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Physica B 275 (2000) 187–190

PHYSICA B

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Hysteresis in a dipolar Ising model

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Abstract

Zero-temperature Monte Carlo simulations are performed to study the magnetic hysteresis in a three-dimensional model with only dipolar interactions among the Ising spins located inside a sphere on a cubic lattice. Relevant differences are found in the site energy distributions between the up and down spins during the magnetization process. Variations of the dipolar energy and the density of incomplete columns are also discussed. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Dipolar interactions; Hysteresis modelling; Monte Carlo simulation

1. Introduction

Numerical simulations have proven to be more and more efficient methods of studying the microscopic features of the hysteretic behaviour. Such investigations have clarified that magnetic hysteresis can be caused by the nucleation barrier for the traditional kinetic Ising model [1,2]. The numerical simulations of the random-field Ising models [3,4] and the Sherrington–Kirkpatrick models [5,6] have exposed some other relevant features and relationship during the time evolution under cyclically varied magnetic field. In these cases the Ising system is modified by the introduction of randomness in either the exchange interaction or in the local field. This randomness results in many local energy minima in the phase space. In real magnetic material, however, the domain structure controlled by the dipolar interaction leads to the presence of many energy traps. Although the long-range dipolar interactions cause serious difficulties for the numerical investigations, there are some recent attempts to study Ising models combined with dipolar interactions [7–11].

In a previous paper [11] we have numerically demonstrated the appearance of magnetic hysteresis in a three-dimensional Ising model taking into account the dipole–dipole interactions too. Varying the strength of the (nearest neighbour) exchange interaction this method has allowed us to clarify the geometrical effects due to the general features of the dipole–dipole interaction. Although the shape effects are reduced by choosing spherical ‘samples’ in the simulations, the point-like dipoles create relevant magnetic field variations in the close vicinity of the surface as indicated by early theoretical calculations [12]. This phenomenon initializes the hysteretic behaviour and affects the further evolution of the magnetization process as well.

The present work can be considered as a continuation of our previous study, concentrating on the effects of the dipolar interaction. For this purpose this study is limited to a simplified model omitting the exchange interaction.

2. The model

Using dimensionless quantities the three-dimensional model is defined by the Hamiltonian:

$$H = \frac{1}{2} \sum_{\substack{r,r' \\ r \neq r'}} V(\boldsymbol{r} - \boldsymbol{r}')\sigma(\boldsymbol{r})\sigma(\boldsymbol{r}') - h \sum_{\boldsymbol{r}} \sigma(\boldsymbol{r}), \tag{1}$$

where the up ($\sigma(\boldsymbol{r}) = 1$) and down ($\sigma(\boldsymbol{r}) = -1$) spins are located on a simple cubic lattice ($\boldsymbol{r} = (x, y, z)$; x, y, and z are integers) within a sphere of radius R ($r^2 = x^2 + y^2 + z^2 < R^2$). The second term describes the contribution of the external magnetic field h and the first term summarizes the contributions of the

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PII: S0921-4526(99)00741-3

dipole–dipole interaction given as

$$V(\boldsymbol{r}) = \frac{r^2 - 3z^2}{r^5}. \tag{2}$$

For zero external field ($h = 0$) the ground state energy and the energies for some periodic spin configurations are well described by previous studies [11,13,14]. The minimal energy is reached when the spins form a columnar antiferromagnetic structure characterized by up (down) spins if $x + y$ is odd (even).

Following our previous analysis [11] the magnetization processes are investigated by performing zero-temperature Monte Carlo simulations for a fixed radius, $R = 15.33$. Initially all the spins are pointed up in the presence of an external magnetic field $h = h_{\max}$. The value of h is varied cyclically between $h_{\max}$ and $h_{\min}$ with a uniform step $|\Delta h| = 0.1$. The major loop is studied in the range $h_{\max} = -h_{\min} = 8$ while 10 different values of $h_{\min}$ are chosen for the systematic investigation of the minor loops.

During the simulations we have recorded the local magnetic field defined as $h_l(\boldsymbol{r}) = h + h_d(\boldsymbol{r})$ where

$$h_d(\boldsymbol{r}) = -\sum_{\substack{\boldsymbol{r}' \\ \boldsymbol{r}' \neq \boldsymbol{r}}} V(\boldsymbol{r} - \boldsymbol{r}')\sigma(\boldsymbol{r}') \tag{3}$$

describes the dipolar contribution dependent on the spin configuration. For a given field a randomly chosen spin is flipped if this elementary process decreases the energy. Having a spin flipped we have upgraded the value of $h_d(\boldsymbol{r})$ for each site. These steps are repeated until the site energy, $\varepsilon(\boldsymbol{r}) = -h_l(\boldsymbol{r})\sigma(\boldsymbol{r})$ becomes negative for all the sites. After the system has reached an energy minimum we have modified the strength of external field as described above.

During this procedure we have monitored the magnetization defined as $m = \sum_r \sigma(\boldsymbol{r})/N$ where N is the number of spins inside the sphere. Furthermore, we have determined the probability distribution of site energy for both the up and down spins where $P(\varepsilon)\,d\varepsilon$ expresses the probability to have a site energy between ε and $\varepsilon + d\varepsilon$ for the given spin direction (the numerical calculations are performed with a resolution of $\Delta\varepsilon = 0.05$). In addition the density of incomplete columns has been also recorded. In order to reduce the statistical errors all these quantities are averaged over 50 runs.

3. Results and discussions

First we discuss the major and minor hysteresis loops obtained as described above. To avoid confusion Fig. 1 demonstrates only the major hysteresis curve and two typical minor loops out of 10 for $h_{\min} = 0$ and -3. Note that the major loop is symmetric, while a delayed increase of m can be observed for the minor loops in the ascending branch.

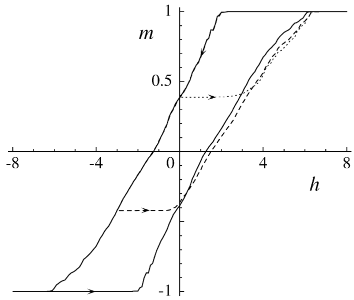

Fig. 1. The major and two minor hysteresis loops obtained by MC simulations for $R = 15.33$.

The difference between the major loop and a minor one can be easily understood when visualizing the subsequent spin configurations appearing during the magnetization process. As demonstrated by a series of spin configurations in Fig. 3 of Ref. [11] the structure with uniform columns is typical and most of the spins flip only once during a half-cycle. The hysteretic behaviour is (strongly) related to the fact that along the same branch of the major loop a state with magnetization m is completely independent of that with $-m$, that is, they cannot be mapped into each other by an overall $\sigma(\boldsymbol{r}) \to -\sigma(\boldsymbol{r})$ reversal of spins. In this model this follows from the striking feature of the consecutive configurations, that the first reversing columns are positioned in the close vicinity of the 'equator', in contrast to the last ones positioned inside the sphere.

For the minor loops a portion of spins remains unchanged. The frozen portion depends on $h_{\min}$ and results in a delay for the magnetization process. As demonstrated in Fig. 1 the 'rising curve' of the minor loops are slightly different and unexpectedly go beyond the major ascending branch.

As mentioned above there is an asymmetry between the up and down spins in the states passed through by the system during the magnetization process. Such a difference can be well illustrated by the site energy distributions. The curves plotted in Fig. 2 correspond to an averaged state formed in the $h = 0$ point of the descending major loop. This is the state where the magnetization process is reversed in the smaller minor loop plotted in Fig. 1. Note that the reversed (down) spins have markedly deeper site energies than those remaining unchanged. Similar results are found for other values of h. Generally, at the peak of these distributions the site energy for the reversed spins is lower than that for the unchanged spins. It is worth mentioning, however, that the area below the site energy distribution changes together with the ratio of spins of given direction.

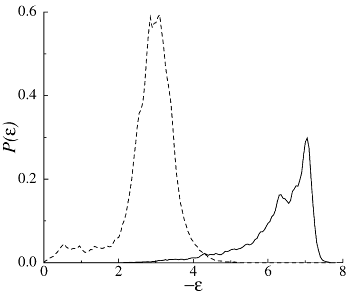

Fig. 2. Site energy distributions as a function of $-\varepsilon$ for up (dashed line) and down (solid line) spins for a state of zero magnetic field when decreasing h along descending major loop.

Some features of the hysteresis loops can be related to these site energy distributions as follows. Let us consider the state whose site energy distribution is given in Fig. 2. A further decrease of the magnetic field along the descending major loop shifts this distribution left (right) for the up (down) spins. As a result in some lattice points the up spin direction becomes unstable (with positive site energy). A spin-flip occurring at any such site can initiate avalanches of spin-flips frequently leading to the reversal of spins in complete columns and decreasing the peak area. In this process the number of reversed spins exceeds the number of originally unstable sites. On the other hand, an increase of the magnetic field will cause an opposite shift of the site energy distributions when a minor loop is initialized. In this case, however, we practically cannot find unstable spins because of the extremely low value of $P(\varepsilon)$ for down spins. This is the reason why the initial susceptibility at the reversal point of the smaller minor loop in Fig. 1 is approximately zero.

The above analysis can be performed at any point of the hysteresis loops. Fig. 3 demonstrates the variation of the dipolar energy per sites with the applied magnetic field along the loops illustrated in Fig. 1. The curves in the upper plot indicate that the average dipolar site energy depends on the history. It is emphasized that at $h = 0$ the system dipolar energy exceeds the equilibrium value calculated previously [11] and marked in the figure. Here it is worth mentioning that this dipolar energy vanishes in the saturated states independently of the system size.

In the plotted curves the irregular small steps come from the finite size effects. These irregularities become less striking when the dipolar energy per sites is plotted as a function of m. In such a plotting the differences between the major and minor loops become comparable to the line width; therefore, the minor loops are omitted in the lower plot. At first glance the dipolar energy can be well approximated with the same parabolic function of m for both the half-cycles with a small systematic deviation of about 1% causing a slight asymmetry in the upper plot too.

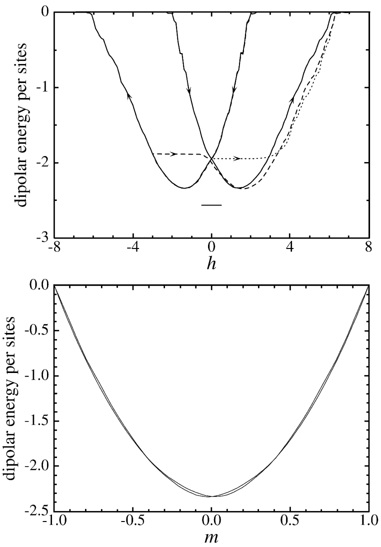

Fig. 3. Average dipolar energy during the magnetization processes as a function of magnetic field (upper plot) and magnetization (lower plot). The solid line represents the results in the major loop, the dashed and dotted lines correspond to $H_{\min} = 0$ and $H_{\min} = -3$. The horizontal marker in the upper plot indicates the ground state energy for $h = 0$.

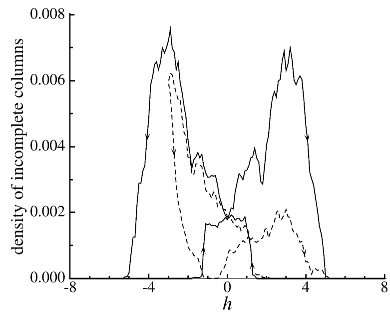

Fig. 4 . Average density of incomplete columns versus magnetic field for the major loop (solid lines) and for a minor loop (dashed lines) if $H_{\min} = -3$.

During the simulations one can easily determine the number of columns whose spins are not ordered. Although the density of such incomplete columns is always less than 1% their role in the hysteretic process is to be investigated. Fig. 4 demonstrates the variation of the average density of incomplete columns for the major loop and for a minor loop (the larger one plotted in Fig. 1). In this case the small number of events results in larger statistical errors illustrated in the figure by the apparent asymmetry between the two branches of the major loop.

Despite its large statistical errors Fig. 4 demonstrates clearly that the incomplete columns disappear immediately after the field reversal point at the 'bottom' of the minor loops. This observation can be related to the short life time (a few steps in h change) of incomplete columns, which may be interpreted as 'soft defects' characterized by small pinning energies. This type of defects play more important role for larger systems since preliminary simulations indicate that their density increases with size. Further systematic analyses are required to clarify their effects on the hysteresis loops.

4. Conclusions

Using Monte Carlo simulations we have studied a three-dimensional dipolar Ising model where dipole–dipole interaction was introduced instead of the usual (short-range) exchange interaction. The unusual behaviour in the ascending branches of the minor loops with respect to the major one can be attributed to geometrical effects of the dipolar interaction in a spherical sample. The asymmetry in the site energy distribution of up spins and down spins is related to the irreversible behaviour that is the difference between the ascending and descending slope at the field reversal points. The role of the incomplete columns deserves further studies. In summary this simplified dipolar model seems to be a good candidate for the investigation of some microscopic features during the magnetization processes.

Acknowledgements

This research was supported by the Hungarian National Research Fund (OTKA) under Grant No. T-23555.

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