Potts Model with Long-Range Interactions in One Dimension

E. Bayong, H. T. Diep,* and Viktor Dotsenko[†]

Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise,
2, Avenue Adolphe Chauvin, 95302 Cergy-Pontoise Cedex, France

(Received 9 February 1999)

We study the nature of the phase transition of the q-state Potts model with long-range ferromagnetic interactions decaying as $1/r^{d+\sigma}$, in dimension $d = 1$, using a histogram Monte Carlo (MC) technique. The model can exhibit a first-order transition or a second-order phase transition with nonstandard critical exponents. The critical value of q above which a first-order transition occurs decreases with decreasing σ, from $q_c = 8$ for $\sigma = 1$ to $q_c = 2$ for $\sigma = 0.3$. Detailed results for various σ will be shown and discussed. Mean-field calculation confirms the tendency of our MC results.

PACS numbers: 05.50.+q, 64.60.Cn, 75.10.–b

The q-state Potts model limited to nearest-neighbor (NN) interactions has been extensively investigated [1]. In particular, the nature of the phase transition is exactly known in low dimensions [1]. For example, in one dimension (1D) there is no phase transition at finite temperature (T) for any q, while in $d = 2$ the transition is of second order for $q \leq 4$ and of first order for $q \geq 5$. However, much less is known when long-range (LR) interactions are included. For instance, when next-nearest-neighbor interactions compete with the NN one, the system becomes frustrated. Though much interesting physics is recently discovered for such systems [2], well-established theoretical methods often fail to predict correct behaviors.

In this paper, we are interested in the effect of LR interactions decaying with distance r as $1/r^{d+\sigma}$, in a 1D system. In the 1D Ising case ($q = 2$) with these LR interactions some studies have been done. It is known that it exhibits LR order at finite T if $\sigma \leq 1$ and no phase transition if $\sigma > 1$ [3–10]. Fisher *et al.* have studied a general system with n-component order parameter [11] using a renormalization group (RG) method. The exponents were shown to depend on the values of n, σ, and d. However, for $\sigma > 2$, they should take the short-range (SR) exponents for all d. A RG expansion in $1 - \sigma > 0$ has been done by Kosterlitz [12] who obtained $1/\nu = [2(1 - \sigma)^{1/2}]$ when $\sigma \to 1$ in 1D. We have recently calculated the critical exponents of the continuous Ising model (i.e., spin value varies continuously between -1 and 1) by Monte Carlo (MC) simulation [13,14]. Though the general aspects of our results are in agreement with the tendency predicted by RG calculations for the discrete Ising model, the details are somewhat different. For instance, in $d = 1$, for the case where $\sigma = 1$, our result shows a large value of ν but far from the divergent value predicted for the Ising model [12]. In $d = 2$, our exponents indicate that they take the SR values only when $\sigma \geq 3$, instead of $\sigma > 2$ given by the RG calculations for the Ising case [11]. Moreover, in the classical regime our results do not verify RG results. In view of this, it would be interesting to perform MC simulations for other models with LR interactions to compare with previous theories.

While the Ising case has been widely investigated, just a few works have been done in non-Ising models among which one can mention our work on the continuous Ising model [13,14], a paper by Glumac and Uzelac [15] investigating the 1D q-state Potts model up to $q = 64$ using a transfer matrix method, and the works by Priest and Lubensky [16] and by Theumann and Gusmao [17] using a RG expansion in $\epsilon = 3\sigma - d$ to calculate critical exponents of the Potts model.

In the LR case, except the early work for $d = 1$ with very small sizes [4], and our previous work [13,14], MC techniques have not been used. This is partially due to the long computing time. The absence of reliable MC results, in particular, in the non-Ising case has motivated the present work.

We investigate here the phase transition in the 1D q-state Potts model using standard MC simulations and the MC histogram method for various σ. One of our striking results is the existence of a phase transition which becomes of first order for $q > q_c$ where q_c depends on σ. The critical exponents when $q < q_c$ are displayed. A mean-field (MF) calculation is shown to confirm our MC tendency.

The q-state Potts model is defined by

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} \delta_{m_i, m_j} , \tag{1}$$

where m_i is a q-state Potts spin at site i, i.e., $m_i = 1, 2, \ldots, q$, and $J_{ij} = 1/|i - j|^{d+\sigma}$. All interactions permitted by the periodic boundary conditions are taken into account, i.e., $|i - j| \leq L/2$ where L is the system size.

We use first the standard MC simulations to localize for each size the transition temperature $T_0(L)$: the equilibrating time is from 100 000 to 200 000 MC steps per spin (MCS/spin) and the averaging time is from 500 000 to 1 000 000 MCS/spin. Next, for histogram measurements at $T_0(L)$, we discard 1×10^6 MCS/spin and measure between 3 and 5×10^6 MCS/spin. The histogram [18] $H(E)$ are then used to calculate canonical probabilities at temperatures T around $T_0(L)$ by $P(E,T) = H(E) \exp[-\Delta\beta E]/\sum_E H(E) \exp[-\Delta\beta E]$

 0031-9007/99/83(1)/14(4)$15.00

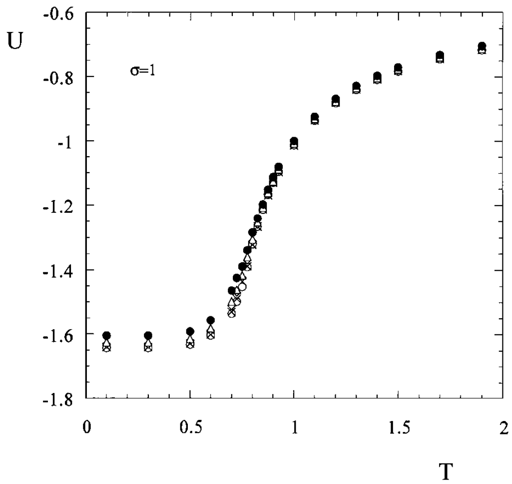

FIG. 1. U vs T for $\sigma = 1$ with $q = 3$. Void circles, filled triangles, void triangles, filled circles, and crosses are for $L = 50$, 100, 150, 400, and 900, respectively.

where $\Delta\beta = 1/k_B T_0(L) - 1/k_B T$. The thermal average of a physical quantity A is then calculated as a continuous function of T by $\langle A \rangle = \sum_E AP(E,T)$.

We have calculated the averaged order parameter $\langle M \rangle$, averaged total energy $\langle E \rangle$, specific heat C_v, susceptibility χ, first-order cumulant of the energy C_U, nth order cumulant of the order parameter V_n for $n = 1$ and 2, defined as follows: $\langle M \rangle = \langle (q\rho - 1)/(q - 1) \rangle$, ρ is defined as $\rho = L^{-d} \max(M_1, M_2, \ldots, M_q)$, M_i being the number of spins in the state i, $\langle E \rangle = \langle \mathcal{H} \rangle$, $C_v = \frac{1}{k_B T^2}(\langle E^2 \rangle - \langle E \rangle^2)$, $\chi = \frac{1}{k_B T}(\langle M^2 \rangle - \langle M \rangle^2)$, $C_U = 1 - (\frac{\langle E^4 \rangle}{3\langle E^2 \rangle^2})$, and $V_n = \langle (\frac{\partial \ln M^n}{\partial(1/k_B T)}) \rangle = (\frac{\langle M^n E \rangle}{\langle M^n \rangle}) - \langle E \rangle$.

Plotting these quantities versus T, we obtain their maximum or minimum, for a given L. A transition temperature can then be identified for each quantity. The transition temperatures for these quantities coincide only at infinite L. For large L, these quantities are expected to scale with L as follows: $V_1^{\min} \propto L^{1/\nu}$, $V_2^{\min} \propto L^{1/\nu}$, $C_v^{\max} = C_0 + C_1 L^{\alpha/\nu}$, and $\chi^{\max} \propto L^{\gamma/\nu}$ at their respective "transition" temperatures $T_c(L)$, $C_U = C_U[T_c(\infty)] + AL^{-\alpha/\nu}$, $M_{T_c(\infty)} \propto L^{-\beta/\nu}$, and $T_c(L) = T_c(\infty) + C_A L^{-1/\nu}$, where A, C_0, C_1, C_A are constants. We estimated ν independently from $V_1^{\min}$ and $V_2^{\min}$. With these values we calculated γ from $\chi^{\max}$. We estimated $T_c(\infty)$ by using the last expression for each observable. Using $T_c(\infty)$ we calculated β from $M_{T_c(\infty)}$. The Rushbrooke scaling law $\alpha + 2\beta + \gamma = 2$ gives α. Finally, using the hyperscaling relationship, we can estimate the effective dimension by $d_{\text{eff}} = (2 - \alpha)\nu^{-1}$ and η by $\gamma = (2 - \eta)\nu$.

The values of σ were chosen in the classical regime ($0 < \sigma < 0.5$) and in the nonclassical regime ($0.5 < \sigma \leq 1$) where exponents are expected to depend on σ, n, and d [11]. For a given set (σ, q), we performed MC simulations where the order parameter per site m, energy per site U, C_v, and χ were measured as functions of T for varying L. Whenever the transition is of second order,

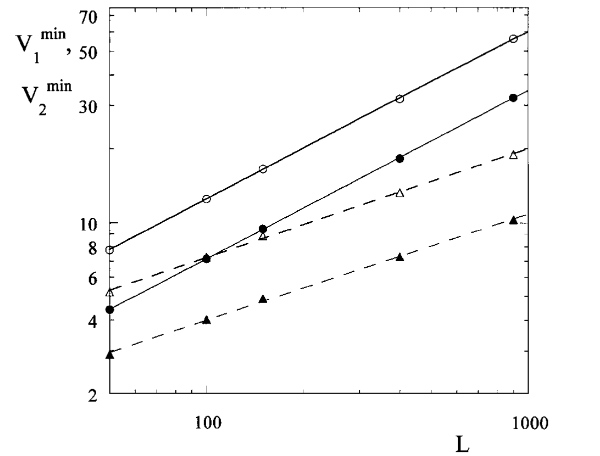

FIG. 2. $V_1^{\min}$ and $V_2^{\min}$ vs L in ln-ln scale for $\sigma = 0.7$, $q = 3$ (filled and void circles are for $V_1^{\min}$ and $V_2^{\min}$, respectively), and for $\sigma = 1$, $q = 3$ (filled and void triangles are for $V_1^{\min}$ and $V_2^{\min}$, respectively). Errors are smaller than the size of data points.

we calculate the exponents using the histogram technique. The first-order transition is signaled by a double-peak distribution of $H(E)$. We show now an example of each kind.

For $\sigma = 1$, the transition is of second order up to $q = 10$. Figure 1 shows U versus T with several L for $\sigma = 1$ and $q = 3$. Histogram measurements have been made and using the formulas given above we obtain the exponents. Figure 2 shows $V_1^{\min}$ and $V_2^{\min}$ versus L in the ln-ln scale. The data lie nicely on straight lines of equal slopes yielding $\nu = 2.272(5)$. The errors were estimated from the line-fitting procedure. Systematic errors from estimates of $T_0(L)$ were much smaller. Figure 3 shows $\chi^{\max}$ versus L in the ln-ln scale where the slope is γ/ν. One obtains $\gamma = 2.196(5)$. The scaling relations then give $\alpha = -0.272(5)$ and $\beta = 0.038(5)$. For $q > 8$, the transition is of first order. We show in Fig. 4

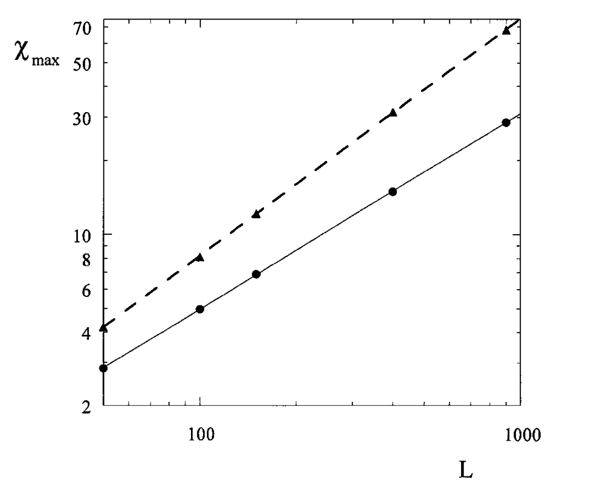

FIG. 3. $\chi_{\max}$ vs L in ln-ln scale for $\sigma = 1$, $q = 3$ (upper curve) and for $\sigma = 0.7$, $q = 3$ (lower curve). Errors are smaller than the size of data points.

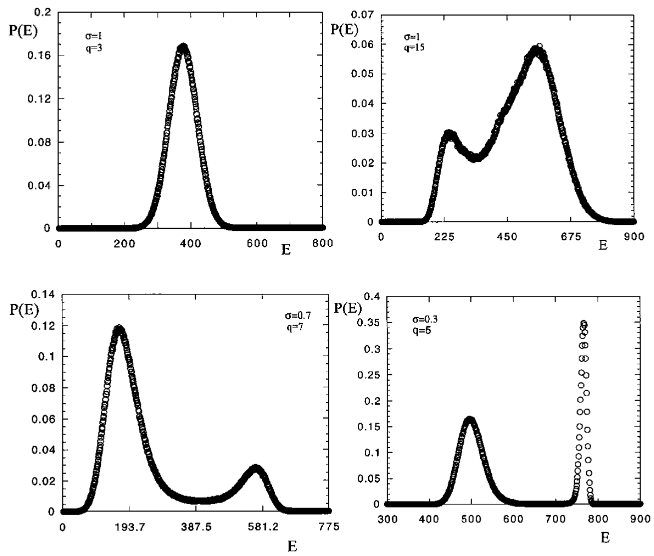

FIG. 4. Energy histograms for $\sigma = 1$, $q = 3$ (upper left); $\sigma = 1$, $q = 15$ (upper right); $\sigma = 0.7$, $q = 7$ (lower left); and $\sigma = 0.3$, $q = 5$ (lower right), at their transition temperatures. The single peak (upper left) shows a second-order transition while double peaks indicate first-order ones ($L = 900$).

the $P(E)$ taken at the transition temperature for various set $(\sigma, q = 15)$. The double-peak structure shows a first-order transition. Our conclusion is that the LR interactions are responsible not only for the existence of a phase transition in the Potts model in 1D but also the existence of a critical q above which the transition is of first order, similar to the SR case in higher d.

The results for several σ and q are displayed in Table I. Several remarks are in order as follows: (i) For a given σ, there exists a critical value q_c above which the transition is of first order. q_c decreases with decreasing σ going from $q_c = 8$ for $\sigma = 1$ to $q_c = 2$ for $\sigma = 0.3$. (ii) For a given σ, below q_c, the value of ν increases with increasing q. We find a large value of ν when $\sigma = 1$, a tendency predicted for the 1D Ising case [12]. (iii) When the transition is of second order, for a given q the value of ν also increases with increasing σ. (iv) Our results for $\sigma = 1$ indicate that the transition becomes first order for $q > 8$, in disagreement with the prediction of Thouless [3], according to which in the Ising case ($q = 2$) with $\sigma = 1$ the transition is either of first order or $\beta = 0$. (v) Our results for ν are far from those obtained by Glumac and Uzelac [15] for the standard Potts model: for $q = 64$ they obtained $\nu = 1$ for $\sigma = 1$ and for $q = 16$ they gave $\nu = 0.22$ for $\sigma = 0.7$, while our results give a first-order transition for these cases.

As seen, when σ becomes small, the transition is of first order at very small q. In order to understand this, we have calculated the Landau-Ginzburg free energy for the limiting case $\sigma = -1$ where J_{ij} is equal to a constant. Let us take, for calculation convenience, $J_{ij} = -1/2N$ where N is the spin total number. We consider a q-state spin at the ith site $\overrightarrow{S}_{\mathbf{i}}$ who can take any of the following states $\overrightarrow{S}^{\mathbf{1}}_{\mathbf{i}}, \overrightarrow{S}^{\mathbf{2}}_{\mathbf{i}}, \ldots, \overrightarrow{S}^{\mathbf{q}}_{\mathbf{i}}$. We assume $|\overrightarrow{S}_i|^2 = 1$ and $\sum_\alpha \overrightarrow{S}^{\alpha}_{\mathbf{i}} = 0$ where $\alpha = 1, \ldots, q$. The last condition which is similar to that of the Potts clock model yields $(\sum_\alpha \overrightarrow{S}^{\alpha}_{\mathbf{i}})^2 = 0$. In other words, $\sum_{\alpha,\beta} \overrightarrow{S}^{\alpha}_{\mathbf{i}} \overrightarrow{S}^{\beta}_{\mathbf{i}} = \sum_\alpha (\overrightarrow{S}^{\alpha}_{\mathbf{i}})^2 + \sum_{\alpha\neq\beta} (\overrightarrow{S}^{\alpha}_{\mathbf{i}} \overrightarrow{S}^{\beta}_{\mathbf{i}}) = 0$. Defining for $\alpha \neq \beta$ $\cos\theta = \overrightarrow{S}^{\alpha}_{\mathbf{i}} \overrightarrow{S}^{\beta}_{\mathbf{i}}$, one obtains $q + q(q-1)\cos\theta = 0$ from which one has $\cos\theta = -\frac{1}{q-1}$.

Using the above definitions, we rewrite the Hamiltonian (1) as $H = -(1/2N) \sum_{i,j=1}^{N} \overrightarrow{S}_i \overrightarrow{S}_j$ where we have $\overrightarrow{S}_i \overrightarrow{S}_j = 1$ for $\overrightarrow{S}_i = \overrightarrow{S}_j$, or $\overrightarrow{S}_i \overrightarrow{S}_j = \cos\theta_{ij}$ for $\overrightarrow{S}_i \neq \overrightarrow{S}_j$.

Calculating the partition function and then the free energy per spin f, one obtains

$$f(\overrightarrow{\phi}) = \frac{1}{\beta}\left(\frac{1}{2}\overrightarrow{\phi}^2 - \ln\left[\sum_{\vec{S}} e^{\beta^{1/2}(\vec{\phi}\cdot\vec{S})}\right]\right), \tag{2}$$

where $\overrightarrow{\phi} = \phi \overrightarrow{S}$. From the notations given above, one has

$$f(\phi) = \frac{1}{\beta}\left(\frac{1}{2}\phi^2 - \ln\left[e^{\beta^{1/2}\phi} + (q-1)e^{-\beta^{1/2}\phi/(q-1)}\right]\right). \tag{3}$$

TABLE I. Critical exponents, the order of the transition, and $T_c(L)$ associated with the peak position of C_v for all studied σ.

σ	q	ν	γ	α	β	η	T_c
1	$q = 3$	2.272(1)	2.196(1)	−0.272(1)	0.038	1.034(1)	0.74
	$q = 5$	1.78(1)	1.72(1)	0.21(1)	0.030	1.03(1)	0.65
	$q = 7$	1.64(1)	1.60(1)	0.36(1)	0.020	1.02(1)	0.60
	$q = 9$			first-order transition			
0.7	$q = 3$	1.46(1)	1.16(1)	0.54(1)	0.15(1)	1.21(1)	1.18
	$q = 5$			first-order transition			
0.3	$q = 3$			first-order transition			
-1[a]	$q = 2$			second-order transition			1
	$q > 2$			first-order transition			$1/(q-1)$

[a]Mean-field results.

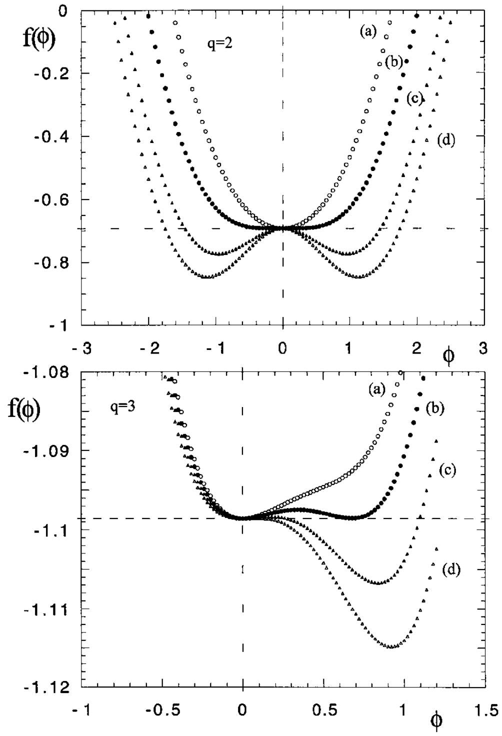

FIG. 5. MF free energy for $q = 2$ (upper) and $q = 3$ (lower) showing second- and first-order transitions, respectively. For the upper figure, (a)–(d) are for $\beta = 0.6$, 1, 1.4, and 1.6. For the lower figure, (a)–(d) are for $\beta = 1.8$, 1.848, 1.9, and 1.94.

For $\phi \ll 1$, an expansion of f gives

$$f(\phi) \approx \frac{1}{2}\left(1 - \frac{\beta}{q-1}\right)\phi^2 + \frac{1}{6}\,\frac{2-q}{(q-1)^2}\,\beta^{3/2}\phi^3 + \frac{1}{4!}\,\beta^2\phi^4 h + \ldots, \quad (4)$$

where h is a constant. Retaining up to the fourth order of ϕ, it is easy to see that f develops two mimima, one at $\phi = 0$ and the other at $\phi \neq 0$ only for $q > 2$ (see Fig. 5). This means that the first-order transition sets in for $q > 2$, confirming the tendency of MC results

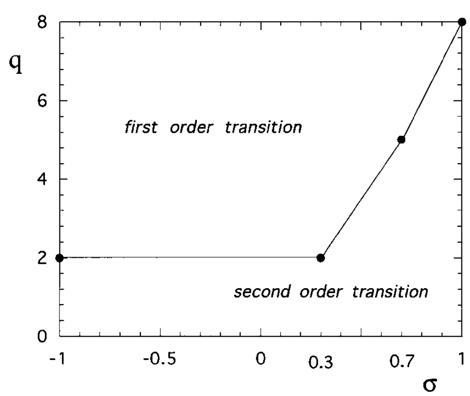

FIG. 6. q_c versus σ. Thin lines are guides to the eye. The value at $\sigma = -1$ is the MF result. The other points are MC results. First-order transitions occur at $q > q_c$.

(Table I). Note that the MF theory becomes exact when the number of interactions goes to infinity. We show in Fig. 6 the whole phase diagram. Note that the values of q_c for a given σ are integers because we studied the discrete q-state Potts model. Finally, we mention that Priest and Lubensky [16] have briefly commented on the stability of the fixed point with respect to σ when LR interactions exist, but their analysis was concentrated on the percolation limit ($q \rightarrow 1$). Therefore no indication on the existence of q_c was given. The same remark is for the work of Theumann and Gusmao [17].

In conclusion, we have studied the standard 1D q-state Potts model with LR interaction algebraically decaying as a power law of distance, using MC method. For each σ we found a first-order transition for q larger than a critical value q_c. This is similar to the case of SR interaction in $d = 2$ and $d = 3$. In some sense, the LR interactions compensate the loss of dimension when going down to 1D. A MF calculation confirms our MC results. We believe that the present work will stimulate future theoretical analysis on the LR Potts model.

"Laboratoire de Physique Théorique et Modélisation" is associated with CNRS (ESA 8089).

*Email address: Hung-The.Diep@ptm.u-cergy.fr
†Permanent address: Landau Institute for Theoretical Physics, 2, Kosygina Street, 117940 Moscow, Russia.

[1] R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, New York, 1992).
[2] For recent reviews, see *Magnetic Systems with Competing Interactions (Frustrated Spin Systems)*, edited by H. T. Diep (World Scientific, Singapore, 1994).
[3] D. J. Thouless, Phys. Rev. **187**, 732 (1969).
[4] D. Rapaport and N. E. Frankel, Phys. Lett. **28A**, 405 (1968).
[5] See references given in E. Luitjen and H. W. J. Blote, Phys. Rev. Lett. **76**, 1557 (1996); **76**, 3662 (1996); (to be published).
[6] Z. Glumac and K. Uzelac, J. Phys. A **22**, 4439 (1989).
[7] Z. Glumac and K. Uzelac, J. Phys. A **24**, 501 (1991).
[8] M. J. Wragg and G. A. Gehring, J. Phys. A **23**, L2157–2164 (1990).
[9] G. Kotliar, P. W. Anderson, and D. L. Stein, Phys. Rev. B **27**, 602 (1983).
[10] J. F. Nagle and J. C. Bonner, J. Phys. C **3**, 352 (1970).
[11] Michael E. Fisher, Shang-keng Ma, and B. G. Nickel, Phys. Rev. Lett. **29**, 917 (1972).
[12] J. M. Kosterlitz, Phys. Rev. Lett. **37**, 1577 (1976).
[13] E. Bayong, H. T. Diep, and T. T. Truong, J. Appl. Phys. (to be published).
[14] E. Bayong and H. T. Diep, Phys. Rev. B (to be published).
[15] Z. Glumac and K. Uzelac, J. Phys. A **26**, 5267 (1993).
[16] R. G. Priest and T. C. Lubensky, Phys. Rev. B **13**, 4159 (1976).
[17] W. K. Theumann and M. A. Gusmao, Phys. Rev. B **31**, 379 (1985).
[18] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **61**, 2635 (1988); Phys. Rev. B **44**, 5081 (1991).