FINITE-SIZE SCALING STUDY OF THE LAPLACIAN ROUGHENING MODEL ☆

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We perform further Monte Carlo simulations of the Laplacian roughening model on a triangular lattice to decide whether two-dimensional defect melting proceeds in a *single first-order* or *two successive continuous* transitions, as predicted by two conflicting theories. Of the two alternatives, the new high-statistics Monte Carlo data favor the single first-order transition.

1. Introduction

Until very recently [1] the nature of the two-dimensional melting transition was very controversial both experimentally and theoretically. The previous status until winter '87 was summarized in an extensive review by Strandburg [2]. In the context of defect models of melting, Strandburg gave special emphasis upon the Laplacian roughening model [3], the dual formulation of a disclination system with long range forces. She argued that, on a triangular lattice, this model undergoes a sequence of two Kosterlitz–Thouless (KT) transitions as suggested by the KTHNY theory [4]. An alternative theory [5], predicting a single first-order transition in this model, due to a coupled transition of dislocations and disclinations, was briefly considered by Strandburg but subsequently ruled out on the basis of Monte Carlo data [6,7] [#1], which she claims to favor the KTHNY scenario. This claim, however, is not consistent with our own Monte Carlo simulations [9,10] [#2] of the same model which showed a single weak first-order transition.

Naturally, Strandburg [2] tried to "resolve" this contradiction by criticizing our numerical analysis. Her arguments will be presented later in the course of the discussion. While we were able to convince ourselves that this critique is unjustified, Strandburg succeeded in attracting a group of renowned experimentalists to her standpoint [11], making Hurlbut and Dash even withdraw (see ref. [12], Response to the Comment cited in ref. [11]) their original interpretation [13] of experimental data. This fact together with the new light shed upon the problem by the most recent theoretical work [1] compelled us to investigate once more the issue of a *single first-order* versus *two successive continuous* melting transitions in the Laplacian roughening model via Monte Carlo simulations, with much higher statistics and better temperature resolution than before.

Although we find that it is impossible to extract from the data a completely unbiased statement about the nature of the transition, a difficulty we share with most other Monte Carlo simulations, the data do help to judge between the two alternative theories: They definitely favor a single first-order transition over two successive KT transitions.

2. The model and its simulation

Adopting the usual conventions, the Laplacian roughening model is described by an energy

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[#1] For work related to ref. [6], on a square lattice, see ref. [8].

[#2] On a square lattice in a dually equivalent form, ref. [9], and on a triangular lattice, ref. [10].

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$$\beta E = \frac{\beta}{2} \sum_{x} [\bar{\nabla}\nabla h(x)]^2$$

$$\equiv \frac{\beta}{2} \sum_{x} \left(\frac{2}{3} \sum_{i} [h(x) - h(x+i)] \right)^2 , \qquad (1)$$

where x denote the sites of a triangular lattice, the i are the displacement vectors to the six nearest neighbors, and $\beta = J/k_B T$. The $h(x)$ are integer variables to be summed over in the partition function. They may be interpreted as the height variable of a surface at site x. Via a standard duality transformation [3], this ensemble of fluctuating surfaces is known to be equivalent to a system of defects with long-range interactions,

$$\beta E = \frac{1}{2} \frac{4\pi^2}{\beta} \sum_{x,x'} m(x) v_4(x - x') m(x') . \qquad (2)$$

The integer valued defect field $m(x)$ describes disclinations at site x. Since the infrared divergence of the potential $v_4(x - x') \equiv 1/(\bar{\nabla}\nabla)^2$ enforces neutrality and dipole neutrality of these defects ($\sum_x m(x) = 0$, $\sum_x x m(x) = 0$), it can be replaced by the twice subtracted finite potential

$$v_4''(x) \equiv v_4''(n_1, n_2)$$

$$\equiv \int_{-\pi}^{\pi} \frac{d^2k}{(2\pi)^2} \frac{\exp(i k \cdot x) - 1 + \frac{1}{4} x^2 \bar{K}K}{(\bar{K}K)^2} , \qquad (3)$$

where

$$\bar{K}K = 4 - \tfrac{4}{3} [\cos(k_1) + \cos(k_2) + \cos(k_1 + k_2)] ,$$

n_1, n_2 are the components of x in the basis $(1, 0)$, $(-1/2, \sqrt{3}/2)$, and k_1, k_2 are those of k in the reciprocal basis $(1, 1/\sqrt{3})$, $(0, 2/\sqrt{3})$. Its asymptotic behaviour has been calculated analytically [14],

$$v_4''(x) \xrightarrow{|x| \to \infty} \frac{\sqrt{3}}{2} \frac{1}{8\pi} [\, |x|^2 \ln(|x| 2\sqrt{3}\, e^{\gamma - 1})$$

$$- \tfrac{1}{2} \ln(|x| 2\sqrt{3}\, e^{\gamma - 1/6})] , \qquad (4)$$

where $\gamma = 0.5772...$ is Euler's constant [#3].

From a study of the asymptotic behaviour of surface correlation functions on a 32×32 lattice, SSC [6] claimed evidence for two continuous transitions at $\beta_c^{(1)} = 1/(1.84 \pm 0.01) = 0.5435 \pm 0.0030$ and $\beta_c^2 = 1/(1.925 \pm 0.015) = 0.5195 \pm 0.0040$. In the dual defect interpretation (2), the first transition is caused by an unbinding of dislocations (which are pictured as tightly bound pairs of disclinations) destroying the translational order. The second transition is caused by an unbinding of disclinations destroying the orientational order. Calculating the specific heat via numerical differentiation of the internal energy, Strandburg, Solla and Chester (SSC) located a single, very sharp peak at $\beta_{pk} \approx 1/1.85 \approx 0.541$. The appearance of two continuous transitions contradicts our findings [9,10] according to which the model undergoes a single first-order transition. This conclusion was deduced in ref. [10] from a finite-size scaling analysis of the height of the specific heat peak, C_{max}, on 37×37, 44×44 and 58×58 triangular lattices, being consistent with the ansatz $C_{max} = aV + b$ ($V = L^2 =$ lattice volume). Indeed, the *location* of the very sharp peak of SSC is in reasonable agreement with our value on a 58×58 lattice, $\beta_{pk} \approx 0.536$ [10].

Strandburg's criticism [2] of our work [10] was based on the following arguments. While the specific heat peak of SSC [6] reaches a height of about 14

[#3] In the literature, the second subtraction is sometimes taken as $\frac{1}{2}(k \cdot x)^2$ instead of $\frac{1}{4} x^2 \bar{K}K$. This has the disadvantage that the asymptotic limit requires a numerical evaluation, the difference to (4) being

$$\tfrac{1}{4} x^2 \int_{-\pi}^{\pi} \frac{d^2k}{(2\pi)^2} \frac{k^2 - \bar{K}K}{(\bar{K}K)^2} .$$

Notice that the asymptotic behaviour of this potential has been given incorrectly in ref. [3], $\tilde{v}_4'' \sim |x|^2 \ln|x| + A|x|^2 - B$, i.e. the term $\sim \ln|x|$ has been missed. Unfortunately, this incorrect result has been used in all subsequent works by Strandburg et al. [2,6,7], with $B \approx 2.1$ determined numerically. Our subtraction in eq. (3) has the virtue that both $v_4''(0, 0) = 0$ and $v_4''(1, 0) = v_4''(0, 1) = v_4''(1, 1) = 0$, so that disclinations as well as dislocations have no explicit self-energy. The natural core-energy of the dislocations is then obtained purely from the long-range part of the interaction

$$-b_i(x)(\delta_{ij}\partial^2 - \partial_i \partial_j) v_4''(x) b_j(0)$$

$$\xrightarrow{|x| \to \infty} -\frac{\sqrt{3}}{2} \frac{1}{4\pi} b_i(x) [\delta_{ij} \ln(|x| 2\sqrt{3}\, e^{\gamma + 1/2})$$

$$- x_i x_j / x^2] b_j(0) .$$

It is therefore equal to $E_c = \frac{1}{2}\sqrt{3}(1/4\pi) \ln(2\sqrt{3}\, e^{\gamma + 1/2}) \approx 0.1599$. For more details, see ref. [15]. When using the $\frac{1}{2}(k \cdot x)^2$ subtraction, this result appears only after adding the non-zero self-energies.

on a 32×32 triangular lattice, we obtained a considerably lower peak height of only 8 on a 37×37 lattice [10]. Compared to SSC, we worked with somewhat larger temperature increments ($\Delta\beta=0.005$ corresponding to $\Delta T\approx0.017$ near the transition point $\beta\approx0.54$). This led Strandburg to suspect that we might have missed the true maximum of the specific heat. Later in fig. 3 we shall see that, on the contrary, their number 14 is exaggerated by statistical fluctuations. Let us recall that, since with increasing lattice size (44×44 and 58×58) we observed a considerable narrowing of the specific-heat peak, we also increased the temperature resolution. On our largest lattice with 58×58 sites we estimated a peak height of about 14 which, accidentally, agrees quite well with the SSC value for the 32×32 lattice. Whereas we interpreted this increase as a typical finite-size scaling signal near a first-order transition, Strandburg [2], taking this accidental agreement serious, speculated that the true height of the specific heat peak is almost independent of the lattice volume as would be necessary for a Kosterlitz–Thouless transition in the KTHNY scenario. In other words, Strandburg attributes the observed scaling of the peak height with the lattice volume solely to the progressive increase of temperature resolution.

It is the purpose of this note to present further evidence for our case, and against Strandburg's. First, we perform further simulations on smaller triangular lattices with carefully chosen temperature resolution and high statistics. In this way we expect to see the onset of the asymptotic scaling behaviour. Second, we reinvestigate the lattice sizes studied in ref. [10] with much higher statistics. Third, we study even larger lattices (66×66 and 72×72) in order to see more clearly the asymptotic scaling behaviour.

In the whole of this work we use periodic boundary conditions. The Monte Carlo program is fully vectorized using a 3×3 checker-board update which explains why the linear lengths L of our lattices are multiples of three. To update the configurations, we employ the standard Metropolis algorithm with trial values of $h(\boldsymbol{x})$ chosen randomly from one above or below the current value at each site. We measure local quantities like the internal energy (per site), $u\equiv\langle e\rangle\equiv\langle(1/V)E\rangle$, and the squared width of the interface

$$w\equiv\left\langle\frac{1}{V}\sum_{\boldsymbol{x}}[h(\boldsymbol{x})-h_{\mathrm{av}}]^2\right\rangle, \tag{5}$$

where $h_{\mathrm{av}}\equiv(1/V)\sum_{\boldsymbol{x}}h(\boldsymbol{x})$ is the average height of one configuration, and the angular brackets denote the usual thermal averages. The specific heat (per site) is calculated from the fluctuations of the energies, $C=\beta^2V(\langle e^2\rangle-\langle e\rangle^2)$.

The statistical errors of the energy and the squared width are estimated by dividing each run into blocks of 1000, 2000 and 5000 sweeps, calculating the block-average, and taking the variance of these partial energies. If the block-averages are uncorrelated (in "Monte Carlo time"), this error estimate does not depend on the block-size. For the two largest blocks this criterion was reasonably satisfied and is in accord with a direct estimate of the energy–energy "Monte Carlo time" correlation length. The errors of the specific heat are estimated similarly, but with a much larger block-size of 50000 sweeps. Since the average of specific heats within individual blocks is always smaller than the specific heat taken over the total run, we have rescaled our errors by this ratio.

The statistics of our samples is relatively large. It varies with lattice size, which is partly motivated by physical considerations and partly dictated by computer-time limitations. After discarding the first 1×10^5 sweeps for thermalization, on the smaller lattices (12×12–30×30) we used averages over 1.5×10^6–3.5×10^6 configurations, depending on the distance from the transition point. On the medium-sized lattices (36×36, 45×45, and 57×57) we worked with extremely high statistics (5×10^6, 10×10^6, and 12×10^6). Unfortunately, due to the computer-time limitations, on the large lattices (66×66 and 72×72), we could gather similar (and physically desirable) statistics (9×10^6) only for a few points. This is clearly reflected by the error bars. In all simulations, the averages of the large blocks were recorded on tape. This allowed us to check for equilibrium by discarding successively $(1, 1.5, 2, \ldots)\times10^5$ thermalization sweeps and taking averages over the rest of the run. Since even near the transition no systematic trends are detectable, we are convinced that our averages display true equilibrium behaviour.

3. Results

The resulting specific-heat (per site) curves are plotted in fig. 1a for various lattice sizes. We observe a pronounced scaling with lattice volume in both the peak height and the "full width at half maximum" (FWHM). From the form of the peaks (which are always rounded to a downward parabolic shape by finite-size effects) it is obvious, that we cannot possibly have missed the true maximum by a considerable amount as suspected by Strandburg [2]. The

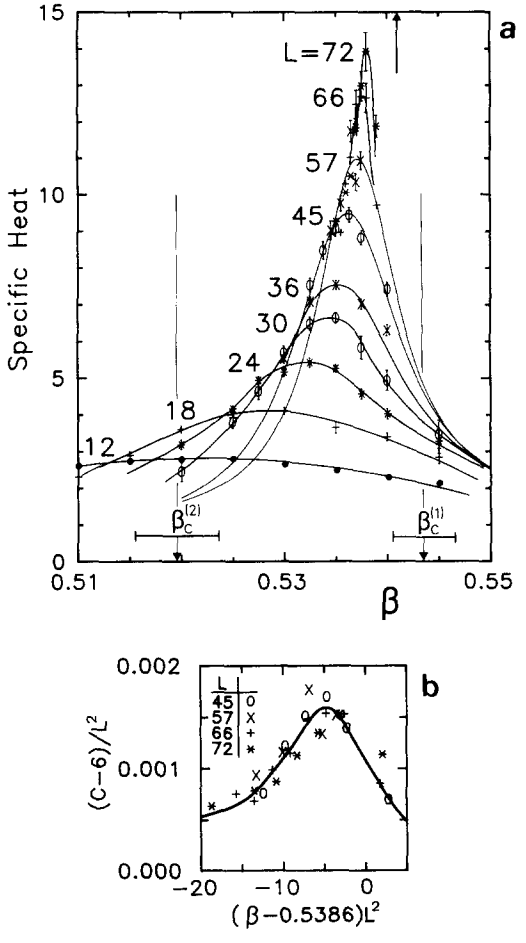

Fig. 1. (a) Finite-size scaling behaviour of the specific heat near the phase transition. $\beta_c^{(1)}$ and $\beta_c^{(2)}$ are the Kosterlitz–Thouless transition points quoted by SSC [6], and the arrow at the top line shows their estimate for the location of the peak maximum on a 32×32 lattice. (b) Finite-size scaling plot of the data shown in (a). We see that they are consistent with the hypothesis of a single first-order transition.

scaling behaviour of our data for the large lattices is seen more clearly in the finite-size scaling plot fig. 1b. It demonstrates that our data are consistent with a single first-order transition.

In fig. 2a we plot the maxima of the specific-heat peaks versus the lattice volume. (Fig. 2b will be discussed later.) We see again that the peak heights on the larger lattices scale with the lattice volume, as required for a first-order transition. Furthermore, for the smaller lattices, the expected corrections to asymptotic scaling are also clearly visible. Fig. 2c shows the location of the peak maxima, β_{pk}, versus inverse lattice volume. Using a linear extrapolation to infinite volume, we estimate for the transition point

$$\beta_{pk}^{\infty}=0.5385\pm0.001\,. \tag{6}$$

In the vicinity of a first-order transition, the system is expected to tunnel between two metastable phases of equal free energy. In a Monte Carlo simulation this is reflected by jumps of the internal energy, $\Delta u\neq0$. Assuming well separated, sharp jumps, the constant a in the ansatz $C_{max}=aV+b$ is easily identified as $a=(\Delta s/2)^2$ where $\Delta s=\beta_{pk}^{\infty}\Delta u$ is the transition entropy (per site), and b is found to be the average of the specific heats in each phase. With $a\approx0.0015$ read off from fig. 2a, we obtain

$$\Delta s\approx0.08 \tag{7}$$

in reasonable agreement with our former estimates [9] on the square lattice (measuring directly Δu).

It should be stressed that our specific heat data are deduced from the fluctuations of the energies. We believe that this method is much more reliable than the numerical differentiation of the internal energy, $C=\partial u/\partial T\approx\Delta u/\Delta T$, which was used in refs. [6–8]. In the latter method, systematic errors can in principle only be avoided by choosing small enough temperature increments $\Delta T=T_2-T_1$. This however, is traded with an increase in statistical error since although $\Delta u\equiv u_2-u_1\equiv u(T_2)-u(T_1)\to0$, the error $\delta(\Delta u)=\sqrt{(\delta u_1)^2+(\delta u_2)^2}$ remains constant. Notice that if ΔT is chosen too small, it is even possible to produce a negative specific heat! As an illustration, we compare in fig. 3 the specific heat on a 30×30 lattice derived from energy fluctuations, $C=\beta^2V(\langle e^2\rangle-\langle e\rangle^2)$, with the results of numerical

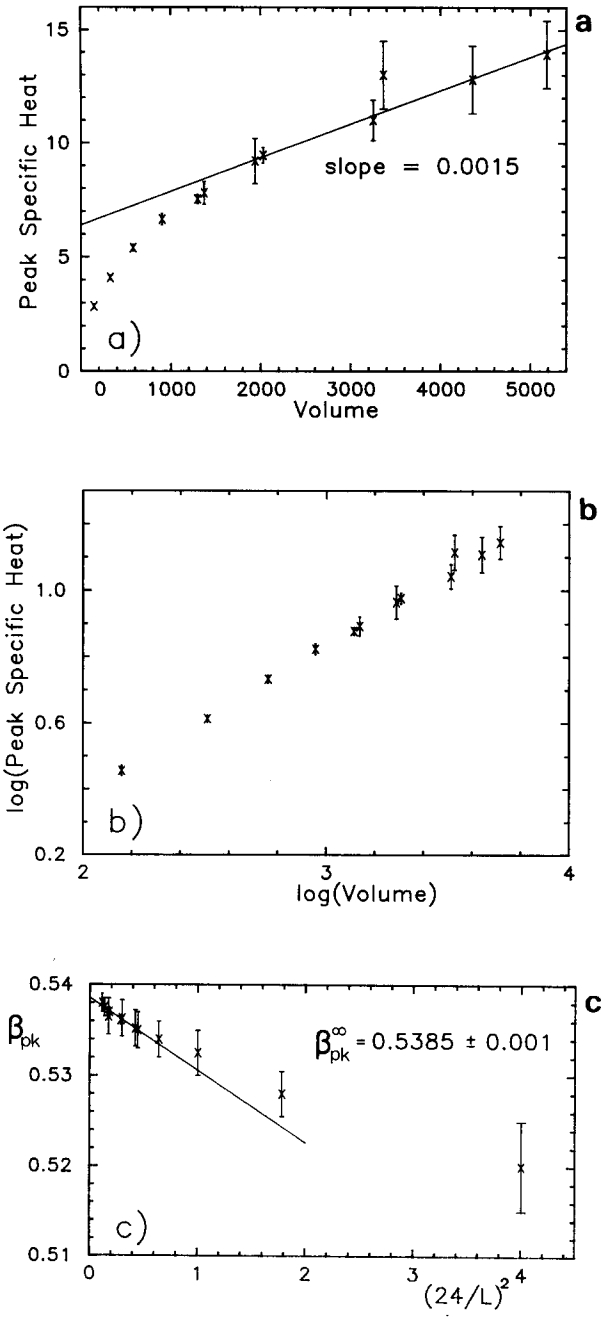

Fig. 2. Maxima of the specific heat (a) versus the lattice volume and (b) in a doubly logarithmic plot. The slope of the linear fit in (a), characteristic for a first-order transition, is related to the transition entropy (see eq. (7)). (c) Locations of the peaks versus the inverse volume. Using a linear extrapolation to infinite volume, we estimate $\beta_{pk}^{\infty} = 0.5385 \pm 0.001$. The data for the 37×37, 44×44 and 58×58 lattices are taken from ref. [10].

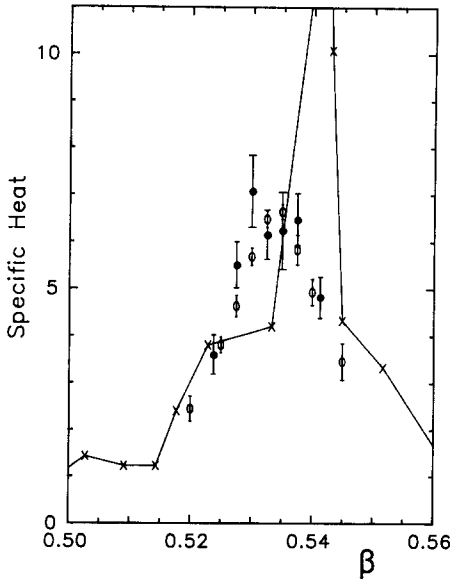

Fig. 3. Comparison of our new specific heat on a 30×30 lattice, calculated from energy fluctuations (○), with the data obtained in the same way as SSC, namely by numerical differentiations (●) of our energies, and with the curve given by SSC [6] (×) on a 32×32 lattice (no error bars are given in this reference). Notice the smallness of the error bars in the fluctuation method.

differentiations [#4] of the energies, $C \approx \Delta u/\Delta T \approx -\beta^2(\Delta u/\Delta\beta)$. We see that both methods are in rough agreement when applied to *our* data. The statistical errors, however, are much larger for the differentiation method. Obviously, our new precise data deviate significantly from the results of SSC for a 32×32 lattice (using numerical differentiation) shown as solid curve. Since no error bars are given for the SSC data, we can only speculate that they must be quite large in order to reconcile both simulations. In fact, it seems that SSC used very small temperature increments (down to $\Delta T = 0.0007$) which considerably blow up the statistical errors of their energies (which are averages over only 20000–50000 configurations).

Finally, in fig. 4, we show some typical surface configurations after 2.05×10^6 sweeps on a 30×30 lattice for temperatures (a) below, (b) very near and (c) above the peak of the specific heat.

[#4] In order to avoid unreasonably large error bars, we have not used the smallest possible distances in β, but the doubled stepwise $\Delta\beta = 0.005$ corresponding to $\Delta T \approx 0.017$.

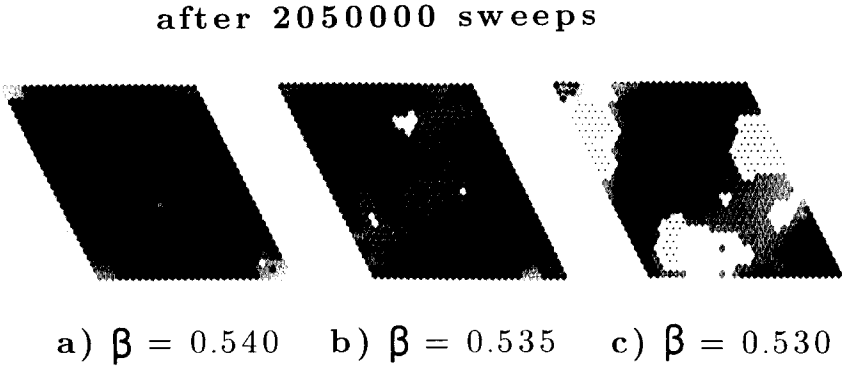

Fig. 4. Typical surface configurations after 2050000 sweeps on a 30×30 lattice for temperatures below (a), near (b) and above (c) the specific-heat peak, $\beta_{pk}\approx0.534$. The different shadings symbolize different surface heights separated by one unit. The black (white) patches with white (black) dots are the highest (lowest) regions.

4. Discussion

Our data show that the Laplacian roughening model on a triangular lattice has a single, very sharp specific-heat peak around $\beta_{pk}^{\infty}=0.5385\pm0.001$. It is located between the two inverse temperatures, $\beta_c^{(1)}$, $\beta_c^{(2)}$, claimed by SSC to be KT transitions. This result is very difficult to understand in the framework of the KTHNY theory. If there were two successive KT transitions, *both* should be accompanied by finite, broad peaks lying above their respective transitions in temperature. Such a behaviour is well-established for, e.g., the discrete Gaussian (DG) roughening model which shows a broad peak lying $\approx20\%$ above the transition temperature. It is true that the shape of the peak and its temperature displacement are non-universal and may be different from the DG model. In fact, this is nicely illustrated by the most recent simulation data of a more generalized defect model [1]. Still, it appears very unnatural that the first ("dislocation"-)transition is connected with a very sharp peak displaced only by $0.5435/0.537-1\triangleq1.2\%$ while the second ("disclination"-)transition seems to produce no peak at all. In fact, our simulations [1] of the generalized model show that a sharp peak can only appear in the regime where both transitions have merged together.

Our most compelling argument that the transition is weakly first-order rather than two successive KT transitions is based on the finite-size scaling analysis which is shown in fig. 1b: While the peak height *increases linearly* with the lattice volume, the width of the peak clearly *decreases*. We see no sign of peak height and width stabilization as required by the KT scenario. This observation is important in view of the interpretation of experimental data [13] which was influenced [12] quite substantially by the SSC claim for a Kosterlitz–Thouless transition with an unusually small width [11].

After the first version of this preprint was circulated, an objection was raised by Strandburg [16] that our present data admit also an excellent fit to a straight line in a doubly logarithmic plot over the entire range of L^2 with a slope ≈0.48, corresponding to $C\approx L$ (see fig. 2b). This might, in principle, suggest that the transition is of *an entirely different nature* not covered by either of the two available theories, with an amazing precocity of its limiting finite-size scaling behaviour. Certainly, our data do not allow us to outrule such an extra possibility. This weakness of our analysis, however, is intrinsic to Monte Carlo studies altogether. Indeed, similar arguments would disqualify many results on the order of phase transitions derived from finite-size scaling analyses, existing in the literature. To illustrate this, we have added such an analysis of the data for one of the best understood first-order transitions in two dimensions, the $q=8$ Potts model, for which rigorous results are available [17] (for a review see ref. [18]). Among the best numerical data for this model are the points of Ferrenberg and Swendsen [19]. We have replotted them here in fig. 5 on a doubly logarithmic scale. Without any theoretical bias, the most natural fit would, also here, be a straight line (with

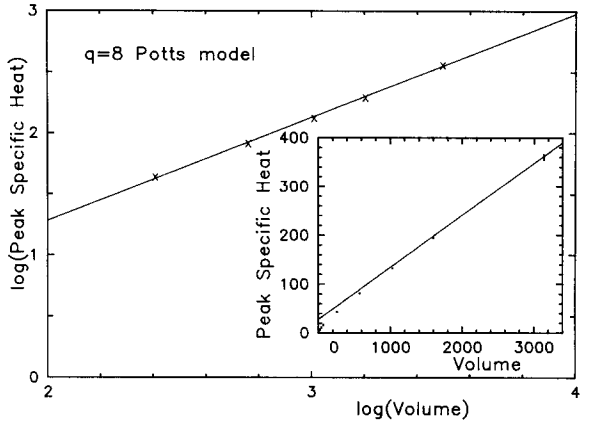

Fig. 5. Peak specific heat data of Ferrenberg and Swendsen [19] for the $q=8$ Potts model replotted on a doubly logarithmic scale. Also here a simple *linear* fit is *apparently* consistent. The insert shows the original plot used in ref. [19] to confirm the rigorously known first-order nature of the transition. The corrections to scaling are qualitatively similar to our fig. 2a.

slope ≈ 0.83). The original plot, on the other hand, used in ref. [19] to confirm the first-order nature of the transition (see the insert in fig. 5), looks qualitatively similar to our fig. 2a. Notice that since the transition entropy is somewhat larger in the $q=8$ Potts model ($\Delta s=0.652914$ [17], compared to $\Delta s \approx 0.1$ (eq. (7))), it is natural that the corrections to asymptotic scaling are smaller than in our case. We therefore believe that, taking into account these corrections, it is reasonable to interpret also our data in favor of a single first-order transition rather than two successive KT transitions.

Finally let us mention that at least for an artificially reduced core-energy in the model (2), also Strandburg [7] identified the transition as first-order. However, to use her data for localizing a splitting point in the transition line as a function of the core-energy seems to be quite dangerous. Her splitting shows unusual variations over her core-energy interval which are themselves of the order of the distance between the two transition lines at the crucial place corresponding to the pure Laplacian roughening model (her $E_c \approx 4.1$).

After this evidence, we believe that the splitting of the two-dimensional melting transition can only arise if the model is extended to incorporate also rotational stiffness with a length scale $l^2 \geqslant 0.2$, as reported recently [1]. We would be pleased if the evidence presented in this note would induce Hurlbut and Dash to return to the original interpretation [13] of their data.

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