Phase transition in two-dimensional magnetic systems with dipolar interactions

L.A.S. Mól\textsuperscript{1,} and B.V. Costa\textsuperscript{2,}\textsuperscript{3}

\textsuperscript{1}Departamento de Física, Universidade Federal de Viçosa, 36570-000, Viçosa, Minas Gerais, Brazil
\textsuperscript{2}Departamento de Física, Laboratório de Simulação, ICEX, UFMG, 30123-970, Belo Horizonte, MG, Brazil

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Abstract

In this work we have used extensive Monte Carlo calculations to study the planar to paramagnetic phase transition in the two-dimensional anisotropic Heisenberg model with dipolar interactions (AHd) considering the true long-range character of the dipolar interactions by means of the Ewald summation. Our results are consistent with an order-disorder phase transition with unusual critical exponents in agreement with our previous results for the Planar Rotator model with dipolar interactions. Nevertheless, our results disagrees with the Renormalization Group results of Maier and Schwabl [PRB, 70, 134430 (2004)] and the results of Rapini et. al. [PRB, 75, 014425 (2007)], where the AHd was studied using a cut-off in the evaluation of the dipolar interactions. We argue that besides the long-range character of dipolar interactions their anisotropic character may have a deeper effect in the system than previously believed. Besides, our results shows that the use of a cut-off radius in the evaluation of dipolar interactions must be avoided when analyzing the critical behavior of magnetic systems, since it may lead to erroneous results.

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I. INTRODUCTION

Magnetism is one of the most studied subjects in physics. In particular, the study of the statistical behavior of spin models was the trend in the years 1960’s and 1970’s. They gave fruitful contribution to the understanding of several phenomena, not only in Physics, but in several other fields. The concept of symmetry breaking and universality transcend the subject of physics to many other areas, being thus of great importance. More recently, mainly due to the growing interest in magnetic thin-films, magnetic nano-dots and arrays of magnetic nanoparticles \(^1\text{–}14\), there were a renewed interest in the study of spin models.

In many magnetic systems a long range dipole-dipole energy term has to be considered beside the exchange interaction between neighboring sites and the anisotropies present in the system. The study of such models is mainly associated with the development of magnetic-nonmagnetic multilayer for the purpose of giant magnetoresistance applications and magnetic nanoparticle arrays as an alternative for new media storage. In addition, experiments on epitaxial magnetic layers have shown that a huge variety of complex structures can develop in the system\(^2\text{–}4,15\). Rich magnetic domain structures like stripes, chevrons, labyrinths, and bubbles associated with the competition between dipolar long-range interactions and a strong anisotropy perpendicular to the plane of the film were observed experimentally. A lot of theoretical work has been done on the morphology and stability of these magnetic structures\(^11\text{–}20\). Beside that, it has been observed the existence of a switching transition from perpendicular to in-plane ordering at low but finite temperature\(^3,4\): at low temperature the film magnetization is perpendicular to the film surface; rising temperature the magnetization flips to an in-plane configuration. Eventually the out-of-plane and the in-plane magnetization become zero. Although the structures developed in the system are well known, the phase diagram of the model is still not completely understood.

Here, our interest is in magnetic thin-films with an out-of-plane anisotropy as described above. For such a system we can write a model Hamiltonian as follows

\[
H = -J \sum_{i,j} \langle \vec{S}_i \cdot \vec{S}_j \rangle - A \sum_i (S^z_i)^2 + D \sum_{i \neq j} \left[ \frac{\vec{S}_i \cdot \vec{S}_j}{r^{3}_{i,j}} - \frac{(\vec{S}_i \cdot \vec{r}_{i,j})(\vec{S}_j \cdot \vec{r}_{i,j})}{r^{5}_{i,j}} \right], \tag{1}
\]

known as anisotropic Heisenberg model with dipolar interactions (AHd). Here, we consider a ferromagnetic system, so that \(J > 0\), \(A\) is an easy-axis anisotropy, and \(D\) is the strength of
Figure 1: (Color online) Phase diagram of the anisotropic Heisenberg model with dipolar interactions (AHd) for fixed $A/J = 1$ in the $(D/J, T)$ space. The black solid line represents the transition lines as obtained using a cut-off in the dipolar interactions and the solid black line are the results obtained when full long-range interactions are considered by means of the Ewald summation (this work). The phase I is an Ising-like phase characterized by an ordered out-of-plane alignment of spins (that may present stripe-like configurations for full long-rang interactions). Phase II is an ordered planar ferromagnetic state and phase III is a paramagnetic one.

The dipolar interactions. $\vec{r}_{i,j}$ is a vector connecting sites $i$ and $j$ while $<i,j>$ means that the first summation is to be evaluated for nearest neighbors only. For the dipolar interactions the summation is evaluated over all pairs $i \neq j$ and in the single-ion anisotropy term the summation is evaluated for all sites in the lattice. For $D \neq 0$ the system is frustrated due to the competition between the dipolar and the anisotropic terms. For small $D/J$ compared to $A/J$ we can expect the system to have an Ising-like behavior since an out-of-plane configuration of the spins is expected. If $D$ is not too small we can expect a transition of the spins from out-of-plane to in-plane configuration. For large enough $D$ out-of-plane configurations become unstable such that, the system lowers its energy by turning the spins into an in-plane ferromagnetic arrangement. Earlier works on this model, which discuss the phase diagram, were mostly done using renormalization group approach and numerical Monte Carlo simulation. They agree between themselves in the main features. The phase diagram for fixed $A/J$ is schematically shown in Fig.1 in the $(D/J, T)$ space. From Monte Carlo (MC) results it is found that there are three regions labeled in Fig.1 as I, II, and III. Phase I corresponds to an out-of-plane magnetization, phase II has in-plane magnetization, and phase III is paramagnetic. The border line between phase I and phase II is believed to be of first order and that between regions I and II is a second order one. The transition line between regions II and III has a non clear character. Some authors reported they found a second order line. In reference the author’s claim that the transition is of
the $BKT$ type. In many cases a second order phase transition can be confused with a $BKT$ transition. This can be due to the analysis of the finite size effects to be done in not large enough lattices. Although the different results point out in the direction of a second order or a $BKT$ transition$^{16,21}$ between region II and III, much care has to be taken because they were obtained by using a cutoff radius $r_c$ in the dipolar interaction. The long-range character of the potential is lost and then long-range order may not develop$^{22}$. As a consequence, it will not be surprising if a completely different scenario emerges when considering the true long-range dipolar interaction, since long-range order is expected to be present$^{22}$. In a recent paper, Maier and Schwabl$^{25}$ analyzed the phase transition in the dipolar planar rotator (dPR) model via renormalization group techniques. It is expected that the dPR model describes the critical behavior of the planar to paramagnetic transition in the anisotropic Heisenberg model with dipolar interactions (AHd) since they have the same simetry. Their results indicate that the dPR model belongs to a new universality class characterized by an exponential behavior of the magnetization, susceptibility and correlation length. Besides that, the specific heat was found to be non-divergent, as occurs in the BKT phase transition. More recently Mól and Costa$^{26,27}$ studied, by using Monte Carlo simulations, the AHd model in a bilayer system and the dPR model. In both cases they found strong evidences for the transition between region II and III to be in another universality class characterized by a mixed behavior between order disorder and BKT transitions. Besides, even in a 2D dipole lattice the scenario is not clear due to some conflicting results (see, for example, references$^{28–31}$). It should be noticed however that in most of these works the full long-range character of dipolar interactions are not taken into account properly. Indeed, the dipolar interaction is conditionally convergent in two dimensions due to its anisotropic character, such that the use of the minimal-image convention or the introduction of cut-offs in the potential may not describe the real behavior of the system.

In this work we have used extensive Monte Carlo simulations to study the transition line between regions II and III (the planar to paramagnetic phase transition) in the easy-axis Anisotropic Heisenberg model with dipolar interactions (AHd) (see Eqn. 1). Although the system in consideration has a significant out-of-plane anisotropy our main interest is in a easy-plane symmetry brought about by the dipolar interactions, so that for a suitable choice of the model parameters the spins lie in the film plane. Indeed, our goal is to compare the results obtained for the above mentioned model when full long-range dipolar interac-
tions are considered by using the Ewald summation$^{32,33}$ (this work) with those where a cut-off radius is introduced in the evaluation of dipolar interactions$^{34}$. Our results clearly indicate that considering the long-range character of dipolar interactions the transition line between the planar and paramagnetic phases is of the order-disorder type, being characterized by a non-divergent specific heat and unusual critical exponents, instead of being a Berezinskii-Kosterlitz-Thouless one as reported in reference$^{21}$. This observation can be of great importance since the effects of dipolar interactions is enhanced in systems in the sub-micrometer scale, as magnetic nano-dot$^{13,14,34,35}$ and arrays of magnetic nanoparticles$^{5,6,36}$ and can shed extra light on some controversial results in the literature$^{28–31}$.

II. SIMULATION BACKGROUND

In this work we followed the same methodology used in Refs. 26,27. The reader is referred to these works for a more detailed description, specially about the determination of critical temperature and exponents. Our Monte Carlo procedure consists of a simple Metropolis algorithm$^{37}$ where one Monte Carlo step (MCS) consists of an attempt to assign a new random direction to each spin in the lattice. To equilibrate the system we have used $100 \times L^2$ MCS which has been found to be sufficient to reach equilibrium, even in the vicinity of the transition. In our scheme, two sets of simulations have been performed. In the first one, we preliminarily explored the thermodynamic behavior of the model in order to estimate the position of the maxima of the specific heat and susceptibilities and the crossings of the fourth order Binder’s cumulant. In this first approach we used lattice sizes in the interval $20 \leq L \leq 50$. Once the possible transition temperature is determined, we refined the results by using single and multiple histogram methods. We produced the histograms for each lattice size in the interval $20 \leq L \leq 120$ and they were built at/close to the estimated critical temperatures corresponding to the maxima and/or crossing points obtained in step 1. To construct the histograms at least $2 \times 10^7$ configurations were obtained using at least 3 distinct runs. These histograms are summed so that we obtain a new histogram that allow us to explore a wider range of temperature (an example of the use of histograms can be found in Ref. 26). Periodic boundary conditions are assumed in the directions $x$ and $y$. To take into account the long range character of the dipolar interaction we use the Ewald summation to calculate the energy of the system$^{32,33}$. 
All simulations were done using a square lattice, $A/J = 1$ and $D = 0.3J$. Energy was measured in units of $J$ and temperature in units of $J/k_B$, where $k_B$ is the Boltzmann constant. Our choice of $D = 0.3J$ was to guarantee that the planar behavior of the system was not much affected by the frustration existent near the multicritical point where the three lines shown in Fig. 1 come together. We have devoted our efforts to determine a number of thermodynamic quantities, namely the specific heat, magnetization, susceptibility, fourth order Binder’s cumulant and moments of magnetization as described elsewhere.26,27

III. SIMULATION RESULTS

Concerning the systems’ magnetization no significant size dependence is observed in low temperatures, unlike the results shown in Ref. 21 where a cut-off radius were used in the evaluation of dipolar interactions. This may be an evidence that as the full long-range character of dipolar interactions are taken into account long-range order develops, as expected by the results of Maleev22.

In figure 2 we show a $\log - \log$ plot of the maxima of the susceptibility as a function of the lattice size for $L = 20, 40, 80$ and $120$. The data are very well adjusted by a straight line with slope $\gamma/\nu = 1.763(1)$ exhibiting a power law behavior. This value of the exponent $\gamma/\nu$ is quite near the expected one for a transition in the Ising universality class ($1.75$). Considering the Ising universality class we were able to determine the critical temperature by using the location of the maxima of the specific heat and susceptibilities and the crossing point of the Binder’s cumulant, which gives $T_{c}^{Ising} = 0.946(1)$. By using this value and plotting $\ln(M_{XY} \times \ln(L))$ at $T = T_c$ we have found $\beta/\nu = = 0.163(6)$, which is quite different from the expected value for the Ising universality class ($0.125$).

The last result may indicate that the assumption of the Ising universality class may not be correct. Indeed, by analyzing the moments of magnetization defined in Ref. 26, we obtain $1/\nu = 0.82(2)$ and $T_{c}^{V} = 0.943(1)$. This value of the exponent $\nu$ contrasts with the expected for the Ising universality class, although the value for the critical temperature is approximately the same. Reanalyzing our previous estimates for the critical temperature obtained using the location of the specific heat and maxima of susceptibilities using this new value of the exponent $\nu$ we obtain: $T_{c}^{cv} = 0.945(1)$ and $T_{c}^{x} = 0.943(1)$ (it is worthy to note that in the analysis of the specific heat data the point corresponding to $L = 20$ was
Figure 2: (Color online) Log-log plot of the maxima of the planar susceptibility as a function of the lattice size. The solid red line shows the best linear fit of the data given the exponent $\gamma/\nu = 1.763(1)$. The error bars are shown inside the symbols.

disregarded in both cases). Looking to the crossing point of the Binder’s cumulant we have found $T_c^U = 0.944(2)$. We have thus, as our new estimate for the mean critical temperature $T_c = 0.944(1)$. Using this new value of the critical temperature we obtain $\beta/\nu = 0.149(7)$ in the analysis of the magnetization data.

To distinguish between these scenarios in figure 3 we show a scaling plot of the magnetization obtained with the multiple histogram technique according to its finite size scaling function ($m \approx L^{\frac{\beta}{\nu}} M (tL^{\frac{1}{\nu}})$) considering two possibilities: (i) the Ising-like behavior ($T_c^{Ising} = 0.946(1), \nu = 1$ and $\beta = 0.125$) and (ii) an order-disorder critical behavior with exponents $\nu = 1.22(3)$ and $\beta = 0.18(1)$ and critical temperature $T_c = 0.944(1)$. As can be seen, the scaling plot obtained assuming the Ising universality class does not describe our data as good as the results considering a new universality class. Besides, doing the same analysis with susceptibility and Binder’s cumulant no significant deviations were observed between these two possibilities. Indeed, the values obtained in this study are in good agreement with those obtained for the same model in a bilayer system and for the dipolar Planar Rotator model. To clarify, in table I we show the exponents for the Ising model, the results obtained by Maier and Schwabl for the dPR model, the results of Refs. 26,27 and the results of this work.

So far, everything corroborates to an order-disorder phase transition with non-conventional critical exponents. However, the scale relations $\alpha + 2\beta + \gamma = 2$ and $\nu d = 2 - \alpha$ are believe to be satisfied. Using the values shown in table I and the first relation we should have $\alpha = -0.51(7)$ and using the second relation $\alpha = -0.44(6)$ indicating the possibility that the
Figure 3: (Color online) Scaling plots of magnetization considering the Ising-like behavior (top) and an order-disorder transition characterized by the exponents shown in the last line of table I (bottom).

Table I: In this table we show the critical temperature and exponents for the 2D Ising model\cite{28} (first line), the results of Maier and Schwabl\cite{25} for the dPR model, the results of MC calculations in the bilayer AHd model with a cut-off in the interactions\cite{26}, the results of MC calculations for the dPR model\cite{27} and the results of this work.

| Model             | $T_c$  | $\nu$ | $\gamma$ | $\beta$  | $\alpha$ |
|-------------------|--------|-------|----------|----------|-----------|
| Ising             | 2.269  | 1     | 1.75     | 0.125    | 0 (ln)    |
| dPR (Maier)       |        | 1     | 1/2      | -2       |           |
| AHd (bilayer)     | 0.890(4)| 1.22(9)| 2.1(2)   | 0.18(5)  | -0.55(15) |
| dPR               | 1.201(1)| 1.277(2)| 2.218(5)| 0.2065(4)| -1.1(1)   |
| AHd (this work)   | 0.944(1)| 1.22(3)| 2.15(5)  | 0.18(1)  | -0.44(18) |

specific heat does not diverges. Indeed, to have an better agreement between the results of this work and those of Refs.\cite{26,27} the specific heat should be non-divergent. As one knows, to distinguish between an logarithmic divergence or an slowly power law divergence or even an non-divergent power law, many orders of magnitude are needed. Nevertheless, a careful analysis of the data could give us a clue. In figure\textsuperscript{4} we show our data for the maxima of the specific heat as a function of the lattice size adjusted by two different methods. The dashed
line represents the best fit of a logarithmic divergence \((a \ln(L) + b)\), the solid line is for a non-divergent power law behavior \((-aL^{-b} + c)\). As can be clearly seen, the non-divergent power law describes better the data. Indeed, the \(\chi^2/\text{dof}\) values obtained are \(4.7 \times 10^{-4}\) for the logarithmic divergence and \(1.4 \times 10^{-6}\) for the non-divergent power law. The value obtained for the exponent \(\alpha/\nu\) from the adjust is \(-0.36(14)\), and it is also shown in table III together with the results for the dPR and a bilayer AHd models.

IV. DISCUSSION

In this work we have studied the phase transition in the anisotropic Heisenberg model with dipolar interactions (AHd). Our main goal was to look for possible differences in the critical behavior of the planar to paramagnetic phase transition when full long-range dipolar interactions are considered or not. We have found that the use of the full long-range interaction by means of the Ewald summation\(^{32,33}\) lead to different results, i.e., while the introduction of a cut-off radius at five lattice spacings lead to a BKT transition (Ref. 21), the use of the Ewald summation lead to a order disorder transition with unusual exponents and a non divergent specific heat. Indeed, it would be interesting to present a detailed study of the effects in the critical behavior of the system as the cut-off radius increases. Nevertheless, this study is beyond the scope of this paper and will be addressed in a near future. On the other hand some points deserves a more detailed discussion.

In what follows we present a discussion very similar to that done in Refs. 26,27. In the low temperature phase \((T < T_c)\) the magnetization of the model does not display
any significant decrease as the lattice size is augmented. That is a clear indication of an order-disorder transition. This fact is in disagreement with the results obtained in the work of Rapini et al.\textsuperscript{21} where was reported a BKT transition. Our results are very well described by a finite size scaling theory based on the existence of a low temperature phase with long range order and finite correlation length\textsuperscript{39}. In a BKT phase transition there is no long-range order in the low temperature phase, consistent with the Mermin Wagner theorem\textsuperscript{40}. Indeed, the results of Maleev\textsuperscript{22} predict the existence of long-range order at low temperatures in the AHd model. Our results are consistent with this scenario. As discussed earlier, recent renormalization group results by Maier and Schwabl\textsuperscript{25} predicted that this system may belong to a new universality class, characterized by the presence of long-range order at low temperatures and by an exponential behavior of thermodynamic quantities in the vicinity of the critical temperature. In the Maier and Schwabl scenario the correlation length diverges as $\chi \sim \exp(bt^{1/2})$ when the critical temperature ($T_c$) is approached from the high temperature side, similar to the behavior of the BKT phase transition, while the behavior of other thermodynamic quantities are given by powers of the correlation length. Nevertheless, our results for the AHd model are very well described by power law divergences of the thermodynamic quantities. As can be seen in figure\textsuperscript{3} we have obtained a very good collapse of the curves from different lattice sizes for the magnetization and similar results were also found for the susceptibility and Binder’s cumulant. These curves show that the critical exponents obtained and the conventional finite size scaling theory, that assumes a power law behavior of thermodynamic quantities, describe the Monte Carlo data accurately, indicating that the phase transition in the AHd model is a conventional order-disorder phenomenon with unusual critical exponents. In order to definitely rule out the possibility of this phase transition being in the new universality class proposed by Maier and Schwabl, we should make a comparison of our Monte Carlo results, using a finite size scaling theory based in their predictions and the conventional finite size scaling theory used here. Unfortunately, it is not very clear in the literature how to obtain a finite size scaling theory for exponential divergences. Using a simple replacement of the correlation length by the lattice size (in a manner similar to that made by Challa and Landau in reference\textsuperscript{41}), which should be the first choice, does not give a good collapse of the curves, mainly because the determination of the critical temperature is quite imprecise in this case and the collapse of the curves depends appreciably on the value used for the critical temperature. In any case, using values for the
critical temperature close to the maxima of the susceptibility we were not able to obtain even a reasonable collapse of the curves. At this point one can argue: Why do renormalization group results not agree with Monte Carlo simulations? Actually, the RG study of Maier and Schwabl\textsuperscript{25} is based upon some approximations, for instance by using a continuous version of the model. Since the dipolar interactions have an intrinsic anisotropy, which depends in a complicated manner on the location of each spin in the lattice, the lattice geometry could have a strong effect in the system. The identification and a detailed discussion of the points of the RG study of the model that are behind the discrepancy between our results is beyond the scope of this paper.

Although it was shown that the unusual exponents describes better the data, specially for the magnetization, the transition may be in the Ising universality class as well, since corrections to scaling were not taken into account and the lattice sizes used may not be large enough. Indeed, as can be seen in figure 3 the use of the Ising universality class exponents describes well the data for the largest lattices studied. Nevertheless, it does not seems to be a good choice simply disregard the data for the lattices with $L = 20$ and 40, leaving only two lattice sizes to be analyzed. Thus it is more prudent to not completely rule out the possibility of this phase transition to belong to the Ising universality class. On the other hand, our previous results for the same model in a bilayer system\textsuperscript{26} and the results for the dPR model\textsuperscript{27} were also well described by the same critical behavior found here, such that we still believe that this phase transition is more likely to belongs to a new universality class with unusual exponents. Studies in much larger lattices could remove this ambiguity, nevertheless the computational time needed for such a study turns it impracticable at the moment.

Concerning the origin of the order disorder transition the question is even more complicated. The long-range order observed at low temperatures is expected to occur only when full long-range interactions are present. Nevertheless, in a recent study of the AHd in a bilayer system\textsuperscript{26} using a cut-off in the dipolar interaction, we found the same critical behavior. The same results were also obtained in a study of the dipole planar rotator model in two dimensions\textsuperscript{27} with the dipole long-range interaction treated by means of the Ewald summation. In both cases the critical exponents agree quite well with those obtained in the present work (see table I). This observation indicates that the anisotropic character of dipolar interactions may be the main factor responsible for the observed critical phenomen-
ena. Indeed, this observation is not new in the literature. As an example, Fernandez and Alonso\textsuperscript{31} stated that “Anisotropy has a deeper effect on the ordering of systems of classical dipoles in 2D than the range of dipolar interactions”. In this work the authors found that the inclusion of a quadrupolar anisotropy drastically changes the phase transition behavior of a system of classical dipoles. Apparently, in our system the intrinsic anisotropy of dipolar interactions plays an essential role in the determination of the universality class of the AHd model. The possible new universality class is not surprising. In the theory of critical phenomena\textsuperscript{42} it is expected that the critical exponents, and thus the universality classes, depend only on the spatial dimensionality of the system, the symmetry and dimensionality of the order parameter, and the range of the interactions within the system, characteristics not shared by the AHd model and models of well known universality classes.

As a final remark we would like to stress that these results are much important when the critical behavior of magnetic systems with dipolar interactions is being considered. They show that the use of a cut-off radius in the evaluation of dipolar interactions may lead to erroneous results. This study may be a guide for future works in what concerns the introduction or not of a cut-off radius in the study of critical behavior of magnetic systems with dipolar interactions (see for example Ref. \textsuperscript{43}).

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\* Electronic address: lucasmol@ufv.br
\dag Electronic address: bvc@fisica.ufmg.br
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