Monte Carlo Simulations of Ultrathin Magnetic Dots

M. Rapini, R.A. Dias, and B.V. Costa
Laboratório de Simulação - Departamento de Física - ICEX - UFMG 30123-970 Belo Horizonte - MG, Brazil

D.P. Landau
Center for Simulational Physics, University of Georgia, Athens, Georgia 30602

In this work we study the thermodynamic properties of ultrathin ferromagnetic dots using Monte Carlo simulations. We investigate the vortex density as a function of the temperature and the vortex structure in monolayer dots with perpendicular anisotropy and long-range dipole interaction. The interplay between these two terms in the hamiltonian leads to an interesting behavior of the thermodynamic quantities as well as the vortex density.

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I. INTRODUCTION

Magnetism at nanoscale, when the size of the structure is comparable to or smaller than both the ferromagnetic (FM) and antiferromagnetic (AF) domain size, offers a great potential for new physics. In the last decade there has been an increasing interest in ultrathin magnetic dots from research groups as well as technological industries. Such an interest is due to numerous unique phenomena related to the low-dimension of these systems.

The modern technology demands techniques capable of producing nanometer-sized structures over large areas. A good perspective is the use of nanodots of nickel that could store terabyte of data in a computer chip just a few centimeters wide. In particular, ferromagnetic nanodots have been widely studied by use of experimental techniques such as MFM (magnetic force microscopy). In addition, some theoretical models were proposed to explain the physical phenomena observed in the experiments, among them the transition from perpendicular to in-plane ordering and the magnetoresistence effect.

Regarding the perpendicular to in-plane ordering transition, experiments were done using epitaxial films to investigate its transition temperature and thickness dependence [2] [3]. In addition, many theoretical approaches were developed, for example, treating a two-dimensional layer by renormalization group [4]. Some lattice models were proposed to take into account long-range dipolar interactions and surface anisotropy [5].

Based on such models, Monte Carlo simulations have been widely used to study the phase diagram of very thin films [6], the nature of this transition [7] as well as its dependence on the magnetic history of the system [8]. On the other hand, magnetic domains [9] and magnetic structures [10] have also been investigated by using computational methods. A topological excitation, the spin vortex, has been found in experiments and also detected in simulations. Vortex structures are believed to drive a Berezinski-Kosterlitz-Thouless (BKT) phase transition in the two dimensional planar-rotator (PR) model [11]. Although vortices are present in thin films with long range interactions, it is not clear if they play any role in the transition.

The model we study is described by the Heisenberg spin hamiltonian with exchange and long-range dipolar interactions as well as single-ion anisotropy

\[ H = -J \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j + D \sum_{i \neq k} \frac{\mathbf{S}_i \cdot \mathbf{S}_k}{r_{ik}^3} - 3 \frac{(\mathbf{S}_i \cdot \mathbf{r}_{ik})(\mathbf{S}_k \cdot \mathbf{r}_{ik})}{r_{ik}^4} - A \sum_i (S_i^z)^2, \tag{1} \]

where we use classical spins $|S| = 1$. Here the first sum is performed over nearest neighbors with exchange coupling strength, $J > 0$, while the second sum runs over all spin pairs in the lattice. The constant of dipole coupling is $D$, $r_{ik}$ is a vector connecting the $i$ and $k$ sites and $A$ is the single-site anisotropy constant along the z-axis [5].

The main task in this work is to study the importance of vortices in the physics of the model. Although preliminary, our results indicate an anomalous behavior of the vortex density at the transition temperature for $\delta = \frac{D}{A} \ll 1$. In the following we present a brief background on the simulation, our results and the conclusions.

Method

The simulations are done in a square lattice of volume $L \times L$ with $L = 20, 40, 60$ by using the Monte-Carlo method with the Metropolis algorithm [12] [13]. Since nanodots are finite per nature we have to use open

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boundary conditions in our simulations. However, we want to emphasize the long range effects of the dipolar term of the model at the boundary of the structure. For that, we have used periodic boundary conditions in the non dipolar terms while for the dipolar term we have used open conditions.

We have studied the model for three different values of the parameters $A$ and $D$, $\delta = \frac{D}{A} = 0.1, 1.0$ and 9.0 for fixed $J = 1$. Energy is measured in units of $JS^2$ and temperature in units of $JS^2/k_B$, where $k_B$ is the Boltzmann constant. For every temperature the first $10^5$ MC steps per spin were used to lead the system to equilibrium and the next $10^5$ configurations were used to calculate thermal averages of thermodynamical quantities of interest.

II. RESULTS

In the case where $\delta = 0.1$, we measured the out-of-plane ($z$) and in-plane ($xy$) magnetizations (Shown in figure 1).

![Figure 1: Out-of-plane and in-plane magnetization for $\delta = 0.1$.](image1.png)

The system comes from an ordered state at low temperature to a disordered state at high temperature. That behavior indicates an order-disorder phase transition at $T_c \approx 0.55$. The in-plane magnetization, $M_{xy}$, grows presenting a maximum close to the order-disorder critical temperature $T_c$. However, the height of the peak diminishes as $L$ grows, in a clear indicative that it is a finite size artifice.

The magnetic susceptibility is shown in figure 2. The position of the maxima give us an estimate for $T_c(\approx 0.55)$.

![Figure 2: Out-of-plane and in-plane susceptibilities for $\delta = 0.1$.](image2.png)

For $\delta = 1.0$ the behavior of the in-plane and out-of-plane magnetizations (See figure 4), suggest that the ground state is disordered in contrast to earlier works of Santamaria [6] and Vedmedenko [10] that argue that the ground state is for spins ordered in the $xy$ plane. A plot of the susceptibility is shown in figure 5 as a function of temperature. Although some authors [6, 10] concluded that this transition is of second order, the curves show well defined maxima that do not seem to indicate any critical behavior.

The vortex density curve in the $xy$ plane is shown in figure 3, and the graphics indicate that the ground state of the system has a significant number of vortices and antivortices in the $xy$ plane. Apparently, the minimum of the vortex curve is connected with the transition to in-plane magnetization, however, we were not able to establish that connection.

![Figure 3: Vortex density for $\delta = 0.1$.](image3.png)

For $\delta = 1.0$ the behavior of the vortex density curve as a function of the temperature suggest that the ground state is disordered, in contrast to earlier works of Santamaria [6] and Vedmedenko [10] that argue the ground state is for spins ordered in the $xy$ plane. A plot of the susceptibility is shown in figure 5 as a function of temperature. Although some authors [6, 10] concluded that this transition is of second order, the curves show well defined maxima that do not seem to indicate any critical behavior.

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We see that the number of vortices increases monotonically from zero as a function of temperature. As temperature grows we observed that the spins in the lattice start to disorder, so that pairs vortices-anti-vortices can unbind inducing a BKT transition. However our results are not refined enough to decide that. In figure 7 we show two typical configurations for $T = 0.8$ and $1.2$ where the vortices are indicated by circles and the anti-vortices by squares.

For systems with larger $\delta$, for example, $\delta = 9.0$, the spins are preferentially in the $xy$ plane but it does not present any magnetic ordering (See figure 5). The vortex density curve is similar to the case where $\delta = 1.0$ (See figure 6).

III. CONCLUSION

In summary, we investigated the Heisenberg spin model with exchange $J$ and dipolar interactions $D$ and an anisotropic term $A$ for different parameters $\delta = \frac{D}{A}$. For small $\delta$, (0.1), we observed that the vortex density has a minimum and is non-zero for low temperatures. Apparently, this minimum is connected with the order-disorder phase transition but this connection has to be
studied more carefully. For larger values of $\delta$ (1.0 and 9.0) the vortex density and the configurations of vortices in the system led us to suspect of a phase transition of the BKT type involving the unbinding of vortices-antivortices pairs. However our results are not refined enough to decide that.

FIG. 8: Out-of-plane and in-plane magnetization (open and full symbols) for $\delta = 9.0$.

FIG. 9: Vortex density in the $xy$-plane for $\delta = 9.0$.

[1] Electronic mail: mrapini@fisica.ufmg.br
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