LAPLACIAN ROUGHENING ON A TRIANGULAR LATTICE

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Monte Carlo simulation of the laplacian roughening model on a triangular lattice indicates that the model has a single first-order phase transition.

1. Introduction

The phase structure of the two-dimensional laplacian roughening model is of special interest because it is related by a duality transformation to a defect model of two-dimensional melting [1]. Inspired by the Kosterlitz–Thouless theory of the vortex induced superfluid transition, Halperin, Nelson and Young [2] (KTHNY) have argued that two-dimensional defect melting should take place through two successive Kosterlitz–Thouless transitions. In contrast to this, the work of Kleinert [3] suggests that due to the possibility of a pile up of neighboring dislocations, defect models of two-dimensional melting should have a single first-order transition. On square lattices, the first-order transition is supported by several analytic [4] and Monte Carlo studies [5,6]. However, in an earlier Monte Carlo simulation of this model on a triangular lattice Strandburg, Solla and Chester [7] (SSC) studied the large distance behavior of correlation functions and concluded that the model has two closely spaced continuous phase transitions of the Kosterlitz–Thouless type, as predicted by the KTHNY theory. According to this study, in the first transition (as temperature increases) the surface becomes rough and in the second transition the local orientation becomes disordered. However, a Monte Carlo study of the model on a square lattice by Janke and Kleinert (JK) found a single first-order transition, with clear evidence for metastable states [6]. In this study an equivalent model (using another duality transformation) involving a "periodic gaussian" form of strain was simulated [3]. This model in turn can be mapped very precisely onto a mixed cosine model

$$H = -\beta\sum\cos(\nabla_i u_j + \nabla_j u_i) - 2\beta\xi\sum\cos(\nabla_i u_i) - \gamma\sum\cos(2\nabla_i u_i) \quad (1)$$

along a particular path in the β–γ plane, and this mixed cosine model was also simulated. Here the additional parameter γ allows one to harden or soften the transition. Extrapolating the somewhat larger and therefore more reliable entropy jumps for $\gamma > 0$ to negative values of γ, both the pure cosine model ($\gamma = 0$) [5] and the "periodic gaussian" model ($\gamma \approx -0.4$) were found to undergo a single first-order transition with $\Delta s \approx 0.2$.

The results of SSC and JK are not necessarily contradictory – it is conceivable that the dif-

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ference in lattice structure changes the parameters of the long distance theory enough that the phase structure of the theory is changed. In order to clarify this situation we have undertaken a high statistics study of the thermodynamic properties of the model on larger triangular lattices. We find a single peak in the specific heat between the temperature quoted by SSC. The height of this peak increases with lattice size in a manner consistent with a first-order transition. Near the transition we see the system tunneling between two phases with distinct energies. The interface width and τ, a measure of local fluctuations in orientation, are both correlated with the jumps in the energy.

2. The simulation

We adopt the notational conventions of SSC. The surface height is denoted by $h(x)$, with h restricted to integral values. The hamiltonian is the square of the lattice laplacian

$$H = 8\beta \sum_x \left(h(x) - \tfrac{1}{6} \sum_{\hat{n}_j} h(x + \hat{n}_j) \right)^2 , \qquad (2)$$

where the $\hat{n}_j$ are the displacement vectors to the six nearest neighbors and $\beta = J/kT$.

We used 37 by 37, 44 by 44, and 58 by 58 lattices in this work. (SSC used a 32 by 32 lattice.) Skewed periodic (helical) boundary conditions were used, so that except for an overall modulus with respect to the volume the neighbors of a site can be found by adding single fixed integers to the index of the site being updated. Since we are using a vectorized updating, some care was required in programming the simulation. Fig. 1 shows the locations of the neighboring sites whose values are needed to update a single site. Clearly it is forbidden to update any other site in this neighborhood until the update of the central site has been completed. This can be accomplished by an appropriate choice of the stride, or distance between points being simultaneously updated. In particular, if the stride is seven and the x dimension of the lattice modulo 7 is equal to 2 (and the vector length is not so long that we go completely through the lattice before the first vector of updates is completed), all these constraints are satisfied. This is the solution we used, which explains our seemingly perverse choice of lattice sizes.

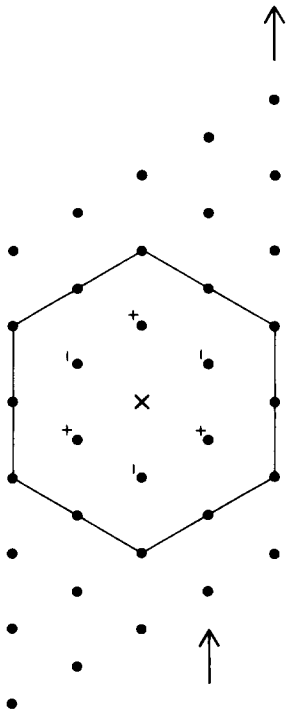
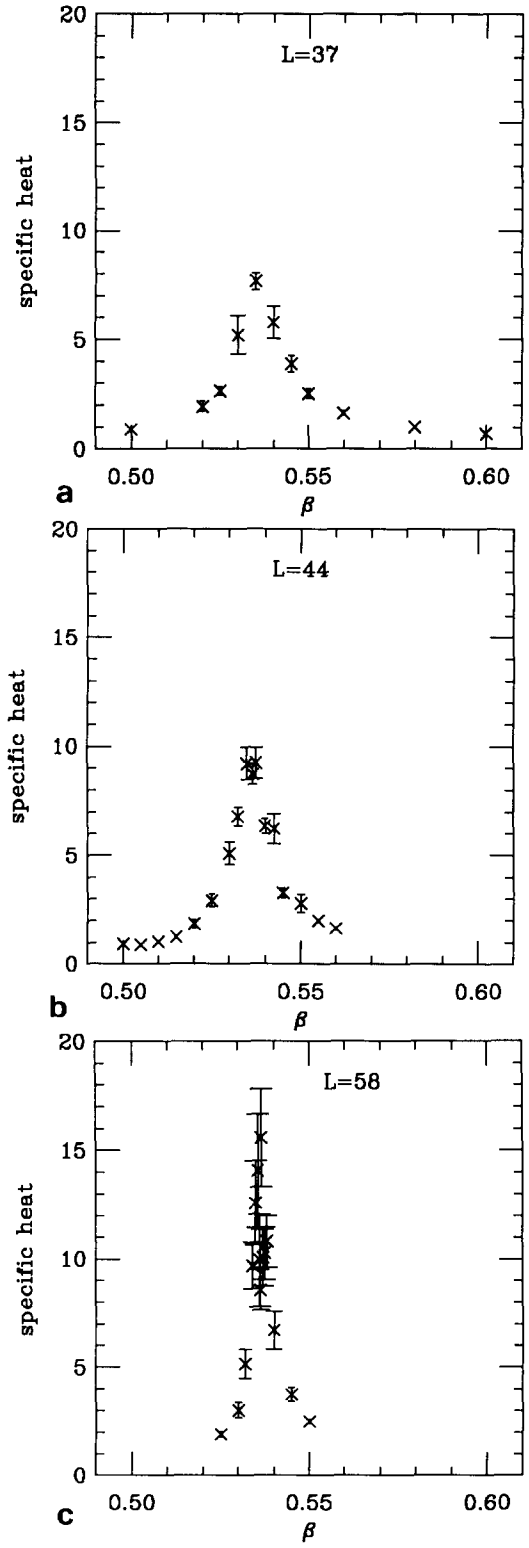


Fig. 1. The neighborhood of a point. Updating the central point requires knowledge of the values at all points in the hexagon. The arrows indicate the skewing of the boundary conditions. When you leave the lattice along the arrow on the right side, you reenter it along the arrow on the left side. The signs on the nearest neighbor points indicate the sign of the contribution to τ.

We used the standard Metropolis algorithm with trial values for $h(x)$ chosen randomly from one above or below the current value at each point. Our calculations were done on an ST100 array processor, and our programs were written in a specialized language for lattice simulations on this machine [8]. The time per update of a single site was 2.8 microseconds.

3. Results

In fig. 2 we plot the specific heat for the three sizes of lattices studied. For most of these points we used 500 000 Monte Carlo sweeps through the



lattice, after discarding 50000 sweeps for thermalization. The values of β quoted by SSC for the transitions are 0.519 and 0.543. It can be seen that on a 32 by 32 lattice these values would both fall inside the broadened peak in the specific heat. However, as the lattice size is increased the peak narrows and becomes higher.

The time histories of our simulations near the phase transition show transitions between two differing phases. In fig. 3 we show a time history of a run on a 58 by 58 lattice, omitting the first 50000 sweeps for thermalization. In addition to the energy we graph the squared width of the interface ω and the local fluctuation in orientation of the interface τ. These quantities are defined by [7]

$$\omega = \frac{1}{V}\sum_x [h(x) - \bar{h}]^2 \tag{3}$$

and

$$\tau = \frac{1}{V}\sum_x \left[\sum_{\hat{n}_j} (-1)^j h(x + \hat{n}_j)\right]^2, \tag{4}$$

where $h = V^{-1}\Sigma_x h(x)$ is the average height of a configuration and V is the lattice volume, or number of sites. The signs of the neighbors j are indicated in fig. 1. This time history includes a particularly dramatic excursion into the rough phase lasting about 100000 sweeps. Note the dramatic increase in the interface width and the concomitant increases in the energy and τ – there is an almost perfect correlation among these three observables.

The specific heat is proportional to the variance of the distribution of energies seen in the simulation. This variance is dominated by the jump in energy between the two phases, although there is a significant contribution from the variance within each phase. Therefore a reliable measurement of the specific heat from the variance of the energies, or from numerical differentiation of the energy, requires a simulation long enough to include a significant number of tunnelings, so that the fraction of time spent in each phase can be reasonably estimated. Because the tunneling time is very long,

Fig. 2. The specific heat near the phase transition. Results are shown for a 37 by 37 lattice (a), 44 by 44 (b), and 58 by 58 (c).

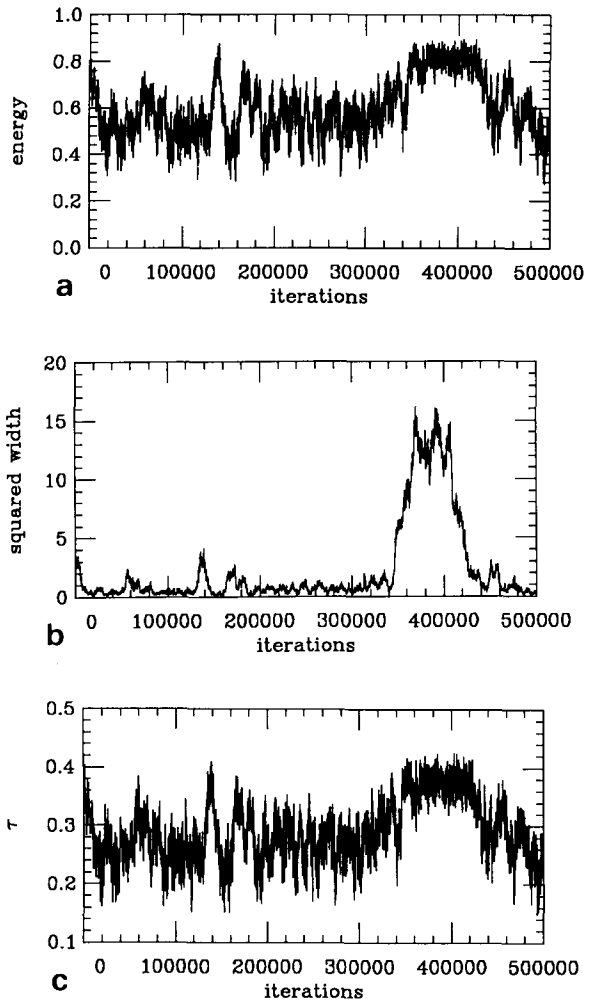


Fig. 3. The time history of a simulation near the phase transition ($\beta = 0.5365$). The quantities plotted versus the number of Monte Carlo sweeps are the energy (a), ω (b), and τ(c).

our specific heat measurements have rather large errors bars. These error bars were estimated by dividing the run into five to ten segments, measuring the specific heat in each segment, and taking the variance of these partial specific heats. However, the values quoted are obtained from averaging the energy and the squared energy over the entire run. This always produces a larger result than the specific heat within the individual blocks, so we have rescaled our error bars by this ratio.

In fig. 4 we show an estimate of the height of

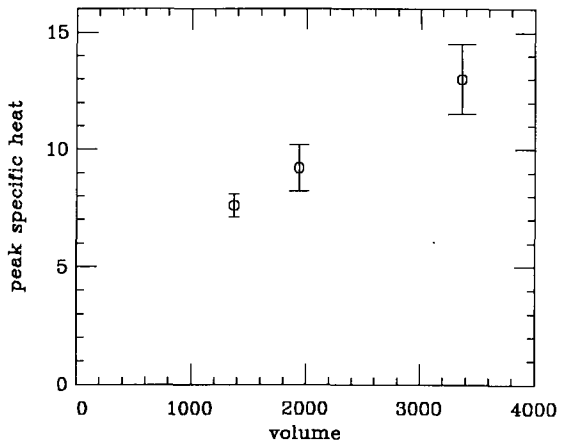


Fig. 4. The maximum specific heat versus the lattice volume.

the specific heat peak as a function of lattice volume. If the transition is first order, and simulations near the transition are well described by tunneling between two states of fixed average energy with a finite specific heat within each of the two phases, then we expect a specific heat

$$C = AV + B, \tag{4}$$

where V is the volume. Although the error bars are large, our result is consistent with this form. It is clearly inconsistent with a constant peak height, as one would expect for a transition of the Kosterlitz–Thouless type.

The scaling of the specific heat and the observed coexistence of metastable phases are strong evidence that the laplacian roughening model on the triangular lattice has a single first-order transition.

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