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1992 J. Phys.: Condens. Matter 4 2035

(http://iopscience.iop.org/0953-8984/4/8/017)

J. Phys.: Condens. Matter 4 (1992) 2035–2042. Printed in the UK

Monte Carlo simulations on Ising dipoles: finite size scaling and logarithmic corrections

Huang-Jian Xu†, Birger Bergersen† and Zoltán Rácz‡§

† Department of Physics, The University of British Columbia, Vancouver, BC, Canada V6T 2A6

‡ Department of Physics, Clarkson University, Potsdam, New York 13676, USA

Received 17 September 1991, in final form 25 November 1991

Abstract. Monte Carlo simulations are presented for Ising dipoles on body centred cubic and tetragonal lattices. A finite size scaling form that includes logarithmic corrections is proposed and found to significantly improve the data collapse. With lattice parameters appropriate to $LiHoF_4$ we obtain a ferromagnetic transition temperature $T_c = 1.51$ K in good agreement with experiment.

1. Introduction

Many systems exhibit Landau-like critical behaviour above a marginal dimensionality d^*. At $d = d^*$, renormalization group theory leads to logarithimic corrections to the mean field behaviour. An example where $d^* = 3$ is an Ising system of permanent dipoles (Larkin and Khmel'nitskii 1969, Aharony 1973) which has a physical realization in the compound $LiHoF_4$ (see e.g. Griffin *et al* 1980 and references therein). Experimental results for this system were compatible with the theoretical prediction of logarithimic corrections.

Logarithmic corrections have also been studied in Ising systems with short-range interactions, for which $d^* = 4$. Computer simulations were carried out for this system by Mouritsen and Knak Jensen (1979a, 1979b) who found logarithmic corrections to the order parameter, in agreement with theory, for a hypercubic four-dimensional (4D) Ising lattice. A finite size scaling analysis of the same model, incorporating logarithmic corrections, was carried out by Lai and Mon (1990). The effect of logarithmic corrections on the high-temperature series in the 4D Ising model was studied by Guttmann (1978) and McKenzie (1979).

In the physically more realistic case of 3D Ising models with dipolar interactions, simulation work was carried out by Knak Jensen and Kjaer (1989) for parameter values appropriate to $LiHoF_4$. The boundary conditions in that calculation were awkward (ellipsoidal sample shape). The ground state will then have a complicated domain structure in the thermodynamic limit (Griffiths 1968, Arrott 1968) and the net magnetization is difficult to interpret. Also, with free boundary conditions finite size effects will be more pronounced than with periodic boundary conditions (Kretschmer

§ Permanent address: Institute for Theoretical Physics, Eötvös University, 1088 Budapest, Pushkin u 5-7, Hungary.

0953-8984/92/082035+08$03.50

and Binder 1979). The transition temperature obtained in the simulation was considerably higher than the experimentally observed temperature for $LiHoF_4$ and it was not possible to determine the critical behaviour. Knak Jensen and Kjaer (1989) suggested that the disagreement with the experimentally observed transition temperature was due to short-range antiferromagnetic couplings (Beauvillain *et al* 1978) which were not included in their simulation. One of the purposes of the present investigation is to show that a more accurate simulation results in an estimate for the critical temperature that is close to the observed value.

More recently, a finite size scaling analysis was made for Ising dipoles on a body centred cubic lattice (Xu *et al* 1991). Again, no attempt was made to estimate the logarithmic corrections. We wish to extend the finite size scaling methods used in that calculation to the more realistic case of the $LiHoF_4$ lattice and to show how the scaling form can be modified to take into account the logarithmic corrections to the critical behaviour.

The remainder of this paper is organized as follows. In section 2 we introduce our version of the finite size scaling methods for a system at marginal dimensionality, while in section 3 we give details and results of our simulations. Finally, a brief discussion is given in section 4.

2. Finite size scaling method

The long-range nature of the dipole–dipole interactions prevents us from applying a cut-off in the simulations. Since every spin will then interact with every other spin it is only possible to handle a moderate number of spins in our Monte Carlo studies. Therefore, it is important to analyse finite size effects carefully. A powerful tool for this purpose is the finite size scaling theory first introduced by Fisher (1972); for a recent collection of reviews see Privman (1990).

We define the reduced temperature

$$t = (T - T_c)/T_c \tag{1}$$

where T_c is the critical temperature.

From Larkin and Khmel'nitskii (1969) we have for the scaling of the square of the total magnetization for the bulk system, when $t > 0$

$$\langle M^2 \rangle \sim \chi N \sim N t^{-1} |\ln t|^{1/3} \tag{2}$$

while for $t < 0$

$$\langle M^2 \rangle \sim \langle M \rangle^2 \sim N^2 t |\ln |t||^{2/3}. \tag{3}$$

Here N is the number of spins and M is the total magnetization.

In order to have a finite size scaling form which agrees with (2) and (3) we conjecture the following finite size scaling forms

$$\langle M^2 \rangle / N^{3/2} = f_+(N^{1/2} t |\ln(t)|^{-1/3}) \tag{4}$$

for $t > 0$ and

$$\langle M^2 \rangle / N^{3/2} = f_-(N^{1/2} t \, |\ln (-t)|^{2/3}) \tag{5}$$

for $t < 0$. We see that (2) and (3) are reproduced in the large-argument limit from (4) and (5) provided $f_-(x) \to x$ as $x \to -\infty$ and $f_+(x) \to 1/x$ as $x \to \infty$. We conclude that (4) and (5) will be valid as $N^{1/2}t \to \infty$.

Our conjecture is somewhat different from the standard finite size scaling form

$$p_L(t)/p_\infty(t) = f(L/\xi_\infty(t)) \tag{6}$$

where p_L and p_∞ are, respectively, thermodynamic quantities for a system of size L and the asymptotic form in the bulk limit. The bulk correlation length is ξ_∞. Brezin (1982) and Brezin and Zinn-Justin (1985) have made extensive studies of the validity of (6) from the point of view of renormalization group theory. For an isotropic system with short-range interactions, (6) holds when $d < d^*$. For $d > d^*$, (6) is no longer valid. However, one can still use a scaling of the form (6) if ξ_∞ is replaced by a 'thermodynamic length' $\lambda \sim t^{-2/d}$ (Brezin and Zinn-Justin 1985, Binder 1990). At $d = d^*$ Brezin (1982) argues that (6) will break down (in his case $d^* = 4$ for ϕ^4-theory) due to logarithmic corrections.

For a system with long-range interactions the concept of length is weakened. In the case of an infinitely correlated system, mean field theory is exact in the thermodynamic limit. 'Dimensionality' and 'length' then lose their meaning. In the spirit of Botet *et al* (1982) we introduce a 'coherence volume' $V_\lambda(t) = \xi_{||}\xi_\perp^2$. Since the Ising dipolar system is anisotropic the correlation lengths $\xi_{||}$, parallel, and $\xi_\perp$, perpendicular to the magnetization will behave differently (Aharony 1973), in fact near the transition $\xi_{||} \sim \xi_\perp^2$ with

$$\xi_{||} \sim t^{-1} \, |\ln t|^{1/3}. \tag{7}$$

The scaling form suggested by Botet *et al* (1982) then gives in our notation

$$p_N(t)/p_\infty = f(N/V_\lambda(t)) \tag{8}$$

which is a form consistent with (4) provided that $p = \langle M^2 \rangle / N^2$. This result is, however, not consistent with (5). We need to use different arguments in the scaling function on the two sides of the transition.

A different approach to ours is that of Lai and Mon (1990) who use the scaling form

$$\chi_N(t)/\chi_N(0) = f(tN^{1/2}(\ln N)^x) \tag{9}$$

where $x = 1/6$ for the Ising model in 4D. In the limit $N \to \infty$, (2) and (3) do not follow from (9) and their scaling is valid when $N^{1/2}t$ is small, unlike our treatment which is valid in the opposite limit $N^{1/2}t \to \infty$. The form (9) was derived from a finite size renormalization group calculation for the $d = 4$ Ising model. In the anisotropic dipolar case the corresponding theory has to the best of our knowledge not been worked out.

3. Monte Carlo simulation

Simulations were performed for both the body centred cubic (BCC) and body centred tetragonal lattices. In the latter case we choose parameter values appropriate to a

specific material: $LiHoF_4$. The reason we choose this material and not, say, $LiTbF_4$, is that it is generally believed that $LiHoF_4$ is a permanent dipole ferromagnet while $LiTbF_4$ has an induced dipole moment (Reich *et al* 1986). The lattice parameters of $LiHoF_4$ are $c = 10.75$ Å, $a = 5.175$ Å (Keller and Schmutz 1965). The g-value for the Ho^{3+} ion is 13.3 (Hansen *et al* 1975). We take our unit cell to have $c = 2a$, while the Monte Carlo cell is cubic. We impose periodic boundary conditions with Ewald summation for the effective dipole–dipole interaction. The advantages of this approach have been discussed by Kretschmer and Binder (1979) and Xu *et al* (1991). The relevant formulae are given by Jansoone (1974). We choose lattice constant and dipole moment in our simulation so that our ground-state energy agrees with Hansen *et al* (1975). We write the bare interaction between dipoles on sites i and j in the form

$$v_{ij} = (\mu^2/4\pi\epsilon_0 r_{ij}^3)\ (1 - 3\cos^2\theta_{ij}) s_i s_j \tag{10}$$

where μ is the dipole moment, r_{ij} is the distance between the spins and θ_{ij} is the angle between the vector connecting the sites and the easy axis. The spins s_i and s_j can take on the values ± 1. In our figures the unit of temperature is

$$T_0 = \mu^2/4\pi\epsilon_0 a^3 k_B \tag{11}$$

where it is assumed that $c = 2a$.

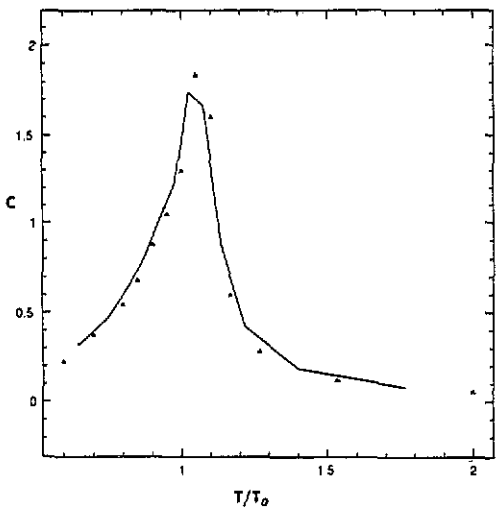

Figure 1. Specific heat of 686 spins on a body centred tetragonal lattice calculated by numerical differentiation of the internal energy (full curve) and the fluctuation formula (triangles).

The simulations were carried out for systems of 128, 250, 432, 686, 1024 and 2000 spins in the case of the body centred tetragonal lattice. In the case of the BCC lattice we did not simulate the largest size system. The simulations start with the ferromagnetic ground state and the temperature is gradually increased. We use a conventional Metropolis algorithm. Since the interactions are long range each energy update is time consuming. At low temperatures, when the acceptance rate is low, we can significantly speed up the algorithm by updating the local fields at each site. This allows us to avoid recalculating the change in the energy at each step which is time

consuming for a system with long range interactions. We check for equilibration by two methods. Firstly we compare specific heats calculated by the fluctuation formula and numerical differentiation of the energy (see figure 1 for the case of $LiHoF_4$). The second method is to follow the time dependence of $\langle M^2 \rangle$ and to check that a steady state has been reached. The temperature dependence of $\langle M^2 \rangle$ is shown in figure 2 again for the body centred tetragonal lattice. In this plot, and in the finite size scaling fits to be discussed below, we have carried out simulation runs for 10–12 different temperatures for each sample size. Between 30000 and 50000 Monte Carlo steps per site (MCS) were used for each size and temperature. For a system of 1024 spins the initial relaxation time for $\langle M^2 \rangle$ was ~30 MCS in the transition region. Let T_i be a simulated temperature and ΔT the difference between neighbouring T_is. We generate two more points at $T_i \pm \Delta T/3$ adjacent to the simulated temperatures, from the simulation data at T_i, using the method of Ferrenberg and Swendsen (1989). The smoothness of the resulting curve then serves as a check of the adequacy of the simulated data.

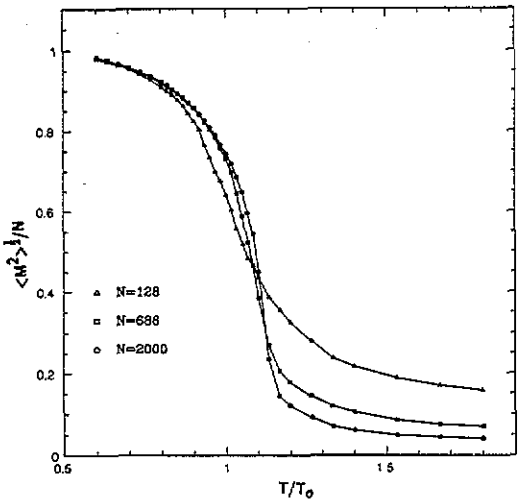

Figure 2. Temperature dependence of $\langle M^2 \rangle^{1/2}/N$ for a body centred tetragonal lattice.

In order to determine the critical temperature we least-square fit the simulated values of $y = \log(\langle M^2 \rangle / N^{3/2})$ to a polynomial of eighth order in the logarithm of the arguments of f in (4) and (5). The procedure is repeated for a number of trial values of T_c. The value of the critical temperature with the smallest statistical quality parameter χ^2 was chosen. The best fit is shown in figure 3. We note that the scaling function for the body centred tetragonal and cubic lattices are identical in the asymptotic region while there is some scatter at small arguments. We also point out that there is only one free parameter in the fit (T_c) and that the slopes in the asymptotic regions are ± 1 to a good approximation which is consistent with the discussion after (5). As a further consistency check we calculate the 'Binder number'

$$U = 1 - \langle M^4 \rangle / 3 \langle M^2 \rangle^2. \tag{12}$$

This quantity goes to zero at high temperatures and approaches 2/3 for low temperatures. When U is plotted against temperatures for systems of different sizes the

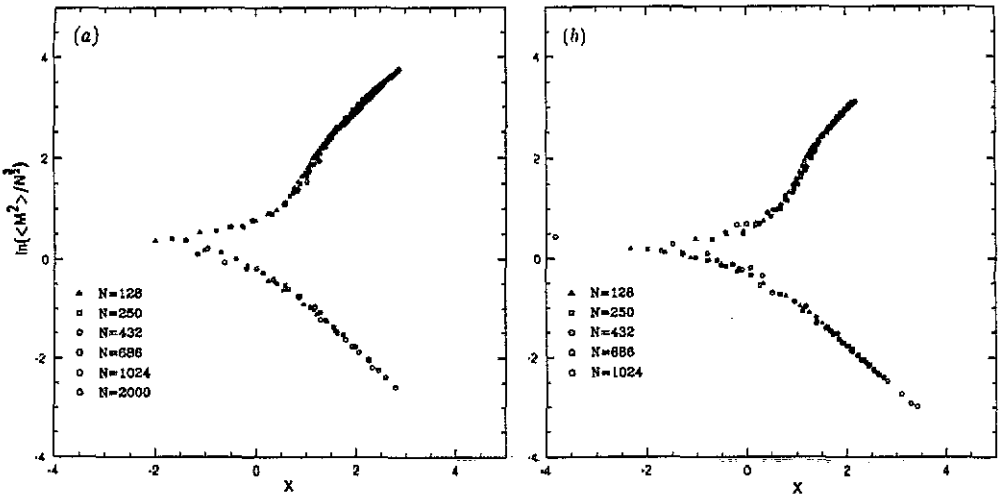

Figure 3. Data collapse using the scaling forms (4) and (5). (*a*) body centred tetragonal lattice with $T_c = 1.145T_0$, (*b*) BCC lattice with $T_c = 0.78T_0$. The abscissa is the log of the argument of the functions $f_\pm$.

curves should intersect at a fixed point value $U = U^*$ and $T = T_c$ (Binder 1990). The theoretical value of U^* from a finite-size renormalization group calculation for the four dimensional Ising model is 0.27 (Brezin and Zinn-Justin 1985) and we expect U^* to be the same for the 3D Ising dipoles considered here. A plot of U versus T is given in figure 4. As can be seen the intersection temperature is close to the best fit temperature 1.15 and U^* is close to the theoretical value.

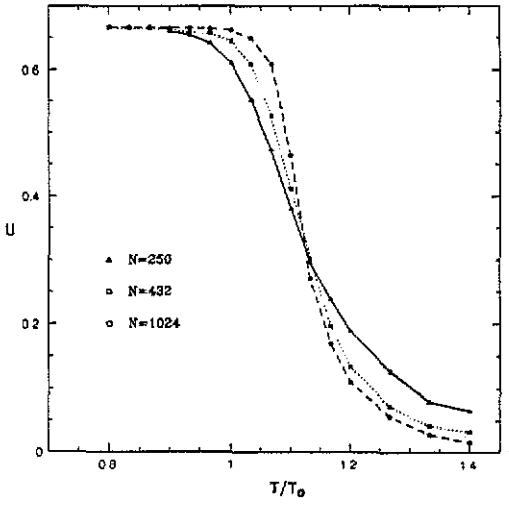

Figure 4. Temperature dependence of 'Binder number', U, for body centred tetragonal lattices of different sizes. The curves are only meant as guides to the eye.

To check the scaling behaviour further we also repeated the analysis using the scaling form

$$\langle M^2\rangle/N^\gamma = f(N^y t) \tag{13}$$

which would have been appropriate if we had critical behaviour without logarithmic corrections. The best fit using (13) with mean-field exponents $x = 1.5$, $y = 0.5$ is shown in figure 5 for the body centred tetragonal lattice (the corresponding fit in the case of the BCC lattice is given in figure 4(*a*) of Xu *et al* (1991)). We note that the fit in figure 5 is inferior to that of figure 3 especially in the low-temperature region. It is possible to get a good fit to the data with three free parameters x, y and T_c in (13), although there seems to be some systematic deviation for low temperatures (figure 6).

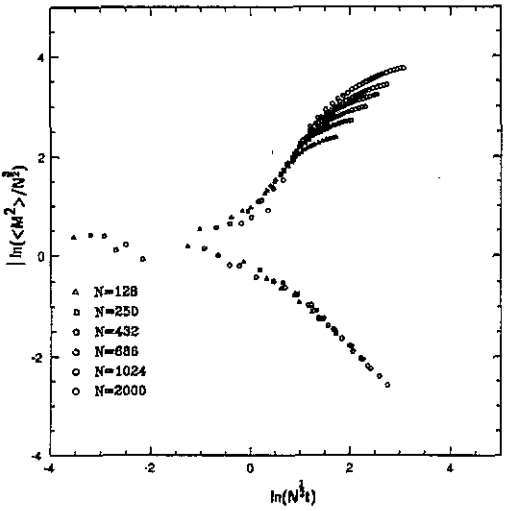

Figure 5. Data collapse using the scaling form (13) and mean-field exponents with $T_c = 1.17T_0$.

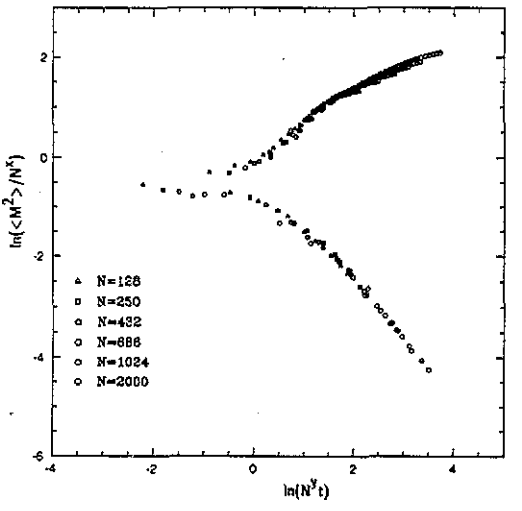

Figure 6. Data collapse using the scaling form (13) with a three-parameter fit $x = 1.72$, $y = 0.59$ $T_c = 1.126T_0$ (order parameter exponent, $\beta = 0.24$; susceptibility exponent, $\gamma = 1.22$).

4. Discussion

We have shown that in the case of Ising dipolar interactions one can get a significant improvement over the mean-field result for the finite scaling fit by including logarithmic corrections to the mean-field expressions. It is also possible to fit the data with non-classical exponents, but this interpretation is not favoured by theory. This suggests (perhaps not surprisingly) that the data-collapse method can give misleading results when theoretical support is not available and many parameters are used. The same difficulty occurs in analysis of experiments where Griffin *et al* (1980) could not unambigously distinguish the logarithmic corrections from weakly non-classical critical behaviour. The best fit for the critical temperature is not very sensitive to the inclusion of logarithmic corrections, e.g. in the case of the BCC lattice our best estimate is $T_c = 0.78T_0$, which should be compared with the value $T_c = 0.79T_0$ found by Xu *et al* (1991) without logarithmic corrections to scaling.

Finally, we conclude that when the calculation is carried out with only one free parameter, we can determine the critical temperature with good accuracy without going to extremes in computational effort. In the case of the body centred tetragonal

lattice we find for the critical temperature $T_c = 1.145T_0$. We compare this with the experimental transition temperature of $LiHoF_4$ by determining the value of T_0 in (11). Our procedure is to equate our ground-state energy (found numerically to be $-0.7211\ k_B T_0$) with the calculated value $-0.9499\ k_B$ K of Hansen *et al* (1975) for $LiHoF_4$. This gives $T_c = 1.51$ K in good agreement with the experimental results 1.538 K of Griffin *et al* (1980). Our results are thus consistent with the interpretation that the dipolar interactions are the dominant ones in this material.

Acknowledgment

We are grateful to Tom Nicol at the UBC Computing Centre for technical assistance. This report has been supported by the Natural Sciences and Engineering Research Council of Canada, US NSF grant CHE-90 08033 and the donors of The Petroleum Research Fund, administered by the American Chemical Society.

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