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Single tensionless transition in the Laplacian roughening model

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We report large scale Monte Carlo simulations of the equilibrium discrete Laplacian roughening (dLr) model, originally introduced as the simplest one accommodating the hexatic phase in two-dimensional melting. The dLr model is also relevant to surface roughening in molecular beam epitaxy (MBE). Our data suggest a single phase transition, possibly of the Kosterlitz-Thouless type, between a flat low-temperature phase and a rough, tensionless, high-temperature phase. Thus, earlier conclusions on the order of the phase transition and on the existence of a hexatic phase are seen as due to finite size effects, the phase diagram of the dLr model being similar to that of a continuum analog previously formulated in the context of surface growth by MBE.

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Two-dimensional (2D) melting has played a driving role in statistical physics for more than two decades. Efforts made at clarifying its nature [1] have aided to understand systems in which topological defects are relevant, from the equilibrium fluctuations of metallic surfaces [2] to superfluidity and superconductivity in thin films, and phase transitions in liquid crystals [3]. One of the most intriguing related notions is the hexatic phase, between a solid at low temperature (T) and an isotropic fluid at high T, transitions between phases being of the Kosterlitz-Thouless (KT) type. Such is the Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) mechanism for 2D melting [3]. Although controversial for some time, the hexatic phase has indeed been found in atomistic model systems [4] and in experiments [5].

A successful approach to systems with defect-mediated phase transitions as the above has been the use of duality to formulate equivalent height models. For example, the discrete Gaussian (dG) model [Eq. (1) below for bending rigidity parameter $\kappa=0$] is dual of the 2D Coulomb gas, and the roughening transition in the former corresponds [6] to the well-known KT phase transition of the latter, driven by the unbinding of vortex-antivortex pairs. With a similar philosophy, the discrete Laplacian roughening (dLr) model was introduced by Nelson [7] to describe the 2D melting. Its Hamiltonian is

$$\mathcal{H} = \frac{1}{2}\sum_{\mathbf{r}} \{\sigma[\nabla_d h(\mathbf{r})]^2 + \kappa[\nabla_d^2 h(\mathbf{r})]^2\}, \qquad (1)$$

where $\mathbf{r}$ denotes the position on a 2D lattice of lateral size L, ∇_d is a discrete gradient, and $h \in \mathbb{Z}$. The original dLr model [7] is obtained by setting to zero the surface tension parameter σ. Note, the dLr model is a *discrete* version of the *linear* approximation to Helfrich's energy functional for 2D membranes [8], and provides a simplified description of fluctuating *tensionless* surfaces, such as biological membranes [8], or, e.g., such as those grown under conditions typical in molecular beam epitaxy (MBE) [9].

For the dLr model, the KTHNY mechanism would imply [1] an intermediate hexatic phase in which the surface disorders in heights, but not in slopes (quasilong range orientational order). For low T, the surface would be in a flat phase, dual of the isotropic fluid in melting, while for high T the surface would disorder in heights and slopes, providing the dual of the solid phase. In terms of the surface structure factor $S(\mathbf{q})=\langle \hat{h}(\mathbf{q})\hat{h}(-\mathbf{q})\rangle$ [10], the rough high T phase implies the power law behavior as $S(\mathbf{q}) \sim q^{-4}$, changing to $S(\mathbf{q}) \sim q^{-2}$ in the hexatic phase [11], and to the existence of a finite correlation length in the flat low T phase. Equivalently, for the stationary height-difference $C(r)$ and slope-difference $C_d(r)$ correlations [12], these behaviors amount to: (i) rough phase $C(r) \sim r^2 \log r$, $C_d(r) \sim \log r$; (ii) hexatic phase $C(r) \sim \log r$, $C_d(r) \sim 1$; (iii) flat phase $C(r) \sim 1$, $C_d(r) \sim 1$. Results supporting this picture were obtained on small ($L \leqslant 32$) square and triangular lattices [13]. However, conflicting evidence for $L \leqslant 64$ was presented that the model had a *single first order* transition, see [14], and references therein. The discrepancy has remained unsolved, in spite of recent analytical studies [15]; elucidation of the phase diagram being important to the diverse contexts mentioned above.

Here, we provide new Monte Carlo (MC) simulations of the dLr model on the square and triangular lattices. Our results for sizes up to 512×512, much larger than those previously studied [13,14], allow us to see previous works as inconclusive due to finite size effects. The model seems to display a single continuous transition, possibly of the KT type, between the flat and the rough phases, there being no sign of a hexatic phase to within our numerical resolution in T. Notably, this provides an instance of a roughening transition in which the rough phase corresponds to a free *tensionless* surface, rather than a free surface with tension, as in the dG model. Moreover, the phase diagram of the dLr model is seen to resemble closely that of a *continuum model* proposed [9,15] for MBE growth, suggesting that both models are in the same universality class, much like the relationship between the dG and the continuum sine-Gordon models [16].

For our MC simulations we follow the same procedure as in [13], fluctuations being treated by the histogram method

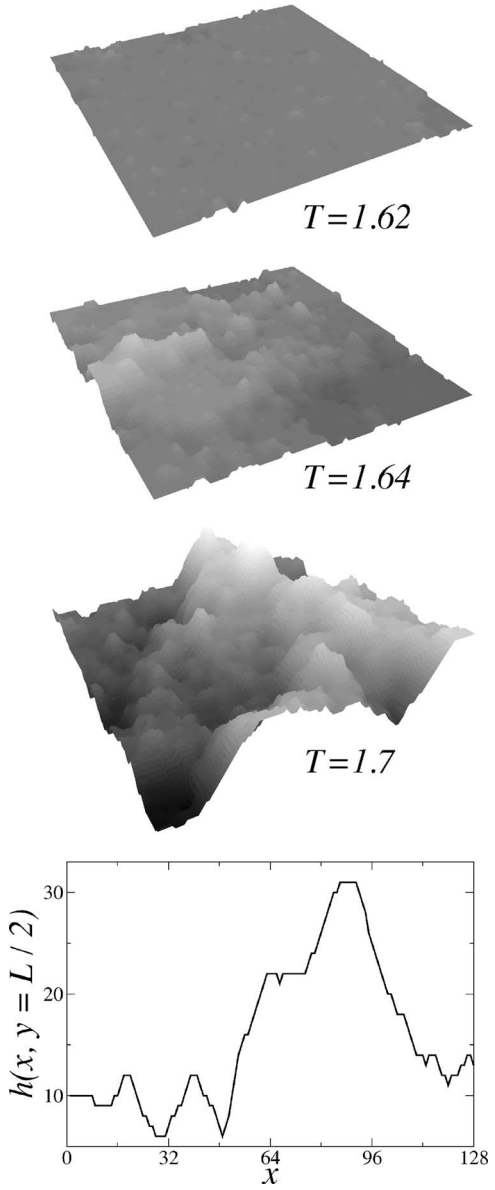

FIG. 1. Surface morphologies for three sample temperatures around T_c on the $L=128$ square lattice for Neumann (zero derivative) boundary conditions. Inset: Lateral cut of the surface for $T=1.7$. All units are arbitrary.

[17], further validated through additional simulations on different points of the extrapolated intervals. Thermalization has been checked by monitoring the behavior of nonlocal observables such as the specific heat and the structure factor at the smallest wave vector on our finite lattices, $S(q=2\pi/L)$, as functions of MC time. Note that the dLr model has a richer ground state structure than the dG model, Hamiltonian (1) with $\sigma=0$ being minimized not only by configurations with uniform heights, but also by configurations with uniform slopes (and by more complex morphologies, see below), see, e.g., the surface morphology made up of patches with various constant slopes shown in Fig. 1 for high T. In simulations, this requires large enough system sizes and appropriate boundary conditions so that the full minima structure can be significatively probed. In particular, for small

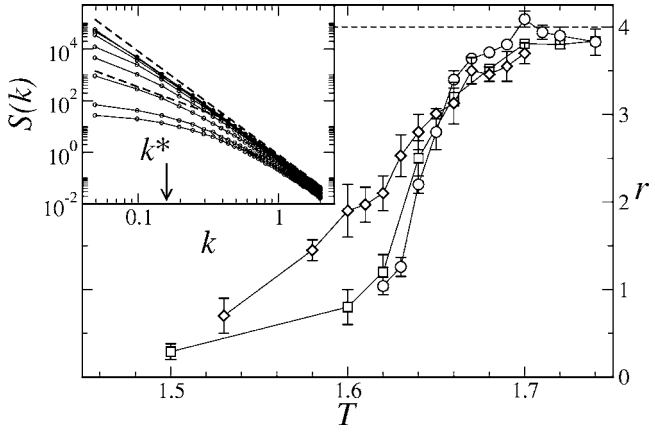

FIG. 2. Effective exponent r in the small wave-vector behavior $S(k)\sim k^{-r}$ [for $k\equiv 2\sin(q/2)<k^*(L)\simeq 3\pi/L$], as a function of T, for $L=32$ ($\diamond$), 64 ($\square$), and 128 ($\bigcirc$) for the square lattice. Inset: surface structure factor $S(k)$ on the $L=128$ square lattice vs k, for $T=1.62$ (bottom) up to $T=1.69$ (top). Dashed reference lines have slopes -2 (bottom) and -4 (top). All other lines are guides to the eye. All units are arbitrary.

sizes and periodic boundary conditions the system is effectively constrained to fluctuating around a single energy minimum (the morphology with zero slope), inducing apparent hystheretic behavior associated with a first order transition [14]. In our simulations, we have employed both periodic and free (Neumann) boundary conditions, and we have made sure that results provided are (qualitatively) independent of these.

As done for the dG model in [18], we study the phase transition through the behavior of the structure factor $S(q)$ for different temperatures. In order to test the KTNHY mechanism, we have studied the behavior of $S(q)$ as a function of T and L, by fitting the small wave-vector part of $S(q)$ to $S(q)\sim q^{-r}$. As seen in Fig. 2 for the square lattice (for the sake of clarity, we omit plots for the triangular lattice, in which completely analogous results are obtained), there is no evidence of a *finite* temperature interval *within* which $r\simeq 2$, that would be the signature of the hexatic phase. Rather, we find a *gradual* change from the flat phase behavior ($r\simeq 0$) to the rough phase one ($r\simeq 4$). This change becomes more abrupt when the system size is increased, so that only the flat and the rough phases remain well defined in the thermodynamic limit. These results may thus explain the apparent observation of a hexatic phase in [13] for small L values, where no systematic finite size effects were assessed. By defining the critical temperature T_c as the value at which curves for different system sizes cross [17], we estimate $T_c=1.65(1)$ for the square lattice and $T_c=1.90(2)$ for the triangular lattice.

Further evidence on the existence of a single phase transition is provided by the behavior of the specific heat $c(T,L)=(\langle\mathcal{H}^2_{\mathrm{dLr}}\rangle-\langle\mathcal{H}_{\mathrm{dLr}}\rangle^2)/(T^2L^2)$ as a function of temperature. Figure 3 shows $c(T)$ on the square and triangular lattices for the largest system sizes in our simulations. Within our statistics, a *single* peak at $T=T^*$ can be detected, rather than two as would be expected within the KTHNY scenario. The height and position of the peak are functions of lattice

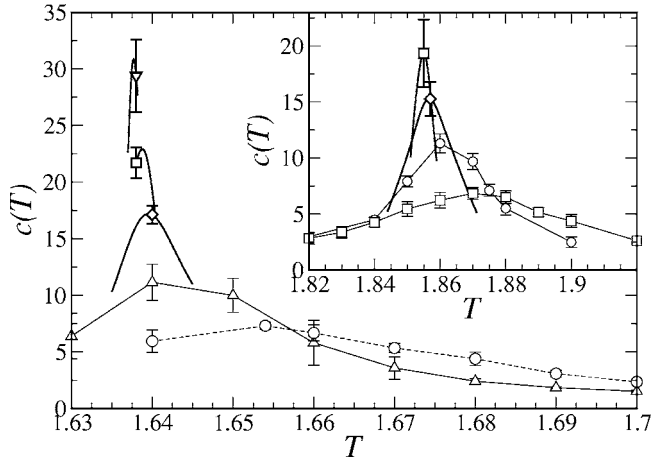

FIG. 3. $c(T)$ vs T on the square (main panel) and triangular (inset) lattices for $L=16$ (*), 32 (△), 64 (◯), 128 (◇), 256 (□), and 512 (▽). Bars are statistical errors and thin lines are guides to the eye. For the larger L values in each case, thick solid lines show the $c(T)$ curve extrapolated by the histogram method [17]. All units are arbitrary.

size L. Figure 4 (inset) provides the results of finite size analysis on the specific heat curves, in which the maximum value $c_{\max}(L)$ obtained for each lattice size is plotted as a function of L. Remarkably, although for lattice sizes $L \lesssim 70$ the specific heat grows approximately as $c_{\max} \lesssim L$—compatible with claims on the apparent weakly first order character of the transition for $L \leqslant 64$ [14]—for larger L values the increase of $c_{\max}(L)$ slows down. For our largest simulated systems, the best fit is logarithmic $c_{\max} \sim \log L$. Actually, for the 2D XY model the specific heat at the transition temperature is known [19] to first grow logarithmically with system size and then saturate for large enough values of L, suggesting that our result might reflect

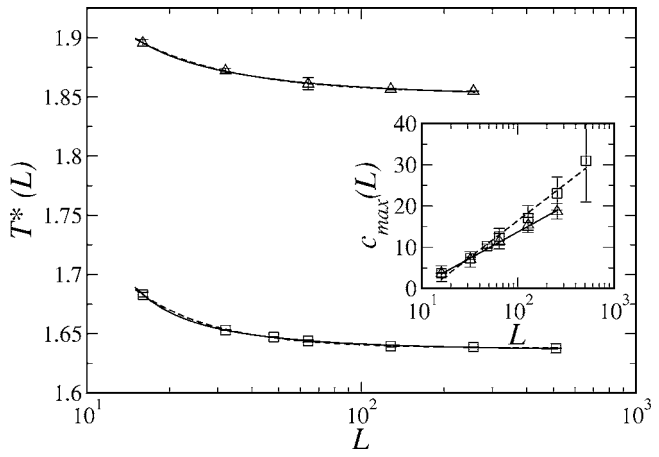

FIG. 4. Transition temperature T^* as obtained from Fig. 1, as a function of L for the square (□) and triangular (△) lattices. For each case, the dashed line is a power-law fit $T^*(L)-T^* \sim L^{-1/\nu}$, and the solid line is a fit to Eq. (2). $L=512$ is not employed for the fit due to low statistics. Inset: $c_{\max}(L)$ vs L on the square (□) and triangular (△) lattices. Lines are logarithmic fits to the data, shown for reference. All bars represent statistical errors and all units are arbitrary.

finite size effects. Indeed, saturation is expected provided that the correlation length at T^* is smaller than L and thus a horizontal plateau would occur at low k for $S(k)$, namely $r=0$ as defined in Fig. 2. The steady decrease of r at T^* for increasing L indicates that such a condition has not been reached. Persistence of logarithmic behavior in the $L \to \infty$ limit would rather suggest that the phase transition is in, e.g., the 2D Ising class [20]. In order to explore this possibility, in Fig. 4 we study the dependence of the specific heat jump position $T^*(L)$ with lateral size L. In a continuous transition, $T^*(L)$ scales as [20] $T^*(L)-T^* \sim L^{-1/\nu}(1+gL^{-\omega})$, where g is a numerical constant and ω is an exponent that accounts for corrections to scaling, and is in the range $7/4 \leqslant \omega \leqslant 2$ for the 2D Ising class [21]. The best multiparameter fit to such scaling forms yields $\nu=1.54(47)$ and $\nu=0.94(16)$ on the square and the triangular lattices, together with $\omega=1.6(3)$ and 2.2(2.0), respectively, to be compared with $\nu=1$ for the 2D Ising class [22]. Although these results might seem compatible with the 2D Ising universality for the present transition, we believe our numerical evidence favors more strongly a different interpretation. Thus, in marked contrast with a 2D Ising and as shown by Fig. 2, the transition in the dLr model is from a phase with finite correlation length to a continuous line of fixed points [in the renormalization group (RG) sense], characterized by an infinite value of the correlation length, as occurs in a KT transition [16]. In order to corroborate the latter interpretation, we can try a phenomenological KT-type form for $T^*(L)$, namely [20]

$$T^*(L) = T^* + \frac{a}{(\log L + b)^2}, \tag{2}$$

for constant a and b. As seen in Fig. 4, this fit is in very good agreement with the numerical data for large sizes. We must caution the reader on the well-known feature of the KT transition, that the peak of the specific heat does *not* occur at the critical temperature but, rather, at a temperature preceding T_c [19,20]. Although the size of this offset can be model dependent, Fig. 3 indeed provides estimates, $T^*=1.63(1)$ on the square lattice, and $T^*=1.85(1)$ on the triangular lattice, that are below the corresponding T_c values, *and are still inside the low T behavior for the spatial correlation functions*, see Fig. 2. Thus, the inexistence of an intermediate phase and the fact that the spatial correlations and the specific heat change behavior at different values of T can be hardly reconciled with a single transition of the Ising class.

Our results seem to replace the KTHNY scenario for the dLr model by a single, tensionless, KT-type phase transition. The absence of the hexatic phase may seem surprising when contrasted with the often accepted argument that, for increasing T, the surface should first disorder in heights and, then, in slopes. However, this is a *sufficient* condition for surface roughening, but it is not *necessary*. For instance, in the dG model slopes are not disordered at any temperature. It is also conceivable, as is our belief, that heights and slopes disorder *at the same temperature* in the dLr model. This remarkable result is also against the expectation that discreteness in surface heights renormalizes the surface tension σ, as it indeed does in the dG model [16]. For the dLr model, a generation

of a nonzero σ would imply that the asymptotic properties of the high T phase coincide with those of the dG model [11]. In order to explore this possibility, various analytical approaches [15] have been applied to the following *continuum* analog of the dLr model, introduced in the context of growth by MBE [9]:

$$\frac{\partial h}{\partial t} = -\kappa\nabla^4 h - \frac{2\pi V}{a_\perp}\sin\left(\frac{2\pi h}{a_\perp}\right) + \sqrt{2k_B T}\zeta, \qquad (3)$$

where ζ is a delta-correlated Gaussian white noise, and $a_\perp$, V, are parameters. Although a dynamical RG study for (3) does predict the generation of a nonzero surface tension, numerical simulations of this Langevin equation [9] give results in complete qualitative agreement with those of the dLr model presented here. The discrepancy between the RG arguments and the numerical results for both the discrete and continuum models might be due to inaccuracies in the treatment of model symmetries in the RG studies. Namely, the dLr model can be written as a model for the *surface slopes* $\mathbf{m} \equiv \nabla_d h$, i.e., $\mathcal{H}_{\mathrm{dLr}} = (\kappa/2)\Sigma_{\mathbf{r}}[\nabla_d \cdot \mathbf{m}(\mathbf{r})]^2$, with the implicit restriction that $\nabla_d \times \mathbf{m} \equiv \mathbf{0}$. Thus, the dLr model has larger symmetries than the dG model, the Hamiltonian being invariant under arbitrary global shifts in the heights, as in the latter, but also in the slopes. Thus the ground state degeneracy here is much larger, with minima occurring for all height configurations for which $\nabla_d \cdot \mathbf{m} = 0$. However, standard perturbative RG analyses [15,23] are oblivious to such an added complexity in the ground state structure of the model. Perhaps in a related fashion, the zero-vorticity constraint for the slope field may be playing a dynamical role in the unbinding of surface defects for $T = T_c$ in the 2D melting transition described by the dLr model.

Summarizing, our numerical study suggests that the dLr model features a single continuous phase transition. Although sizes of our simulations are confined to a regime in which the specific heat still grows logarithmically with L, rather than saturating as in proper KT scaling, the combined information from the spatial correlations and the specific heat are consistent with a KT transition. This behavior is remarkably similar to that of the continuum model (3), including the *tensionless* nature of the high T phase. Progress in the analytical description of these phenomena might improve our understanding of nonperturbative effects in defect-mediated transitions, and of dynamical effects of geometrical constraints (such as the curl-free condition above) in equilibrium systems.

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[10] Here, $\hat{h}(\mathbf{q})$ is the Fourier transform of $h(\mathbf{r}) - \bar{h}$, with $\bar{h}$ the mean surface height.
[11] The hexatic behavior $S(q) \sim 1/(\sigma q^2)$ is also the asymptotics of the free Gaussian model [20], and of the dG model in the high T phase, induced by surface tension.
[12] $C(r) = \langle[h(\mathbf{r}) - h(\mathbf{0})]^2\rangle$; $C_d(s) = \langle[\nabla_d h(\mathbf{s}) - \nabla_d h(\mathbf{0})]^2\rangle$.
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