INSTANTANEOUS CONFIGURATIONS OF THE BLOCH WALLS IN A TWO-DIMENSIONAL AND S=1/2 MODEL

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Abstract

We show that instantaneous configurations of 180^o domain walls constructed on a square lattice in a two-dimensional and $S = 1/2$ Ising-type model exhibit fractal structure. The fractal dimension depends on the coupling parameters and it is a continuous function of the temperature. The wall thickness in the neighbourhood of T_c presents scaling properties in good agreement with the classical theory by Landau.

1. Introduction

The theory for the average configuration of the Bloch walls is known since the famous paper of Landau and Lifsitz [1]. In this paper we study the instantaneous configurations of the 180^o Bloch walls for $S = 1/2$ spins on a two-dimensional square lattice. The hamiltonian of the problem is considered of Ising-type [2]. For square lattice, considering interactions between first-nearest neighbours only, the Ising model is well understood theoretically [3]. If we introduce interactions with next-nearest neighbours or domain boundaries the problem becomes much more difficult and usually studied by computer simulation [4, 5, 6]. This is the method we followed in the present paper too. In the meantime the fractalness of the Ising configurations near the critical temperature [7, 8], or the fractal structure of domains in a random Ising magnet [9], suggest that fractal theory [10, 11] could be very adecvat to characterize instantaneous configurations of domain walls. This problem, in the more general context of the roughening of interfaces and their fractal character, was considered in several papers [12, 13, 14]. One can learn from these that the problem also presents interest in the study of the diffusion front for interacting particles, invasion and corrosion. Experiments [15] show that similar structures appear for two-phase liquid flow, where the interface of two immiscible fluids exhibit fractal structure dependent of the Reynolds number characteristic for the flow.

However computer simulations performed in [12, 13, 14] for the diffusion front of interacting particles or Ising models do not reveal the possibility of variation for the fractal structure in correlation with relevant physical parameters of the problem. So in this context we proposed to study the Bloch wall structure obtained by a computer model in function of temperature and characteristic interaction parameters. In this way the problem could present interest not only for magnetism but in a more general view completing the basic ideas of [12, 13, 14].

2. The Method

We constructed a heatbath dynamics model to simulate the dynamics of $S = 1/2$ spins on a square lattice, considering first-nearest neighbour and next -nearest neighbour interactions between the spins. We imposed periodic boundary conditions in the direction parallel to the wall, and mirror-symmetrical boundary conditions in the direction perpendicular to the wall. The size of the lattice were also varied in the interval 100-160 lattice sites for the direction perpendicular to the wall (vertical direction), and 300-600 lattice sites for the direction parallel to the wall (horizontal direction). At each step of the simulation we choose spins randomly , and apply the well-known heatbath dynamics [16]. In this dynamics the spin flip probability for the spin $S_{i,j}$ is given by:

$$W_{i,j} = \frac{exp(\beta E_{i,j})}{exp(-\beta E_{i,j}) + exp(\beta E_{i,j})}. \tag{1}$$

where $E_{i,j} = E^o_{i,j} + E^1_{i,j}$, is the sum of the interaction energies of the considered spin with his first-nearest neighbours , $E^o_{i,j}$, and next-nearest neighbours ,$E^1_{i,j}$.

$$E^o_{i,j} = -J_o \sum_k (S_{i,j}S_{i+k,j} + S_{i,j}S_{i,j+k}), \tag{2}$$

$$E^1_{i,j} = -J_1 \sum_k (S_{i,j}S_{i+k,j+k} + S_{i,j}S_{i+k,j-k}). \tag{3}$$

(Summations are for $k = +/-1$ only.) To verify our model first we studied some single-domain dynamics with first-nearest neighbour interactions. Starting the simulation from completly random or completly ordered configurations we compared our results with theoretical ones. So , we got for the critical temperature ,T_c, the value predicted by the theory [3] :

$$T_c = \frac{1}{2ln(1+\sqrt{2})}.\frac{J_o}{k} \approx 0.5673...\frac{J_o}{k} \tag{4}$$

Starting the simulation from a perfect strait-line 180^o Bloch wall (Fig.1a) we looked for the equilibrium shape of the domain boundaries. We define the instantaneous domain boundary (interface) as the curve separating the two inversly magnetized domains, and which is continuously connected by first-nearest neighbours with the same spin orientation. Every site of this curve must have at least one first-nearest neighbour with inverse spin orientation, and the curve must realize a percolation in horizontal direction. This interface was detected by a special program after the equilibrium configurations were reached. Characteristic result is presented in Fig.2 .

The thickness of the interface ,λ , is considered as the number of rows in which the average magnetization performs the transition between the two $+m$ and $-m$ equilibrium values for the two domains. (This is λ in Fig. 3).

Due to the complexity of these boundaries we used also the fractal theory for their description. The fractal structure was studied by calculating the fractal dimension ,D, with the simple box-counting method [10]. Working on lattices with the mentioned sizes, we could apply our box-counting method on the length-scale of 1-100 lattice constants. This interval is large enough for evidencing fractal structures.

We considered the equilibrium configuration reached when the fractal dimension and the wall-thickness of the interface had no monotonic variations, only statistical fluctuations in time. This happend, depending on the considered temperature between 700-10 000 iterations/spin. The obtained interfaces, after this equilibrium was reached had complicate shapes and large fluctuations in time, but in statistical sense were stable (Fig. 1 f,g).

3. Results

Characteristic time evolution of the structure is presented in Fig. 1. Once the statistical equilibrium configuration reached we studied the structure of the interface. The equilibrium shape of our domain walls had important structural variations with temperature. This is illustrated in Fig. 4. for a model with only first-nearest neighbour interactions. As we mentioned earlier we studied two main aspects of the structure : the fractal properties by the fractal dimension and the wall thickness.

a. Fractal dimension of the interface

Considering only first-nearest neighbour interactions with $T_c = 1000K$ we studied the variation of the fractal dimension ,D, with the temperature. The results are plotted in Fig.5 . Including now next-nearest neighbour interactions too, with $T_o = 560K$ and $T_1 = 110K$ ($T_o = 0.5673\frac{J_o}{k}$, $T_1 = 0.5673\frac{J_1}{k}$, $T_c = 720K$), we got the results presented in Fig. 6 . As mentioned earlier the fractal dimension was calculated on the interval of 1-100 lattice constants. Characteristic result for the fit is shown in Fig. 7. In general for all the studied boundaries the fit quality was good, indicating nice fractal structures on the whole interval of 1-100 lattice constants. The fit was made using at least 80 points, and the worst value for the percent of residuals about mean explained for fitting the log-log plot with a line in the box-counting method was 98% !

Our results from Fig.5 and Fig. 6 suggest that at temperatures small enough comparative to the critical one, the instantaneous configuration of the considered Bloch walls can be well described by a normal one-dimensional curve. For temperatures between a value ,T_f, and T_c the fractal dimension is, in a good approximation, a linear function of the temperature. This T_f , characteristic temperature depends on the chosen interaction parameters. So, the results qualitatively are not affected by the interaction parameters, the only difference that appear is the shifting of the characteristic temperature , T_f. Extrapolating our results for the limit $T = T_c$, the interface tend to a structure with the $D = 1.25$ fractal dimension for both of the considered models.

Identical results were found in [15] ,by studying the dynamical behaviour of the interphase between two immiscible fluids flowing in a tube. A clear increase of the fractal dimension of the interface as a function of total fluid velocity was found, and the fractal dimension had the same kind of variation with the fluid velocity as those obtained in Fig.5 and Fig.6 .

b. Wall thickness

For the equilibrium configurations the wall thickness exhibits the variations plotted in Fig. 8. Considering temperatures close to the critical one, we found that the variation could be well-described by the classical theory , which predict:

$$\lambda \sim \sqrt{\frac{J}{K}}, \tag{5}$$

(here J is the exchange constant and K the anisotropy constant) see for example [17]. The only source of the anisotropy in our lattice is due to the preferenced spin orientation. In this sens, one can consider for our model the anisotropy constant proportional with the average magnetization of the domains.

For our system the magnetization ,M ,scales like:

$$M \sim \sqrt{1 - \frac{T}{T_c}}, \tag{6}$$

in the vicnity of the critical temperature ($T < T_c$). This fact is in accordance with the theory [3] which predict this scaling law for every row with finite distance from the boundary.

So ,by applying equation (5) the theory predict:

$$\lambda \sim (1 - \frac{T}{T_c})^{-\frac{1}{4}}. \tag{7}$$

In Fig. 7 we plotted the variation of λ in function of $(1 - \frac{T}{T_c})$. By fitting these with a power-law function we found for the scaling exponent the value -0.256 for simulations with first-nearest neighbour interactions only, and -0.268 for the case when we included next-nearest neighbour interactions too.

With the assumption made, that for our model one should consider the anisotropy constant proportional with the average magnetization, we got that our results are in good agreement with the classical theory for the Bloch wall thickness.

4.Conclusions

We obtained in our two-dimensional model, that the instantaneous configurations of the 180^o Bloch walls for $S = 1/2$ spins exhibit fractal structure in the $T_f < T < T_c$ temperature interval. In this region the fractal dimension is a linear function of the temperature. The fractal dimension is in a strong correlation with relevant physical quantities of the considered problem, it is very adecvat for characterizing the considered domain walls, and for detecting the equilibrium configuration in computer simulations. The wall thickness presents a power-law scaling in the neighbourhood of T_c ($T < T_c$) in accordance with classical theories. The observed connection with geometrical aspects of two-phase liquid flow is interesting, and suggests, universalities in the geometry of two-phase boundaries. This problem, of the universality or not, could be interesting and suggests further studies.

Acknowledgements

This work was done during a scholarship offered by the Physics Department of the University of Bergen. So, we are grateful to the staff of the Theoretical- and Reservoire- Physics groups, and especially for the generous help from L. Csernai. Discussions with J. P. Hansen are gratefully acknowledged. During our visit at the Energy Technology Institute in Oslo we had interesting discussions with the team of A. Skjeltorp. We also thank to Y. Brechet of ENSEEG-LTPCM Grenoble, M. Coldea of the Babes-Bolyai University of Cluj, and to J. Kertesz of BME-Budapest for their continuous help they given to us in elaborating this paper.

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Figure Captions

Fig.1. Time evolution of a domain wall after 0, 1, 8, 50, 100, 1000 and 10000 simulation steps per pixel (A, B, C,...G respetively).

Fig.2. Detection of the domain wall.

Fig.3. Typical variation for average spin per row , $< S >$, through the wall. λ is the wall thickness.

Fig.4. Equilibrium shapes for the instantaneous configuration of the domain wall at different temperatures (the temperatures are in K). The critical temperature is $T_c = 1000K$.

Fig.5. Variation of the fractal dimension of the domain wall with temperature for simulations considering first-nearest neighbour interactions only and $T_c = 1000K$ (the temperatures are in K).

Fig.6. Variation of the fractal dimension of the domain wall with temperature for simulations considering first- and next-nearest neighbour interactions. $T_o = 560K$, $T_1 = 110K$, $T_c = 720K$ ($T_o = 0.5673\frac{J_o}{k}$, $T_1 = 0.5673\frac{J_1}{k}$).

Fig.7. Characteristic result for the fit applying the box-counting method. Here L is the linear size of the box (the units for L are lattice constants) and $N(L)$ represents the number of boxes necessary to cover our structure with boxes of size L. The slope of the best-fit line is the fractal dimension of the considered interface.

Fig.8. Variation of the wall thicness, λ, (the units are in lattice constants) in function of $T - T_c$ (T the temperature, and T_c the critical temperature). The "first model" are results for considering first-nearest neighbour interactions only, the "second model" are results considering next-nearest neighbour interactions too. In the neighbourhood of T_c the datas were fit by : $\lambda = 103 \cdot (T - T_c)^{-0.256}$ for the first model and $\lambda = 126 \cdot (T - T_c)^{-0.268}$ for the second one.