FIRST-ORDER TRANSITION IN A TWO-DIMENSIONAL LAPLACIAN ROUGHENING MODEL ON A SQUARE LATTICE

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In order to understand why Strandburg, Solla and Chester find, in the laplacian roughening model of two-dimensional defect melting, two successive continuous transitions, we study another form of this model on a square lattice and find a single first-order phase transition. Since our model equilibrates much faster than theirs we conclude that either there is an essential dependence on the lattice structure or their result is not trustworthy.

Inspired by the theoretical work on two-dimensional defect melting of Kosterlitz, Thouless, Halperin, Nelson and Young (KTHNY) [1], Strandburg, Solla and Chester (SSC) [2] have recently studied the correlation lengths of the laplacian roughening model (LRM) on a triangular lattice in great detail. The partition function reads

$$Z = \sum_{\{h(x)\}} \exp\left(-\tfrac{1}{2}\beta_{\mathrm{LR}} \sum_{x} |\Delta h(x)|^2\right) , \tag{1}$$

where

$$\Delta h(x) = \frac{2}{3} \sum_{\mu} [h(x+\mu) - h(x)] \tag{2}$$

is the lattice laplacian, with μ running through the six nearest neighbors of x. Via Poisson's formula

$$\sum_{n} = \int_{-\infty}^{\infty} \mathrm{d}\varphi \sum_{m} \exp(2\pi i m\varphi)$$

this model is seen to describe an ensemble of point disclinations with a partition function

$$Z_{\mathrm{discl}} = (2\pi\beta_{\mathrm{LR}})^{-N/2} \sum_{\{m(x)\}} \exp\left(-4\pi^2\beta_{\mathrm{LR}} \frac{1}{2} \sum_{x \neq x'} m \frac{1}{\Delta\cdot\Delta} m\right) , \tag{3}$$

where

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$$\left(\frac{1}{\Delta\cdot\Delta}\right)(x,x') = N^{-1} \sum_{k} \{\exp[\mathrm{i}k\cdot(x-x')] + \tfrac{1}{2}[k\cdot(x-x')]^2 - 1\}$$

$$\times \{\tfrac{2}{3}[6 - 2[\cos k_1 + \cos(\tfrac{1}{2}k_1 - \tfrac{1}{2}\sqrt{3}\,k_2) + \cos(\tfrac{1}{2}k_1 + \tfrac{1}{2}\sqrt{3}\,k_2)]]\}^{-2} \quad (4)$$

is the twice subtracted finite triangular lattice version of the $1/k^4$ correlation which behaves asymptotically like

$$\int \frac{\mathrm{d}^2k}{(2\pi)^2} \frac{\exp(\mathrm{i}k\cdot x)}{(k^2)^2} \sim (1/8\pi)|x|^2 \log|x| + A|x|^2 + B + \mathrm{O}(1/|x|)\,. \quad (5)$$

The disclination gas is neutral ($\Sigma_x m(x) = 0$) and has no dipole moment ($\Sigma_x x m(x) = 0$). According to SSC, this model has two successive continuous phase transitions of the Kosterlitz–Thouless type, one at

$$T_{\mathrm{LR}}^{(1)} = 1/\beta_{\mathrm{LR}}^{(1)} = 1.84 \pm 0.01\,, \quad (6)$$

where the surface formed by the integers $h(x)$ roughens with a height–height correlation

$$H(x) = \langle (h(x) - h(0))^2 \rangle = 2\langle h(0)^2 \rangle - 2\langle h(x)h(0) \rangle \quad (7)$$

changing from a constant to a logarithmic behavior at large distances and another one at

$$T_{\mathrm{LR}}^{(2)} = 1/\beta_{\mathrm{LR}}^{(2)} = 1.925 \pm 0.015\,, \quad (8)$$

where it changes from logarithmic to $|x|^2$ behavior with a proportionality constant which diverges logarithmically with the lattice size.

To us, this result came somewhat unexpected. Following a different motivation we had constructed another model of defect melting, on a simple cubic lattice, in which stresses and defects in a lattice are described by a partition function involving a periodic form of strain

$$Z = \int_{-\pi}^{\pi} \prod_{x,i} \frac{\mathrm{d}u_i(x)}{2\pi} \sum_{\substack{\{n_{ij}(x)\} \\ i\leqslant j}} \exp\left\{-\beta_{\mathrm{v}}\left[\frac{1}{2}\sum_{x,i<j} (\nabla_i u_j + \nabla_j u_i - 2\pi n_{ij})^2 + \xi_{\mathrm{v}} \sum_{x,i} (\nabla_i u_i - 2\pi n_{ii})^2 \right.\right.$$

$$\left.\left. + \frac{\lambda}{2\mu} \sum_{x} \left(\sum_{i} [\nabla_i u_i(x-i) - 2\pi n_{ii}(x-i)] \right)^2 \right]\right\}. \quad (9)$$

Here $\beta_{\mathrm{v}} = \mu a^2/(2\pi)^2 T_{\mathrm{v}}$ is the inverse temperature in reduced units (μ times cell volume a^2) and the constants $\mu = C_{44}$, $\lambda = C_{12}$, $\xi_{\mathrm{v}} = (C_{11} - C_{12})/2C_{44}$ account for the elastic properties of the cubic crystal whereas the integer numbers n_{ij} describe (similar to the Villain model of superfluidity) the plastic properties, i.e. the jumps of $u_i(x)$ across the Volterra surfaces whose boundaries are defect lines. By a standard duality transformation it is possible to show [3] that for $D = 2$ the model describes the same gas of disclinations as the laplacian roughening model, albeit on a square lattice.

When studying a cosine approximation of this model, at $\lambda = 0$ (similar to the classical planar spin model)

$$Z = \int_{-\pi}^{\pi} \prod_{x,i} \frac{\mathrm{d}u_i(x)}{2\pi} \exp\left(\beta \sum_{x,i<j} \cos(\nabla_i u_j + \nabla_j u_i) + 2\beta\xi \sum_{x,i} \cos(\nabla_i u_i)\right)\,, \quad (10)$$

we found in three [4,5] as well as two dimensions [6], that defect melting proceeds in a single first-order transition. At first sight, there can be three reasons for the discrepancy:

(1) The approximation of the periodic gaussian by a cosine model can change the order.

(2) Defects on a square lattice can have a phase transition of different order than those on a triangular lattice.

(3) The findings of SSC of two successive Kosterlitz–Thouless transitions is unreliable since the distinction of different long-range behaviors of correlation functions on a finite lattice (SSC used 32 × 32 points and extracted the behavior up to $|x| = 16$) can be problematic.

The purpose of this note is to eliminate the first of the three possibilities. Before starting it is worth noting that the difference between cosine and Villain types of models have recently become a subject of interest in connection with U(1) lattice gauge theories. The motivation is the equivalence of this model to an abelian Higgs model [7], for which there are theorems that the transition should always be of first order [8]. According to a more subtle analysis [9,10], however, there should exist a tricritical point and the discovery of such a point has been claimed [11]. It lies somewhere between the cosine and the periodic gaussian version of the pure U(1) lattice gauge models. The latter can be shown to be equivalent to the former with a mixed field energy ("action") [12]

$$\beta \cos \text{“}\theta\text{”} + \gamma \cos \text{“}2\theta\text{”} , \tag{11}$$

where $\gamma \approx -0.18$. The tricritical point is estimated to lie at $\gamma \approx -0.11$, implying a first-order transition for the cosine version and a second-order transition for the Villain model, respectively.

A similar study was recently undertaken for the $D = 3$ classical planar spin model [13]. There, the tricritical point seems to lie at $\gamma = 0.33$, which explains why both forms of the model have a second order transition. Thus the crucial question to be answered in this note is whether the $D = 2$ melting transition is more like the U(1) lattice gauge theory or like the $D = 3$ classical planar spin model, or whether it chooses the third option that *both* forms of the model have a first-order transition. It turns out that the evidence is for the last option. We have therefore investigated the 2D Villain model (9) and the cosine model with mixed field energy (11) with great care by Monte Carlo simulations [‡1].

[‡1] In all Monte Carlo simulations, we worked with the heat-bath algorithm and approximated the phase variables θ_i by N discrete angles $(2\pi/N)n_i$, $n_i = 0, \ldots, N-1$ with $N = 16 \ldots 32$. All data shown in this note were taken on 60×60 square lattices with periodic boundary conditions.

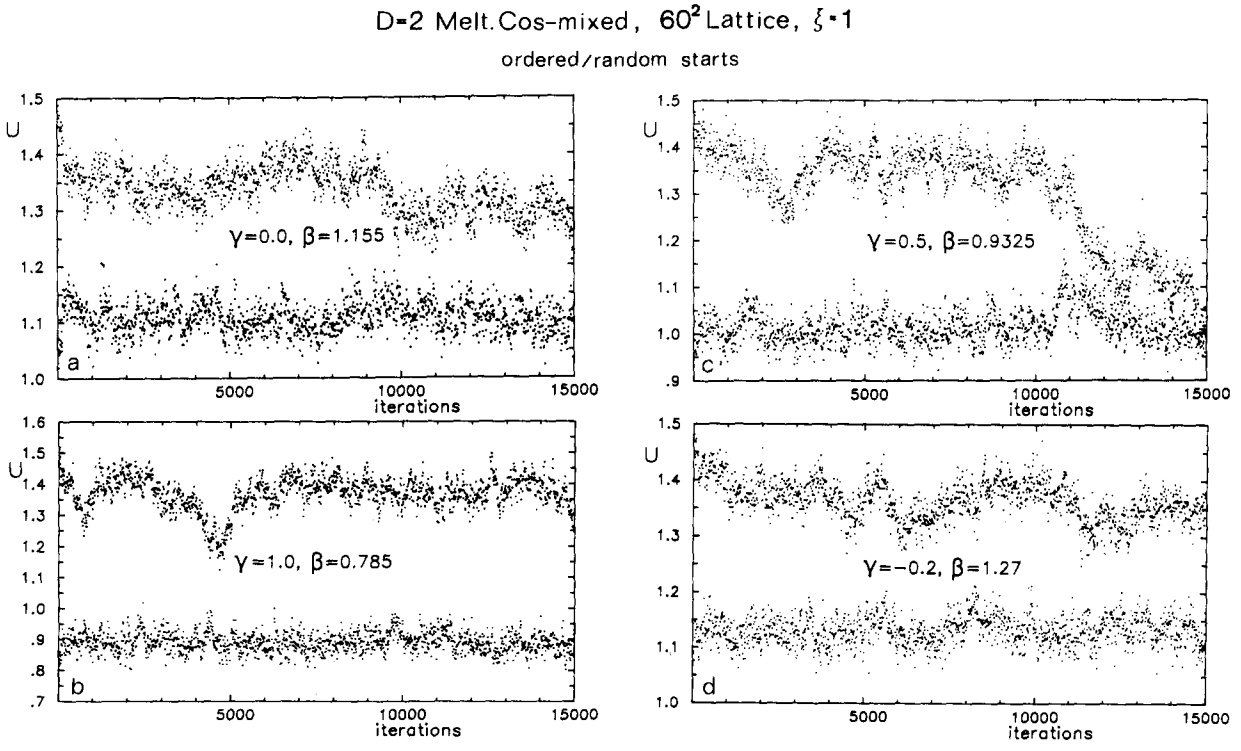

Fig. 1. The development of the internal energies of the crystalline and disordered initial state in the mixed cosine model for various γ near the transition point.

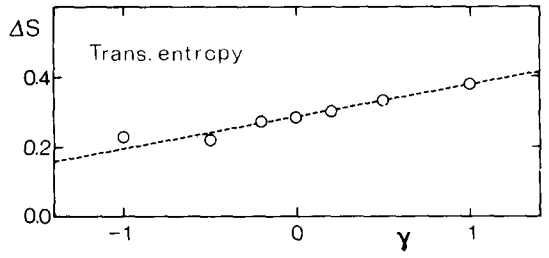

Fig. 2. The γ dependence of the transition entropy in the mixed cosine model.

Our work consists of three parts:

(1) First we confirm once more the first-order nature of the transition in the cosine melting model by going to the transition point, putting the system once in the ordered (o.s.) and once in a random initial state (r.s.) and study the development of the internal energy over 15000 (!) sweeps. The energies converge very fast to two very stable states which we identify with the uniform crystal and liquid, respectively (see fig. 1a). From the energy difference $\Delta U \approx 0.25$ and $\beta_m \approx 1.155$ we find the transition entropy $\Delta S \approx 0.29$ ($\xi = 1$).

It should be pointed out that after waiting for many sweeps the model presents us with a phenomenon which we had not seen in the earlier investigation [6] since there the number of sweeps had been limited to 4000. The crystalline state makes a sudden jump towards the liquid state (about 1/3 of the distance), and continues to remain in that state for another large number of sweeps. A look at the defect picture informs us that what has happened is the formation of a *mixed state* in which chunks of crystal have molten. Since the size of these chunks is about 10^2 lattice sizes we conclude that the mutual approach of the two internal energies is not a signal of a second-order transition (in which there would be no finite length scale).

(2) The second part of our work consisted in looking at the modified model in which the cosine term involving the links (i.e. the $\beta\xi$ term) is modified to

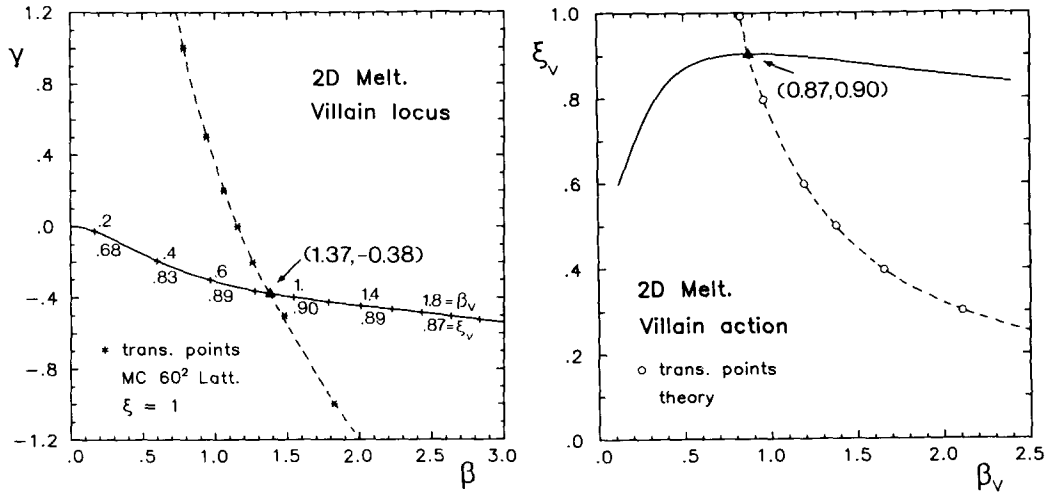

Fig. 3. The solution of eq. (14) for $\xi = 1$. Along the continuous curve in (a), the mixed cosine model is a good approximation of the Villain model with running ξ_V, shown as a continuous line in (b). The stars in (a) and the open circles in (b) mark the transition line in the $\beta-\gamma$ and $\beta_V-\xi_V$ plane, respectively. In (a), they are determined by our Monte Carlo experiments on a 60^2 lattice whereas in (b) they follow from a theoretical analysis (comparison of high- and low-temperature expansions of the free energy). The dotted lines are only guides for the eye. We see that the intersection of the Villain locus and the transition line of the mixed model in (a) ($(\beta, \gamma) = (1.37, -0.38)$) is mapped precisely onto the transition line of the Villain model in (b) ($(\beta_V, \xi_V) = (0.87, 0.90)$).

$$2\beta\xi \cos(\nabla_i u_i) \to 2\beta\xi \cos(\nabla_i u_i) + \gamma \cos(2\nabla_i u_i) . \quad (12)$$

According to our earlier analysis [12,13], this permits hardening or softening the transition, depending on $\gamma > 0$ or $\gamma < 0$. Indeed, when calculating the transition entropy obtained from runs like the previous one for various values of γ, we do find a tendency to harden for $\gamma \approx 1.0$ and to soften for $\gamma \approx -0.2$ (see figs. 1b–d). In contrast to the 3D planar spin model or the 4D U(1) lattice gauge model, however, the γ dependence of ΔS is extremely weak (see fig. 2).

The fact that ΔS at $\gamma \approx -0.4$ is $\gtrsim 0.2$ and definitely looks > 0 can now be used as evidence that also the Villain form of the melting model, which is dually equivalent to the laplacian roughening model on a square lattice, has a first-order transition. The arguments for this are the same as those given in ref. [12] for the planar spin or U(1) gauge models; so we can restrict ourselves to a few comments why this is so. When performing a high-temperature analysis of both the cosine and the Villain form of the model, there are diagrams describing the thermal genera-

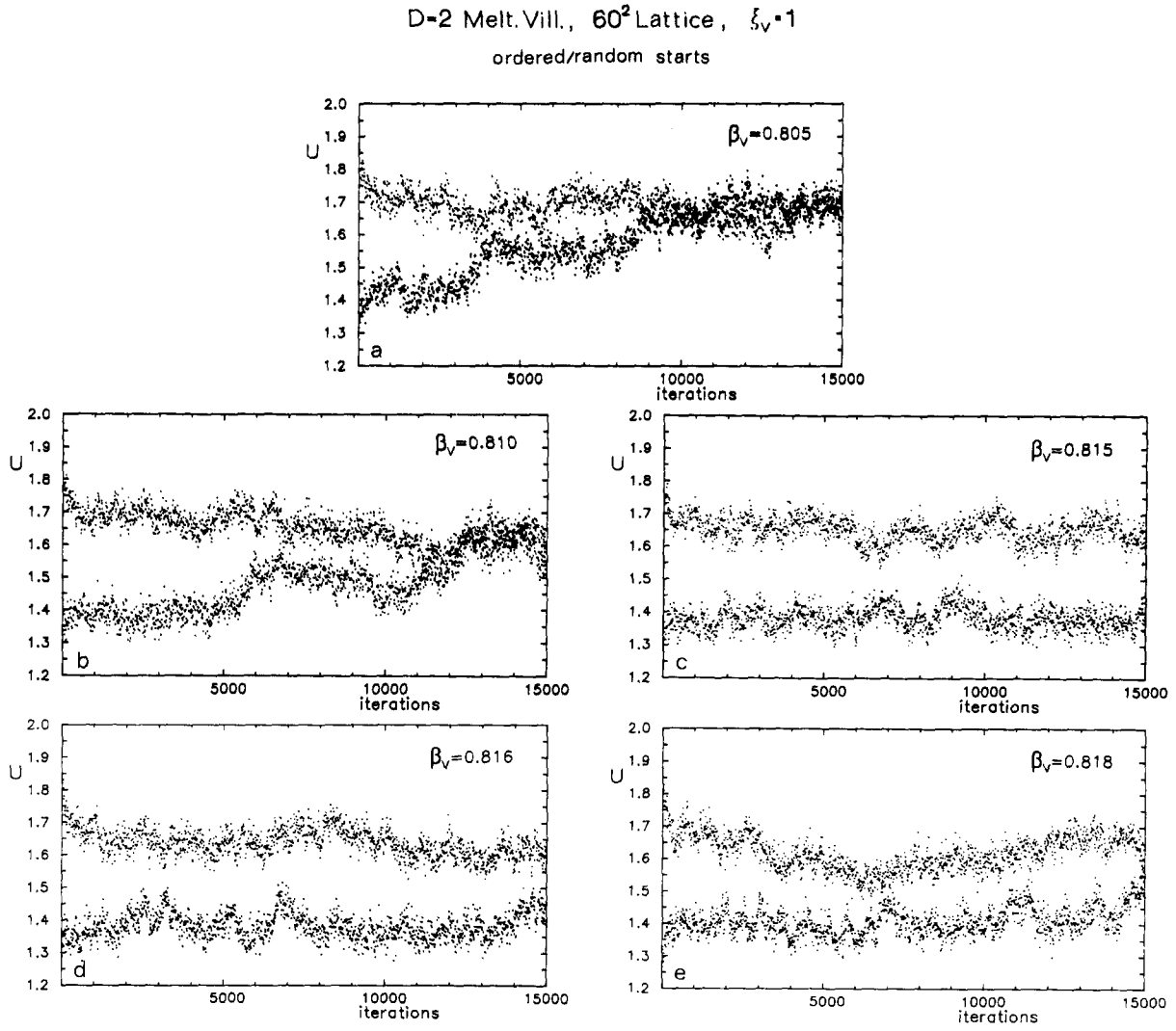

Fig. 4. The development of the internal energies of the crystalline and disordered initial state in the Villain model for $\xi_V = 1$ and various β_V near the phase transition.

tion of small stress configurations. These involve exponentials $\exp(-\sigma_{ij}^2/2\beta_v)$, $\exp(-\sigma_{ii}^2/4\beta_v\xi_v)$ in the Villain case and $I_{\sigma_{ij}}(\beta)$, $I^{\gamma}_{\sigma_{ii}}(2\beta\xi)$ in the cosine case where I_σ are Bessel functions and for the mixed cosine case (12),

$$I^{\gamma}_{\sigma}(2\beta\xi) \equiv \int_0^{2\pi} \frac{d\theta}{2\pi} \cos(\sigma\theta) \exp[2\beta\xi \cos\theta + \gamma \cos(2\theta)] \,. \tag{13}$$

The diagramatic analysis shows that a large number of diagrams have at most weights $\sigma_{ij} = 0, 1$; $\sigma_{ii} = 0, 1, 2$. Thus it is possible to make the statistical weight of all these graphs agree by equating

(i) $\exp(-1/2\beta_v) = I_1(\beta)/I_0(\beta)$,

(ii) $\exp[-1/2(2\beta_v\xi_v)] = I^{\gamma}_1(2\beta\xi)/I^{\gamma}_0(2\beta\xi)$,

(iii) $\exp[-4/2(2\beta_v\xi_v)] = I^{\gamma}_2(2\beta\xi)/I^{\gamma}_0(2\beta\xi)$. (14)

Hence the Villain model with a running ξ_v is approximated by the mixed cosine models along a curve in the β–γ

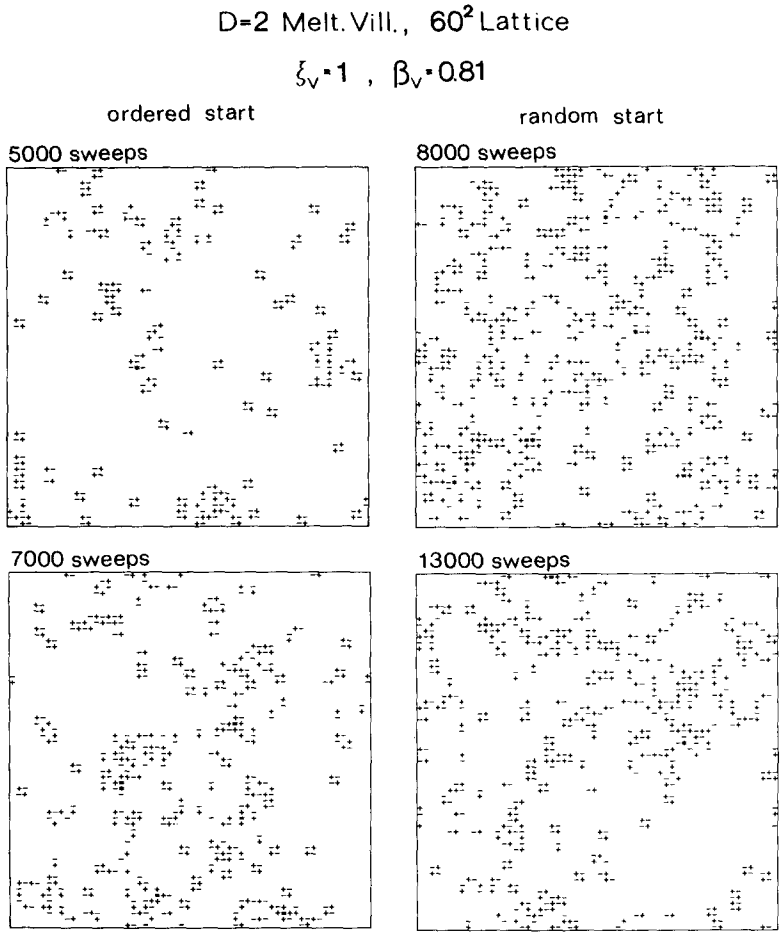

Fig. 5. Defect configurations of the Villain model at $\beta_v = 0.81$, $\xi_v = 1$, after several thousand iterations, starting from a crystalline or disordered state. Notice that the phases are not completely uniform, as discussed in the text.

plane (see fig. 3) intercepting the line of phase transitions at $\beta_m \approx 1.37$, $\gamma_m \approx -0.38$. Inserting these values into formula (14) we calculate from this the transition values of the Villain model

$$\beta_{vm} \approx 0.87\,, \quad \xi_{vm} \approx 0.90\,. \tag{15}$$

From fig. 2, the transition entropy is found to be

$$\Delta S \approx 0.24\,. \tag{16}$$

(3) In order to confirm this result we have performed a direct simulation of the Villain model at $\xi_v = 1$, where β_{vm} is only slightly different from (15), namely $\beta_{vm} \approx 0.81$–0.82. The development of the internal energies of the crystalline and disordered initial state is shown in figs. 4a–e for various β_v near the transition point. For $\beta_v = 0.81$, the two energies approach very fast the values ≈ 1.4 and ≈ 1.7, which they keep for a long time. After 5000 sweeps there is again a jump in the crystalline energy. Plotting the defects in the crystalline state we can again see that a mixed state is beginning to form in which domains of liquid (i.e. calescent patterns of defects) invade into the crystal (see fig. 5). Thus we conclude that the transition is first-order despite the final convergence of the energy and that the transition entropy is as stated above.

The formation of mixed states in simulations of two-dimensional melting has been observed before by Toxvaerd and Abraham [14] in molecular dynamics simulations. It has been shown that it is capable of giving rise to correlations which look just like those of an intermediate phase in a continuous two-step melting process [15]. Our results seem to confirm this phenomenon.

In conclusion we can state that the simple melting model on a square lattice undergoes a first-order transition in the cosine form, in the Villain form, and in the dual laplacian roughening form. The model's tendency to form a mixed phase can easily suggest the existence of two successive continuous transitions. A closer examination of the evidence seems to rule out this possibility.

Let us finally mention that experimentally, one observes first-order as well as continuous transitions, depending on the coverage [16].

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