HAL
open science

First-Order Transition in XY Fully Frustrated Simple Cubic Lattice

V. Thanh Ngo, D. Tien Hoang, Hung The Diep

To cite this version:

V. Thanh Ngo, D. Tien Hoang, Hung The Diep. First-Order Transition in XY Fully Frustrated Simple Cubic Lattice. 2010. hal-00480790v2

HAL Id: hal-00480790

https://hal.science/hal-00480790v2

Preprint submitted on 29 Dec 2010

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

First-Order Transition in XY Fully Frustrated Simple Cubic Lattice

V. Thanh Ngo[a,b], D. Tien Hoang[a] and H. T. Diep*

Laboratoire de Physique Théorique et Modélisation,

Université de Cergy-Pontoise, CNRS UMR 8089

2, Avenue Adolphe Chauvin, 95302 Cergy-Pontoise Cedex, France

[a] *Institute of Physics, P.O. Box 429, Bo Ho, Hanoi 10000, Vietnam*

[b] *Division of Fusion and Convergence of Mathematical Sciences,*

National Institute for Mathematical Sciences, Daejeon, Republic of Korea

We study the nature of the phase transition in the fully frustrated simple cubic lattice with the XY spin model. This system is the Villain's model generalized in three dimensions. The ground state is very particular with a 12-fold degeneracy. Previous studies have shown unusual critical properties. With the powerful Wang-Landau flat-histogram Monte Carlo method, we carry out in this work intensive simulations with very large lattice sizes. We show that the phase transition is clearly of first order, putting an end to the uncertainty which has lasted for more than twenty years.

PACS numbers: 75.10.-b General theory and models of magnetic ordering ; 75.40.Mg Numerical simulation studies

I. INTRODUCTION

One of the most fascinating tasks of statistical physics is the study of the phase transition in systems of interacting particles. Much progress has been made in this field since 50 years. Finite-size theory, renormalization group analysis, numerical simulations, ... have contributed to the advance of the knowledge on the phase transition. Exact methods have been devised to solve with mathematical elegance many problems in two dimensions. But as improvements are progressing, new and more complicated challenges also come in from new

* Corresponding author, E-mail:diep@u-cergy.fr

discoveries of materials and new applications. Renormalization group which has predicted with success critical behaviors of ferromagnets has many difficulties to deal with frustrated systems. Numerical simulations which did not need huge memory and long calculations for simple systems require now new devices, new algorithms to improve convergence in systems with extremely long relaxation time, or in systems whose microscopic states are difficult to access. One class of these systems is called 'frustrated systems' introduced in the seventies in the context of spin glasses. These frustrated systems are very unstable due to the competition between different kinds of interaction. However they are periodically defined (no disorder) and therefore subject to exact treatments. This is the case of several models in two dimensions[1], but in three dimensions frustrated systems are far from being understood even on basic properties such as the order of the phase transition (first or second order, critical exponents, ...). Let us recall the definition of a frustrated system. When a spin cannot fully satisfy energetically all the interactions with its neighbors, it is "frustrated". This occurs when the interactions are in competition with each other or when the lattice geometry does not allow to satisfy all interaction bonds simultaneously. A well-known example is the stacked triangular antiferromagnet with interaction between nearest-neighbors.

The frustration in spin systems causes many unusual properties such as large ground state (GS) degeneracy, successive phase transitions with complicated nature, partially disordered phase, reentrance and disorder lines. Frustrated systems still constitute at present a challenge for investigation methods. For recent reviews, the reader is referred to Ref. 2.

In this work, we are interested in the nature of the phase transition of the classical XY spin model in the fully frustrated simple cubic lattice (FFSCL) shown in Fig. 1. Although phase transition in strongly frustrated systems has been a subject of intensive investigations in the last 20 years, many aspects are still not understood at present. One of the most studied systems is the stacked triangular antiferromagnet (STA) with Ising[3], XY and Heisenberg spins[4,5]. The cases of XY ($N = 2$) and Heisenberg ($N = 3$) STA have been intensively studied since 1987[6–13] , but only recently that the 20-year controversy comes to an end.[14–23] For details, see for example the review by Delamotte et al[4].

The paper is organized as follows. Section II is devoted to the description of the model and the technical details of the Wang-Landau (WL) methods as applied in the present paper. Section III shows our results. Concluding remarks are given in section IV.

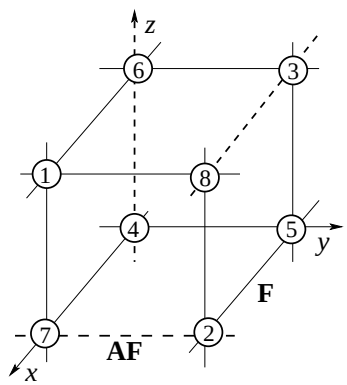

FIG. 1: Fully frustrated simple cubic lattice. Discontinued (continued) lines denote antiferromagnetic (ferromagnetic) bonds.

II. MODEL AND WANG-LANDAU ALGORITHM

We consider the FFSCL shown in Fig. 1. The spins are the classical XY model of magnitude $S = 1$. The Hamiltonian is given by

$$\mathcal{H} = -\sum_{(i,j)} J_{ij}\mathbf{S}_i.\mathbf{S}_j, \tag{1}$$

where $\mathbf{S}_i$ is the XY spin at the lattice site i, $\sum_{(i,j)}$ is made over the NN spin pairs $\mathbf{S}_i$ and $\mathbf{S}_j$ with interaction J_{ij}. Hereafter we suppose that $J_{ij} = -J$ ($J > 0$) for antiferromagnetic (AF) bonds indicated by discontinued lines in Fig. 1, and $J_{ij} = J$ for ferromagnetic (F) bonds. This model is a generalization in three dimensions (3D) of the 2D Villain's model[24] which has been extensively studied[25–27]: every face of the cube is frustrated because we know that a plaquette is frustrated when there is an odd number of AF bonds on its contour[2,24]. To describe the model, let us look first at the xy plane (Fig. 1). There, all interactions are F, except one AF line out of every two in the y direction. The same is for the yz (zx) plane: one AF line of every two in the z (x) direction. Note that there is no intersection between AF lines. Each plane is thus a 2D Villain's model.

Let us recall some results on the present model. For the classical XY model on the FFSCL, the GS is 12-fold degeneracy with non collinear spin configurations[28]. For convenience, let us define the local field acting on the spin $\mathbf{S}_i$ from its neighbors as $\mathbf{h}_i = \sum_j J_{ij}\mathbf{S}_j$. The GS can be calculated by noticing that the local field is the same at every site and is equal to $|\mathbf{h}| = 2\sqrt{3}$ so that[28]

$$\mathbf{h}_5 \;=\; 2(\mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4) \tag{2}$$

$$\mathbf{h}_6 = 2(\mathbf{S}_1 + \mathbf{S}_3 - \mathbf{S}_4) \tag{3}$$

$$\mathbf{h}_7 = 2(\mathbf{S}_1 - \mathbf{S}_2 + \mathbf{S}_4) \tag{4}$$

$$\mathbf{h}_8 = 2(\mathbf{S}_1 + \mathbf{S}_2 - \mathbf{S}_3) \tag{5}$$

where the factor 2 results from the symmetric neighbors lying outside the cube and $J_{ij} = \pm 1$ depending on the bond has been used. Putting into square these equalities and using $\mathbf{h}^2 = 12$, $\mathbf{S}_i^2 = 1 (i = 1, ..., 8)$, one has three independent relations which determine the relative orientation of every spin pair

$$\mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_4 + \mathbf{S}_2 \cdot \mathbf{S}_4 = 0 \tag{6}$$

$$-\mathbf{S}_1 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_4 + \mathbf{S}_1 \cdot \mathbf{S}_4 = 0 \tag{7}$$

$$\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_4 - \mathbf{S}_1 \cdot \mathbf{S}_4 = 0 \tag{8}$$

There are 12 solutions of these equations which can be described as follows[28,29]. Consider just one of them shown in the upper figure of Fig. 2: On a yz face, the spins (displayed by continued vectors) on a diagonal are perpendicular, i.e. $\mathbf{S}_1 \perp \mathbf{S}_2$, $\mathbf{S}_7 \perp \mathbf{S}_8$. In addition, the orthogonal dihedron $(\mathbf{S}_1, \mathbf{S}_2)$ makes an angle $\alpha = \arccos(\frac{1+\sqrt{2}}{\sqrt{6}})$ with the dihedron $(\mathbf{S}_7, \mathbf{S}_8)$. On the other yz face the spins (displayed by discontinued vectors in Fig. 2) are arranged in the same manner: $\mathbf{S}_5 \perp \mathbf{S}_6$, $\mathbf{S}_4 \perp \mathbf{S}_3$ and the dihedron $(\mathbf{S}_4, \mathbf{S}_3)$ makes an angle α with the dihedron $(\mathbf{S}_5, \mathbf{S}_6)$. Note that the dihedron $(\mathbf{S}_5, \mathbf{S}_6)$ makes a turn angle $\beta = \pi/4$ with respect to the dihedron $(\mathbf{S}_7, \mathbf{S}_8)$, and that the sum of the algebraic angles between spins on each face of the cube is zero.

There is another choice shown in the lower figure of Fig. 2 where every thing is the same as described above except $\beta = -3\pi/4$. One has therefore two configurations with the choice of the yz faces. If one applies the same rule for the spins on the xy faces and the xz faces, one obtains in all 6 configurations. Finally, together with their 6 mirror images, the total degeneracy is 12.[29]

The above description of the GS shows an unusual degeneracy which can help to understand the first-order transition shown below by relating this system to a Potts model where the GS degeneracy plays a determinant role in the nature of phase transition. Note however that all simulations have been carried out with the initial Hamiltonian (1), no GS rigidity at finite temperature (T) has been imposed.

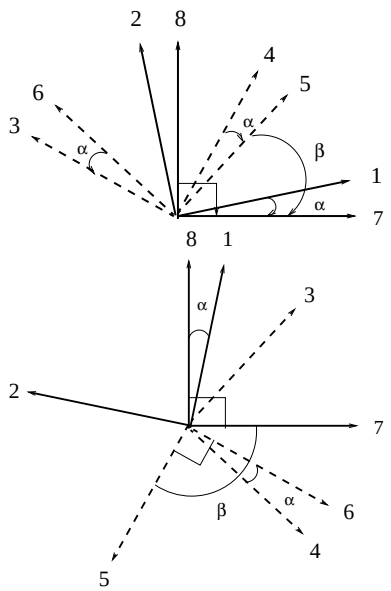

FIG. 2: Two of the 12 ground-state configurations of the fully frustrated simple cubic lattice. The numbers indicate the spins at the sites defined in Fig. 1. The angle α is $\alpha = \arccos(\frac{1+\sqrt{2}}{\sqrt{6}})$. Upper: $\beta = \pi/4$, lower: $\beta = -3\pi/4$.

The first investigation of the nature of the phase transition of this model by the use of Metropolis Monte Carlo (MC) simulations has shown a second order transition with unusual critical exponents[29]. However, MC technique and computer capacity at that time did not allow to conclude the matter with certainty. Recently, Wang and Landau[30] proposed a MC algorithm for classical statistical models which allowed to study systems with difficultly accessed microscopic states. In particular, it permits to detect with efficiency weak first-order transitions[22,23] The algorithm uses a random walk in energy space in order to obtain an accurate estimate for the density of states $g(E)$ which is defined as the number of spin configurations for any given E. This method is based on the fact that a flat energy histogram $H(E)$ is produced if the probability for the transition to a state of energy E is proportional to $g(E)^{-1}$.

We summarize how this algorithm is implied here. At the beginning of the simulation, the density of states (DOS) is set equal to one for all possible energies, $g(E) = 1$. We begin a random walk in energy space (E) by choosing a site randomly and flipping its spin with a probability proportional to the inverse of the temporary density of states. In general, if E and E' are the energies before and after a spin is flipped, the transition probability from E

to E' is

$$p(E \to E') = \min\left[g(E)/g(E'), 1\right]. \tag{9}$$

Each time an energy level E is visited, the DOS is modified by a modification factor $f > 0$ whether the spin flipped or not, i.e. $g(E) \to g(E)f$. At the beginning of the random walk, the modification factor f can be as large as $e^1 \simeq 2.7182818$. A histogram $H(E)$ records the number of times a state of energy E is visited. Each time the energy histogram satisfies a certain "flatness" criterion, f is reduced according to $f \to \sqrt{f}$ and $H(E)$ is reset to zero for all energies. The reduction process of the modification factor f is repeated several times until a final value f_{final} which close enough to one. The histogram is considered as flat if

$$H(E) \geq x\%.\langle H(E)\rangle \tag{10}$$

for all energies, where $x\%$ is chosen between 70% and 95% and $\langle H(E)\rangle$ is the average histogram.

The thermodynamic quantities[30,31] can be evaluated by $\langle E^n\rangle = \frac{1}{Z}\sum_E E^n g(E)\exp(-E/k_BT)$, $C_v = \frac{\langle E^2\rangle - \langle E\rangle^2}{k_BT^2}$, $\langle M^n\rangle = \frac{1}{Z}\sum_E M^n g(E)\exp(-E/k_BT)$, and $\chi = \frac{\langle M^2\rangle - \langle M\rangle^2}{k_BT}$, where Z is the partition function defined by $Z = \sum_E g(E)\exp(-E/k_BT)$. The canonical distribution at any temperature can be calculated simply by $P(E,T) = \frac{1}{Z}g(E)\exp(-E/k_BT)$.

In this work, we consider a energy range of interest[32,33] $(E_{\text{min}}, E_{\text{max}})$. We divide this energy range to R subintervals, the minimum energy of each subinterval is E^i_{min} for $i = 1, 2, ..., R$, and maximum of the subinterval i is $E^i_{\text{max}} = E^{i+1}_{\text{min}} + 2\Delta E$, where ΔE can be chosen large enough for a smooth boundary between two subintervals. The WL algorithm is used to calculate the relative DOS of each subinterval $(E^i_{\text{min}}, E^i_{\text{max}})$ with the modification factor $f_{\text{final}} = \exp(10^{-9})$ and flatness criterion $x\% = 95\%$. We reject the suggested spin flip and do not update $g(E)$ and the energy histogram $H(E)$ of the current energy level E if the spin-flip trial would result in an energy outside the energy segment. The DOS of the whole range is obtained by joining the DOS of each subinterval $(E^i_{\text{min}} + \Delta E, E^i_{\text{max}} - \Delta E)$.

III. RESULTS

We used the system size of $N \times N \times N$ where N varies from 24 up to 48. We stop at $N = 48$ because, as seen below, the transition at this size shows a definite answer to the

problem studied here. Periodic boundary conditions are used in the three directions. $J = 1$ is taken as the unit of energy in the following.

We show in Fig. 3 the magnetization and the susceptibility and in Fig. 4 the energy per spin and the specific heat, for $N = 24$. All these quantities show a transition with an second-order aspect. However, we know that many systems show a first-order transition only at very large sizes. This is indeed the case. The energy histograms obtained by WL technique for three representative sizes $N = 24$, 36 and 48 are shown in Fig. 5. As seen, for $N = 24$, the energy histogram, though unusually broad, shows a single peak indicating a continuous energy at the transition as observed before in Fig. 4. The double-peak histogram starts already at $N = 36$ and the dip between the two maxima becomes deeper with increasing size, as observed at $N = 48$. We note that the distance between the two peaks, i. e. the latent heat, increases with increasing size and reaches $\simeq 0.03$ for $N = 48$. This is rather large compared with the value $\simeq 0.009$ for $N = 120$ in the XY STA[17–19,22] and with 0.0025 for $N = 150$ in the Heisenberg case[23]. We give here the values of T_c for a few sizes: $T_c = 0.68080 \pm 0.00010$, 0.67967 ± 0.00010 and 0.67919 ± 0.00010 for $N = 24$, 36 and 48, respectively.

Note that the double-peak structure is a sufficient condition, not a necessary condition in old-fashion MC simulations (i. e. not WL method), for a first-order transition. This is because in old-fashion MC simulations performed at a given T, we often encounter the situation where, at the transition, the system is spatially composed of two (or more) parts: the ordered phase with energy E_1 and the disordered phase with energy E_2. Since in old-fashion MC simulations, we make histogram from the total system energy, i. e. $E_1 + E_2$, the histogram will record the 'average' energy $E_1 + E_2$, therefore the double peak structure will not be seen. Such a coexistence at any time of the ordered and disordered phases in some first-order transitions makes it impossible in old-fashion MC simulations to detect two peaks. In our present WL flat-histogram method, the double-peak structure is obtained from the DOS histogram which gets rid of the problem of spatial coexistence of the two phases discussed above. Therefore, the double-peak structure is a necessary condition for a first-order transition as it should be.

Let us say a few words on the correlation length. It is known that the correlation length is finite at the transition point in a first-order transition. For very strong first-order transitions, this correlation length is short so that the first-order character is detected in simulations

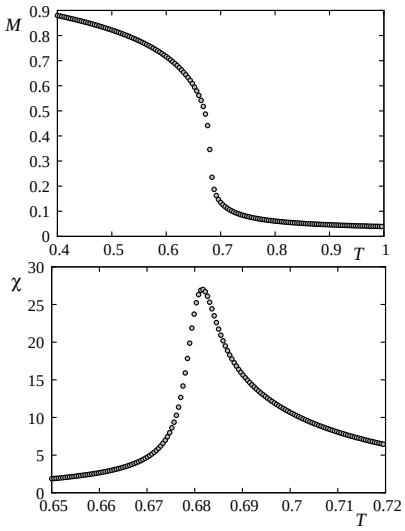

FIG. 3: Magnetization and susceptibility versus T for N =24.

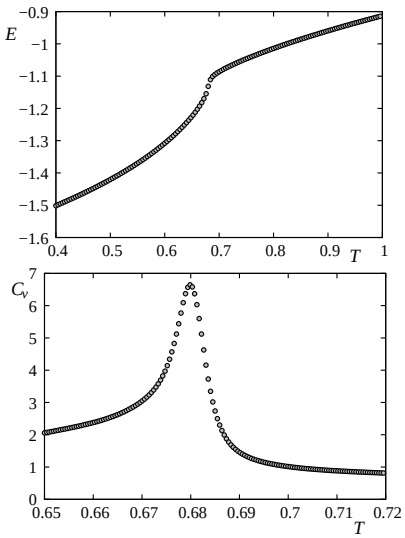

FIG. 4: Energy per spin and specific heat versus T for N =24.

already at small lattice sizes. For weak first-order transitions, the correlation length is very long. To detect it one should study very large lattice sizes as in the present paper. Direct calculation of the correlation length is not numerically easy. Fortunately, one has other means such as the WL method to detect more easily weak first-order transitions.

To close this section, let us emphasize two points: i) First, the first-order transition observed here may come from the fact that the GS of the present XY FFSCL model has a 12-fold degeneracy which is reminiscent of the 12-state Potts model. In three dimensions, the latter model has a first order transition. Note however that this conclusion is not

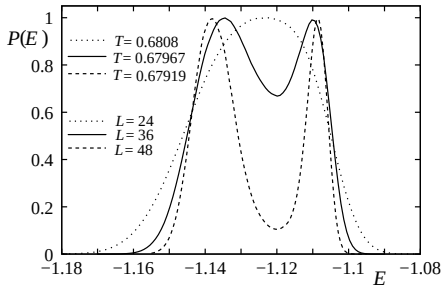

FIG. 5: Energy histogram for several sizes $N = 24$, 36, 48 at T_c indicated on the figure.

always obvious because the continuous degrees of the order parameter mask in many cases the symmetry argument based on discrete models[27], ii) Second, some other XY frustrated systems such as the FCC[34], HCP[35] and helimagnetic[36] antiferromagnets show also a first-order transition in MC simulations. Though the nonperturbative renormalization group has been extensively used for the STA case[4] due to its long-lasting controversy, we believe that the other cases are worth to study in order to verify that the validity of that theory is not limited to the STA but is universal for frustrated systems of vector spins.

IV. CONCLUDING REMARKS

Using the powerful WL flat histogram technique, we have studied the phase transition in the XY fully frustrated simple cubic lattice. The technique is very efficient because it helps to overcome extremely long transition time between energy valleys in systems with a first-order phase transition. We found that the transition is clearly of first-order at large lattice sizes in contradiction of early studies using standard MC algorithm and much smaller sizes[29]. The result presented here will serve as a testing ground for theoretical methods such as the renormalization group which still has much difficulty to deal with frustrated systems[4].

One of us (VTN) would like to thank the University of Cergy-Pontoise for a financial support during the course of this work. He is grateful to Nafosted of Vietnam National Foundation for Science and Technology Development, for support (Grant No. 103.02.57.09). He also thanks the NIMS (National Institute for Mathematical Sciences, Korea) for hospi-

tality and financial support.

---

[1] H. T. Diep and H. Giacomini, in *Frustrated Spin Systems*, Ed. H. T. Diep, World Scientific (2005).

[2] See reviews on theories and experiments given in *Frustrated Spin Systems*, Ed. H. T. Diep, World Scientific (2005).

[3] M. L. Plumer, A. Mailhot, R. Ducharme , A. Caillé and H.T. Diep Phys. Rev. B **47**, 14312 (1993).

[4] See references cited by B. Delamotte, D. Mouhanna, and M. Tissier, Phys. Rev. B **69**, 134413 (2004); ibid in Ref. 2.

[5] See review by D. Loison in Ref. 2.

[6] Hikaru Kawamura, J. Phys. Soc. Jpn. **56**, 474 (1987).

[7] Hikaru Kawamura, Phys. Rev. B **38**, 4916 (1988).

[8] P. Azaria, B. Delamotte and T. Jolicoeur, Phys. Rev. Lett. **64**, 3175 (1990).

[9] D. Loison and H. T. Diep, Phys. Rev. B **50**, 16453 (1994); T. Bhattacharya, A. Billoire, R. Lacaze and Th. Jolicoeur, J. Physique I (France) **4**, 122 (1994).

[10] E. H. Boubcheur, D. Loison and H. T. Diep, Phys. Rev. B **54**, 4165 (1996).

[11] A. Dobry and H. T. Diep, Phys. Rev. B **51**, 6731 (1995); D. Loison and H. T. Diep, J. Appl. Phys. **76**, 6350 (1994).

[12] S. A. Antonenko, A. I. Sokolov and V. B. Varnashev, Phys. Lett. A **208**, 161 (1995).

[13] D. Loison, A.I. Sokolov, B. Delamotte, S.A. Antonenko, K.D. Schotte and H.T. Diep, Pis'ma v ZhETF **72**, No 6, 487 (2000), JEPT Lett. **72**, 337 (2000).

[14] M. Tissier, D. Mouhanna and B. Delamotte, Phys. Rev. B **61**, 15327 (2000).

[15] M. Tissier, B. Delamotte and D. Mouhanna, Phys. Rev. Lett. **84**, 5208 (2000).

[16] M. Tissier, B. Delamotte and D. Mouhanna, Phys. Rev. B **67**, 134422 (2003).

[17] M. Itakura, J. Phys. Soc. Jap. **72**, 74 (2003).

[18] A. Peles, B. W. Southern, B. Delamotte, D. Mouhanna, and M. Tissier, Phys. Rev. B **69**, 220408(R) (2004).

[19] Kazuki Kanki, Damien Loison and Klaus-Dieter Schotte, J. Phys. Soc. Jpn. **75**, 015001 (2006).

[20] S. Bekhechi, B. W. Southern, A. Peles and D. Mouhanna, Phys. Rev. E **74**, 016109 (2006).

[21] M. Zelli, K. Boese and B. W. Southern, Phys. Rev. B **76**, 224407 (2007).

[22] V. Thanh Ngo and H. T. Diep, J. Appl. Phys. **103**, 07C712 (2008).

[23] V. Thanh Ngo and H. T. Diep, Phys. Rev. E **78**, 031119 (2008).

[24] J. Villain, J. Phys. C **10**, 1717 (1977).

[25] B. Berge, H. T. Diep, A. Ghazali and P. Lallemand, Phys. Rev. B **34**, 3177 (1986).

[26] J. Lee, J. M. Kosterlitz and E. Granato, Phys. Rev. B **43**, 11531 (1991).

[27] E. H. Boubcheur and H. T. Diep, Phys. Rev. B **58**, 5163 (1998) and references therein.

[28] P. Lallemand, H.T. Diep, A. Ghazali and G. Toulouse, J. Physique-Lettres **46**, 1087 (1985).

[29] H.T. Diep, A. Ghazali and P. Lallemand, J. Phys. C **18**, 5881 (1985).

[30] F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001); Phys. Rev. E **64**, 056101 (2001).

[31] G. Brown and T.C. Schulhess, J. Appl. Phys. **97**, 10E303 (2005).

[32] B. J. Schulz, K. Binder, M. Müller, and D. P. Landau, Phys. Rev. E **67**, 067102 (2003).

[33] A. Malakis, S. S. Martinos, I. A. Hadjiagapiou, N. G. Fytas, and P. Kalozoumis, Phys. Rev. E **72**, 066120 (2005).

[34] H. T. Diep and H. Kawamura, Phys. Rev. B **40**, 7019 (1989).

[35] H. T. Diep, Phys. Rev. B **45**, 2863 (1992).

[36] H. T. Diep, Phys. Rev. B **39**, 397 (1989).