radii ranging from three to twelve lattice spacings. The critical field of the phase boundary between the antiferromagnetic and paramagnetic phases is also investigated as a function of temperature, and good agreement with the spin-wave theory is observed in the region of very low temperatures.

In Section 2, we present the model and the calculations in the mean-field approximation. In Section 3, we describe our Monte Carlo simulations, and finally, in Section 4, we present our results and summarize our conclusions.

2. The model

To describe the antiferromagnetic particle, we consider a set of spherical layers centered at a given site, inscribed into a simple cubic lattice. Each site of the lattice harbours a magnetic moment of the particle, which is represented by a vector of magnitude $|\vec{S}_i| = 1$ and with components $\vec{S}_i = (S_{ix}, S_{iy}, S_{iz})$.

The model is described by the following classical Heisenberg Hamiltonian

$$\mathcal{H} = \frac{J}{2}\sum_{i=1}^{N}\sum_{j=1}^{q}(S_{ix}S_{jx} + S_{iy}S_{jy} + S_{iz}S_{jz}) - H\sum_{i=1}^{N}S_{iz} - k\sum_{i=1}^{N}S_{ix}^2, \tag{1}$$

where only the couplings among nearest-neighbors are considered. N is the number of spins of the particle, q is the coordination number of the magnetic moments ($q = 6$ for the internal spins), J is the exchange coupling, H represents the magnitude of the external magnetic field and k is the single-ion anisotropy constant. We assume that the magnetic field lies in the z-direction and the easy axis of the particle is along the x-direction. The exchange couplings are of the antiferromagnetic type, and we assume they have the same value for all pairs of spins of the particle, that is, $J > 0$.

The equilibrium magnetic properties of the particle are obtained through mean-field approximation via the Bogoliubov's inequality [18]. In this case, the expression for the mean-field free energy [19,20] of the particle is

$$\begin{aligned} G_{MF} = {} & -\frac{J}{2}\sum_{i=1}^{N}\sum_{j=1}^{q}(m_{ix}m_{jx} + m_{iz}m_{jz}) \\ & - k_BT\ln\left(\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} e^{\beta[-J\sum_j^q m_{jx}S_{ix}+(H-J\sum_j^q m_{jz})S_{iz}+kS_{ix}^2]}\delta\big(|\vec{S}_i|-1\big)\,dS_{ix}\,dS_{iy}\,dS_{iz}\right), \end{aligned} \tag{2}$$

where $|\vec{S}_i| = \sqrt{S_{ix}{}^2 + S_{iy}{}^2 + S_{iz}{}^2}$,

$$m_{ix} = \langle S_{ix}\rangle = \frac{\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} S_{ix} e^{\beta[-J\sum_j^q m_{jx}S_{ix}+(H-J\sum_j^q m_{jz})S_{iz}+kS_{ix}^2]}\delta(|\vec{S}_i|-1)\,dS_{ix}\,dS_{iy}\,dS_{iz}}{\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} e^{\beta[-J\sum_j^q m_{jx}S_{ix}+(H-J\sum_j^q m_{jz})S_{iz}+kS_{ix}^2]}\delta(|\vec{S}_i|-1)\,dS_{ix}\,dS_{iy}\,dS_{iz}}, \tag{3}$$

$$m_{iz} = \langle S_{iz}\rangle = \frac{\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} S_{iz} e^{\beta[-J\sum_j^q m_{jx}S_{ix}+(H-J\sum_j^q m_{jz})S_{iz}+kS_{ix}^2]}\delta(|\vec{S}_i|-1)\,dS_{ix}\,dS_{iy}\,dS_{iz}}{\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} e^{\beta[-J\sum_j^q m_{jx}S_{ix}+(H-J\sum_j^q m_{jz})S_{iz}+kS_{ix}^2]}\delta(|\vec{S}_i|-1)\,dS_{ix}\,dS_{iy}\,dS_{iz}}. \tag{4}$$

The total magnetization of the particle is given by

$$m(T,H) = \frac{1}{N}\sum_{i}^{N}\sqrt{m_{ix}^2 + m_{iz}^2}, \tag{5}$$

where m_{ix} and m_{iz} are the components of the magnetic moment of the ith spin in the x and z directions, respectively.

The components of the staggered magnetization are calculated by

$$m_{sx} = \frac{1}{N}\sum_{i=1}^{N}\big(m_{ix}^{(a)} - m_{ix}^{(b)}\big), \tag{6}$$