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# Intrinsic structure of the phase-separation line in the two-dimensional Ising model

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**Abstract.** Monte Carlo simulations are performed on the two-dimensional square-lattice Ising model to calculate the intrinsic structure, in the sense of Bricmont *et al*, of the phase-separation line. Based on the calculated temperature dependence and the system-size dependence, the critical behaviour of the intrinsic structure is discussed.

## 1. Introduction

The one-dimensional interface is known to be rough and delocalised globally at any finite temperature $T$. A typical example is the phase-separation line (PSL) in the two-dimensional Ising model below the critical temperature $T_c$. Detailed studies (Fisher and Ferdinand 1967, Gallavotti 1972, Abraham and Reed 1976, Aizenman 1980) have led us to a good understanding of the long-distance (global) fluctuation properties of the PSL. It has been established that for a PSL with length (i.e. end-to-end distance) $N$, the global fluctuation width $W(T)$ of the PSL is $O(N^{1/2})$ and diverges as $N \to \infty$. Nevertheless, after scaling by $N^{1/2}$, the interface width and the interface profile have well defined limits; the scaled interface profile is expressed in terms of the integral of a Gaussian function with the variance $\sigma(T) = W(T)/N^{1/2}$ which is the scaled interface width. As $T \to T_c$, $\sigma(T)$ itself diverges as $|T - T_c|^{-1/2}$.

As for the short-distance (local) behaviour of the PSL, it has been believed that the PSL should have a well defined *intrinsic structure* such as the *intrinsic width*. The intrinsic structure of the PSL is itself quite an interesting problem to study and is important since many problems (for example, the interface dynamics) are related to such local properties of the interface. There are two ways of defining the intrinsic structure of the PSL (see, e.g., Abraham 1986): one was proposed by Abraham (1984) (see also Huse (1986), Abraham and Davies (1986)) and the other was proposed by Bricmont *et al* (1981, hereafter referred to as BLP). In the former, the magnetisation profile and the interface tension are utilised to define and calculate exactly the intrinsic width through a convolution. In the latter, which is more microscopic than the former, although a *rigorous qualitative* analysis was made by BLP, no detailed quantitative analysis has yet been undertaken, which would be important in clarifying the relation between the two ways of defining the PSL.

The purpose of this paper is to study quantitatively the local property of the PSL for the two-dimensional Ising model following the line of BLP.

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## 2. Intrinsic structure of the PSL

The Ising model Hamiltonian with a ferromagnetic coupling $J$ is given by

$$H = -J \sum_{\langle m,n \rangle} \sigma_m \sigma_n \tag{2.1}$$

where $\sigma_m \in \{1, -1\}$ and the sum is taken over all nearest-neighbour spin pairs on a square lattice. The critical temperature $T_c$ is given by $k_B T_c/J = 2/\log(1+\sqrt{2}) = 2.26$. We consider an $N \times N$ size system with a special boundary condition where all the uppermost (lowermost) boundary spins are fixed to be $-1$ $(+1)$. For simplicity, the linear size $N$ is chosen to be even. Under this boundary condition, we can draw one and only one PSL as a path connecting the dual lattice sites corresponding to the antiphase boundary (figure 1). Any PSL with length $L$ starts from the dual lattice site $(x_0, y_0) = (-N/2, 0)$ and ends at the dual lattice site $(x_L, y_L) = (N/2, 0)$, forming a path $(x_0, y_0) \to (x_1, y_1) \to (x_2, y_2) \to \cdots \to (x_L, y_L)$. Note that the second coordinate $y_i$ of a point $(x_i, y_i)$ in the path represents the height of the PSL at the point. If we wish to express the height $y$ of the PSL as a function of the first coordinate $x$ as $y = f(x)$, the function $f$ is multivalued in general due to the presence of the kinks and overhangs. At low temperatures, the PSL is well described by the solid-on-solid (SOS) model (Burton *et al* 1951) where the overhang configurations are forbidden and the excitations are limited to the kink type ones. At higher temperatures where large non-SOS type excitations are present, we have several choices of how to draw the PSL. We fix the drawing rule of the PSL in the following.

Let us briefly summarise the basic ingredients of the BLP theory on the intrinsic interface structure of the two-dimensional Ising model. A *deformation* of the PSL is a portion of the PSL where the heights $y$ (as a function of $x$) are multivalued (figure 2).

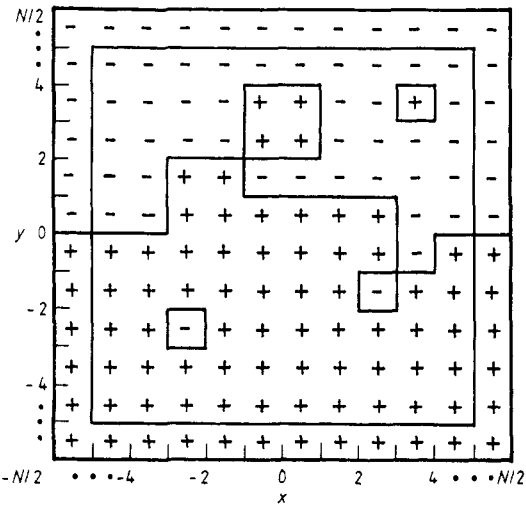


**Figure 1.** Adopted boundary condition and an example of PSL. An Ising spin with $+1$ $(-1)$ state is denoted by $+$ $(-)$. Spins on the upper-half (lower-half) rim are fixed to be $-$ $(+)$. Under the boundary condition, we can always draw a PSL starting (ending) at the middle of the left (right) side, passing through the dual lattice sites. Bubbles, the clusters of flipped spins, not belonging to the PSL are also shown.

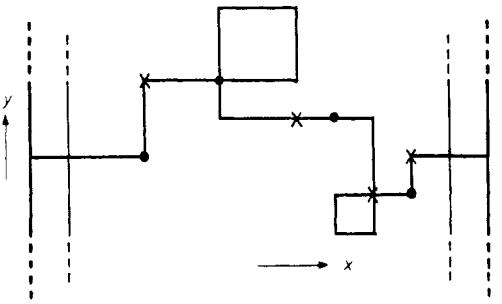


**Figure 2.** Four deformations in the PSL of figure 1. Entry point (exit point) of each deformation is denoted by ● (×). We have $D_{-3}=2$, $D_{-1}=-1$, $D_2=-2$ and $D_4=1$. For other values of $x$, we have $D_x=0$.

In a single PSL, there may exist many deformations connected by *regular components* where heights are single valued. For a deformation starting at some path position s and ending at a path position e (figure 2), the height difference $\Delta y = y_e - y_s$ measures the amount of deformation. The most important quantity in the discussion of BLP is the variable $D_i$ defined by

$$D_i = \begin{cases} y_e - y_s & \text{if a deformation starts (ends) at path position s(e) with } x_s = i \\ 0 & \text{otherwise.} \end{cases} \tag{2.2}$$

We remark here that $D_i$ has a favourable property that does not depend on the drawing rules of the PSL.

Local statistical properties of the deformations are characterised by a sequence of moments $\{d_n\}_{n=1}^{\infty}$ defined by

$$d_n = \langle |D_i|^n \rangle \tag{2.3}$$

which is independent of $i$ in the $N \to \infty$ limit (thermodynamic limit). Since any one of $\{d_n\}$ represents the 'local thickness' of the PSL in some sense, the quantity $w_n^{\mathrm{BLP}}$ given by

$$w_n^{\mathrm{BLP}} = (d_n)^{1/n} \tag{2.4}$$

can be used as a measure of the local interface width which we call the $n$th intrinsic width of the PSL. In particular, the quantities $d_2$ and $w_2^{\mathrm{BLP}}$ were originally introduced and discussed by BLP. As was pointed out in their discussion, $d_2$ and $w_2^{\mathrm{BLP}}$ are related to the scaled *global* width $\sigma(T)$ of the PSL as

$$\begin{aligned} \sigma^2(T) &= \lim_{N\to\infty} \sum_{i=-N/2}^{N/2} \langle D_0 D_i \rangle \\ &= \langle D_0^2 \rangle + \lim_{N\to\infty} \sum_{\substack{i=-N/2 \\ i\neq 0}}^{N/2} \langle D_0 D_i \rangle. \end{aligned} \tag{2.5}$$

In the above, translational invariance of the system has been taken into account. If the first term in (2.5) dominates as $T \to T_c$, as was *conjectured* by BLP, we have

$$d_2 \sim \sigma^2 \sim (T_c - T)^{-1} \qquad \text{as } T \to T_c \tag{2.6}$$

where the exact result $\sigma^2 = 1/\sinh[2(K-K^*)]$ (Abraham and Reed 1976) has been utilised, with $K = J/(k_B T)$ and $K^* = -\frac{1}{2}\log\tanh K$. At low temperatures where the PSL is correctly described by the SOS model, $D_i$ corresponds to a kink excitation ($D_i = h_{i+1} - h_i$). In this low-temperature region, $\langle D_i D_j \rangle \sim 0$ for $i \neq j$ due to the statistical independence of the kink excitations in the SOS model. Hence, from (2.5) we have the obvious low-temperature behaviour of $d_2$

$$d_2 \approx \sigma^2 \qquad \text{at low temperatures.} \tag{2.7}$$

The conjectured critical behaviour (2.6) is less obvious and requires further study. Also, the quantity $d_n$, with other values of $n$, should be studied to investigate the local structure of the PSL in more detail.

We are also interested in the number of deformations $N_d$ and its density $n_d$:

$$n_d = \lim_{N\to\infty} N_d / N \tag{2.8}$$

from which the $n$th moment of fluctuation *per deformation*, denoted by $\Delta_n$, is calculated as

$$\Delta_n = d_n / n_d. \tag{2.9}$$

To discuss the critical behaviour of the intrinsic structure, we introduce the following critical exponents:

$$d_n \sim (T_c - T)^{-\delta_n} \qquad T \to T_c \tag{2.10}$$

$$\Delta_n \sim (T_c - T)^{-\bar{\delta}_n} \qquad T \to T_c \tag{2.11}$$

$$n_d(T) \sim (T_c - T)^{\theta} \qquad T \to T_c \tag{2.12}$$

$$\bar{\delta}_n = \delta_n + \theta. \tag{2.13}$$

## 3. SOS model results

The one-dimensional SOS model describing the low-temperature behaviour of the PSL in the Ising model defined by (2.1) has the Hamiltonian

$$H^{SOS} = 2J \sum_{i=0}^{N-1} |h_{i+1} - h_i| \qquad h_0 = h_N = 0. \tag{3.1}$$

We can calculate the intrinsic interface structure exactly in the SOS model. The results presented below will serve as the reference frame for understanding the actual behaviour of the PSL.

In terms of the kink variables $\{k_i\}$ defined by $k_i = h_{i+1} - h_i$, the Hamiltonian (3.1) takes the following separable (non-interacting) form:

$$H^{SOS} = 2J \sum_{i=0}^{N-1} |k_i|. \tag{3.2}$$

To be precise, the $k_i$ above are not independent due to the constraint $h_0 = h_N = 0$ which amounts to $k_1 + k_2 + \ldots + k_N = 0$. However, this constraint is irrelevant in the $N \to \infty$ limit as can easily be proved and is neglected for calculation of the quantities with which we are concerned.

The quantity $d_n$ defined in (2.3) can be calculated as the $n$th moment of the kink variable:

$$d_n^{\mathrm{SOS}} = \langle |k_i|^n \rangle = \left( \sum_{k=-\infty}^{\infty} |k|^n \exp(-2\beta J|k|) \right) \left( \sum_{k=-\infty}^{\infty} \exp(-2\beta J|k|) \right)^{-1} \tag{3.3}$$

where we have denoted $\beta = (k_B T)^{-1}$. In particular, we have

$$d_1^{\mathrm{SOS}} = 1/\sinh(2\beta J) \tag{3.4}$$

$$d_2^{\mathrm{SOS}} = 1/2\sinh^2(\beta J). \tag{3.5}$$

The deformation number density $n_d^{\mathrm{SOS}}$ is calculated as

$$\begin{aligned} n_d^{\mathrm{SOS}} &= \lim_{N\to\infty} \frac{1}{N} \left\langle \sum_i (1-\delta_{k_i,0}) \right\rangle \\ &= \left( \sum_{k=-\infty}^{\infty} (1-\delta_{k,0}) \exp(-2\beta J|k|) \right) \left( \sum_{k=-\infty}^{\infty} \exp(-2\beta J|k|) \right)^{-1} \\ &= 2\exp(-2\beta J)[1+\exp(-2\beta J)]^{-1} \end{aligned} \tag{3.6}$$

which is a monotonically increasing function of temperature. From (3.4)-(3.6) we have

$$\Delta_1^{\mathrm{SOS}} = d_1^{\mathrm{SOS}}/n_d^{\mathrm{SOS}} = [1-\exp(-2\beta J)]^{-1} \tag{3.7}$$

$$\Delta_2^{\mathrm{SOS}} = d_2^{\mathrm{SOS}}/n_d^{\mathrm{SOS}} = [1+\exp(-2\beta J)][1-\exp(-2\beta J)]^{-2}. \tag{3.8}$$

## 4. Monte Carlo calculation

We performed standard Monte Carlo simulations on the two-dimensional square-lattice Ising model with $N \times N$ system size under the same boundary condition as shown in figure 1, varying the temperature $T$ and the linear system size $N$ (16-128). To improve the statistics, $d_1$ and $d_2$ are actually calculated as

$$d_1 = \frac{1}{N} \sum_i \langle |D_i| \rangle \tag{4.1}$$

$$d_2 = \frac{1}{N} \sum_i \langle D_i^2 \rangle \tag{4.2}$$

which is justified from the $i$ independence of $\langle |D_i| \rangle$ and $\langle D_i^2 \rangle$ in the $N \to \infty$ limit. Note that in (4.2) we are not calculating $(1/N)\langle (\Sigma_i D_i)^2 \rangle$ which is just $\sigma^2(T)$ in the $N \to \infty$ limit.

We calculated the temperature dependences (figures 3 and 4) and the system-size dependences at $T_c$ (figures 5 and 6) of $d_1$ and $d_2$. At low temperatures, both $d_1$ and $d_2$ lie close to the curves of corresponding SOS model results $d_1^{\mathrm{SOS}}$ and $d_2^{\mathrm{SOS}}$. For $d_2$, we see a good agreement of (2.7) for a very wide range of temperatures. In figures 5 and 6, the following behaviour is clearly seen:

$$d_1(T_c) \sim N^0 \text{ (finite)} \qquad \text{for large } N \tag{4.3}$$

$$d_2(T_c) \sim N \qquad \text{for large } N. \tag{4.4}$$

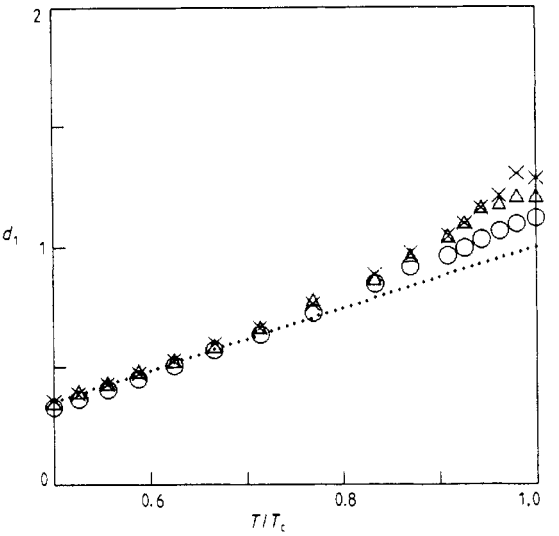


**Figure 3.** Temperature dependence of $d_1$ obtained by Monte Carlo simulation (○: $32\times32$; △: $64\times64$; ×: $128\times128$). Each point, except those at $T=T_c$, represents the average over $4\times10^4$ steps per site. For $T=T_c$, averages over $10^5$ steps per site are shown. The broken curve represents $d_1^{SOS}$.

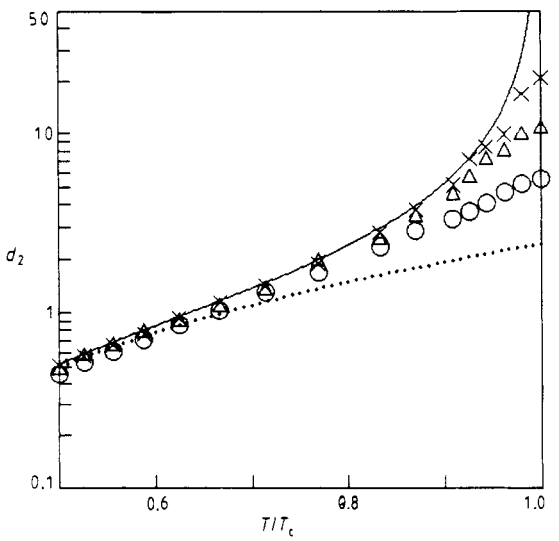


**Figure 4.** Temperature dependence of $d_2$, with details as figure 3. The broken curve represents $d_2^{SOS}$ and the full curve the values of $\sigma^2$.

From the standard arguments of finite-size scaling theory (see, e.g., Barber 1983), results (4.3) and (4.4) imply

$$d_1 \sim |T-T_c|^0 \text{ (finite)} \qquad \text{as } T\to T_c \tag{4.5}$$

$$d_2 \sim |T-T_c|^{-1} \qquad \text{as } T\to T_c. \tag{4.6}$$

In particular, the behaviour (4.6) confirms the relation (2.6). Thus, we obtain the

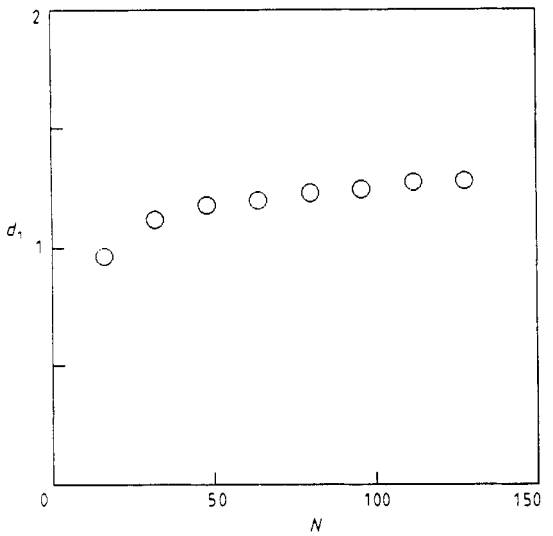


**Figure 5.** Size dependence of $d_1$ at $T = T_c$. We denote the linear size of the system by $N$. Each point represents an average over $10^5$ steps per site.

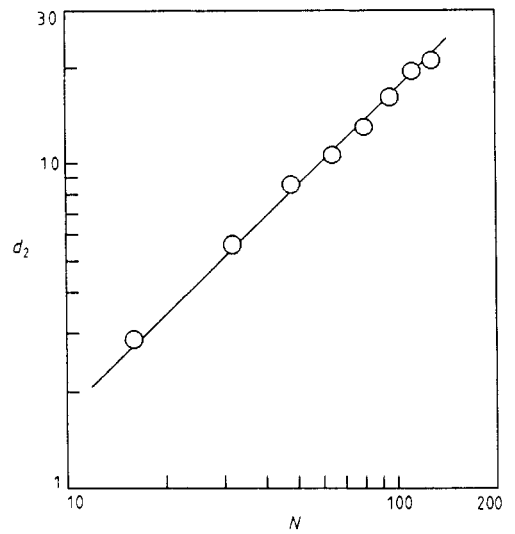


**Figure 6.** Size dependence of $d_2$ at $T = T_c$, similar to figure 5. The line has a slope of one.

values of exponents $\delta_1$ and $\delta_2$ defined in (2.10) as

$$\delta_1 = 0 \tag{4.7}$$

$$\delta_2 = 1. \tag{4.8}$$

The number of deformations $N_d$ is also calculated and the results are shown in figure 7 (temperature dependence of $N_d$), figure 8 (size dependence of $N_d$ at $T_c$) and figure 9 (temperature dependence of $n_d$). As opposed to the SOS model result (3.6), $n_d(T)$ has a maximum around $T^* = 0.85\ T_c$. This is the effect of large deformation (figure 10) as can be explained in the following. At low temperatures, very small

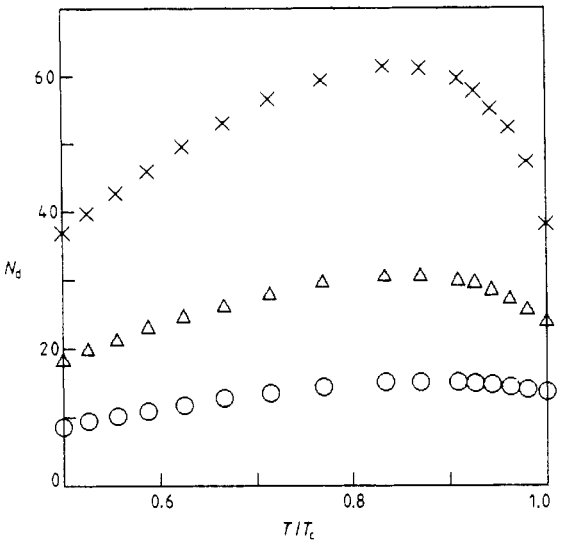


**Figure 7.** Temperature dependence of $N_d$ (○: $32\times32$; △: $64\times64$; ×: $128\times128$). Each point, except those at $T = T_c$, represents the average over $3\times10^4$ steps per site. For $T = T_c$, averages over $4\times10^4$ steps per site are shown.

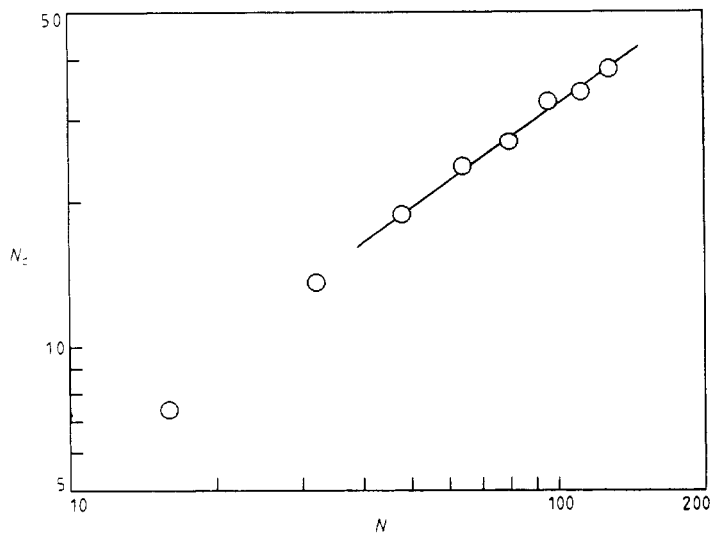


**Figure 8.** Size dependence of $N_d$ at $T = T_c$. Each point represents an average over $4\times10^4$ steps per site. The line has a slope of $0.68\pm0.04$.

numbers of deformations are present. By raising the temperature, we have more and more deformations. At the same time, the mean horizontal extent of deformations becomes larger and larger. Then, for finite size ($N\times N$) system, there should exist a temperature above which $N_d$ do not increase any further but decreases as $T$ increases.

From figure 8, we obtain

$$N_d(T_c)\sim N^{\theta'} \qquad \theta' = 0.68\pm0.04 \qquad \text{for large } N. \tag{4.9}$$

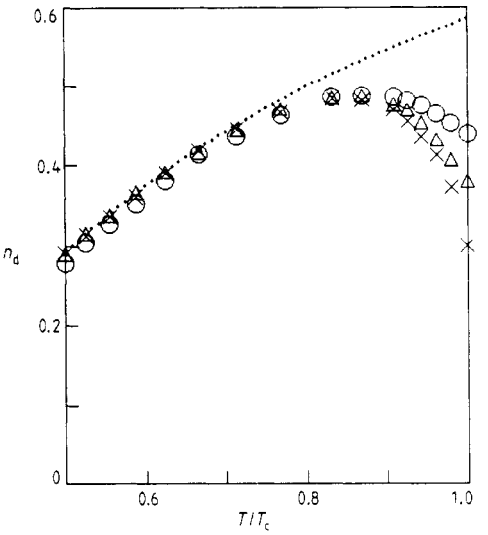


**Figure 9.** Temperature dependence of $n_d$ with details as figure 7. The broken curve represents $n_d^{SOS}$.

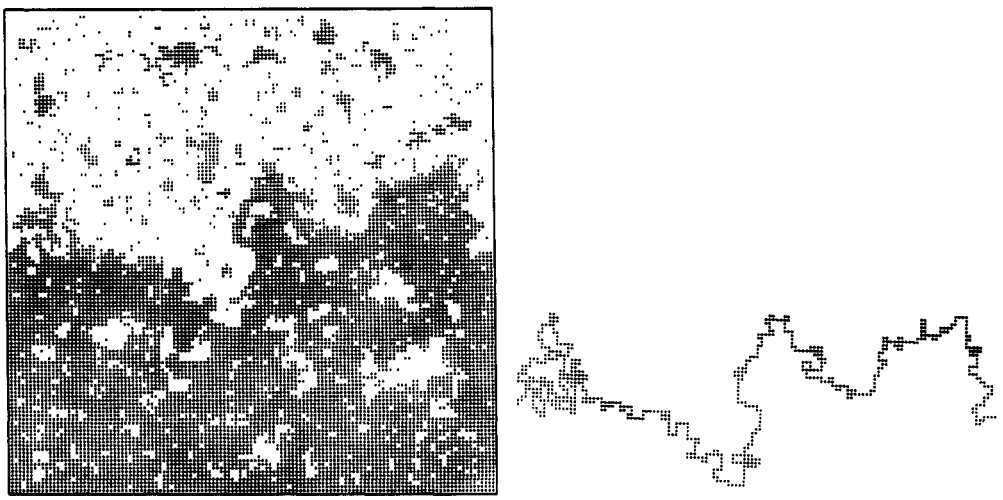


**Figure 10.** (*a*) Typical snapshot of the spin configuration ($\cdot = +1$) at $T = T_c$. The system size is $128 \times 128$. (*b*) Corresponding dual lattice points forming the PSL which contains large deformations.

Then from (2.8) and from the finite-size scaling theory we have

$$n_d(T) \sim (T_c - T)^{\theta} \qquad T \to T_c$$
$$\theta = 1 - \theta' = 0.32 \pm 0.04. \tag{4.10}$$

Combining (2.9)-(2.13) and (4.7)-(4.10), we have

$$\bar{\delta}_1 = \theta = 0.32 \pm 0.04 \tag{4.11}$$

$$\bar{\delta}_2 = 1 + \theta = 1.32 \pm 0.04. \tag{4.12}$$

## 5. Summary

In this paper we have presented a quantitative analysis of the intrinsic interface structure in the sense of Bricmont *et al* (1981) by using the Monte Carlo method. As a summary of this paper, we should like to remark on the following three points.

(i) Agreements of (2.6) and (2.7) are clearly seen. Moreover, interestingly enough, $d_2$ (= local quantity) and $\sigma^2$ (= global quantity) behave very much alike over a very wide range of temperature.

(ii) Quite different critical behaviours between $d_1$ (non-divergent) and $d_2$ (divergent) may cause a problem in choosing the most suitable quantity among $\{w_n^{\mathrm{BLP}}\}$ as the definition of the intrinsic width.

(iii) The deformation number density $n_d$, calculated for the first time, shows non-trivial behaviour. In particular, the critical behaviour $\lim_{T\to T_c} n_d(T)=0$ is observed.

In respect of point (ii), it is an important task to obtain the full form of the probability distribution function of $\{D_i\}$. As for the behaviour of $n_d$, we do not have a satisfactory explanation for the obtained value of the exponent $\theta$, for which calculation of the deformation size distribution may be helpful. These tasks are left for future study and will be published elsewhere.

Analysis of the intrinsic interface structure made in this paper is restricted to that in the sense of Bricmont *et al.* Our calculation presented in this paper is the first step towards clarifying the relation between the BLP theory and the Abraham theory, which is also an important future problem.

## Acknowledgments

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