Kosterlitz-Thouless-Berezinskii transition in the one-dimensional quantum roughening model

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We present numerical simulations of the one-dimensional quantum roughening model. We show that the system undergoes a zero-temperature phase transition of the Kosterlitz-Thouless-Berezinskii type. This transition leads to a superfluid state (nondissipative mass transfer). The mechanism responsible for this transition is very similar to that of the phase transition in two-dimensional smectic crystals.

I. INTRODUCTION

The idea of a phase transition between different phases of a crystal surface dates back to 30 years ago. The transition to a rough state has been extensively studied in terms of classical solid-on-solid models. These models define an integer valued variable at each lattice point of the interface that describes the number of atoms that occupy that particular point (i.e., the height of the interface). In the smooth phase the interface has a finite width and the fluctuations decay exponentially, while in the rough phase the correlations are unbound and the interface width grows with the dimensions of the system.

A number of years ago, Andreev and Parshin¹ pointed out that the surface of a quantum crystal may be rough at zero temperature due to quantum fluctuations. Later work of Fisher and Weeks² challenged this suggestion showing that quantum interfaces should be smooth at zero temperature; however they did not rule out the possibility of a phase transition at $T=0$. The quantum solid-on-solid (QSOS) model was firstly discussed by Fradkin in Ref. 3.

Single steps on the free surface of a quantum crystal can be described by the one-dimensional version of QSOS, the Hamiltonian in this case reads

$$H = \sum_i \left[\frac{U}{2} (n_{i+1} - n_i)^2 - Y \cos(\varphi_{i+1} - \varphi_i) \right], \quad (1)$$

where n is the discrete height variable which describes the distance of the step from some fixed reference, φ is the conjugate variable of n , and the subscript i refers to the position of the step. The first term in Eq. (1) represents the energy of a certain step configuration while the second is the kinetic energy associated with the quantum tunneling of atoms from one site to a nearest neighbor

(U and Y are the respective coupling energies). The model described by the Hamiltonian (1) possesses two different types of symmetries; the simultaneous shift of all the n 's and the global gauge symmetry associated with the phases φ_i . While the transition to a rough state is associated with the amplitude of the fluctuations of the height variables n_i , the system can undergo a transition to a superfluid state due to the breaking of the gauge symmetry (we will specify this point later). In this context, the superfluidity is related to the possibility of non-dissipative mass transfer.

The model defined in Eq. (1) was studied in Refs. 4 and 5; these authors mapped the $T=0$ problem onto a classical Coulomb gas model in $1+1$ dimensions. The charges of this gas interact via a very anisotropic potential which grows with the distance faster than the logarithm. From this observation they concluded that the charges are always bound in dipoles and therefore the system does not undergo any phase transition at the absolute zero (it is always in the disordered, not superfluid, phase).

Very recently Korshunov⁶ reanalyzed the phase diagram pointing out the very important role of the charge-anticharge pairs of small separation. These dipoles renormalize the interaction between the pairs of larger dimensions in an analogous way as the renormalization of the interaction of disclinations by free dislocations in two-dimensional smectic crystals.⁷ The resultant screened potential is logarithmic, therefore at a certain strength of the coupling constant the dipoles dissociate and the KTB transition takes place.

In this work we present a Monte Carlo simulation of the one-dimensional quantum roughening problem defined above and we will show that a phase transition occurs when the ratio U/Y is of the order of one. As it is well known the $T=0$ quantum problem can be translated in a corresponding classical model in $1+1$ dimension; for

the case we are interested in, various representations can be obtained by the standard duality transformations.

The paper will be organized as follows: in the next section we will briefly review the mapping among the various representations on the one-dimensional quantum roughening problem both for the Hamiltonian and the correlation functions. The duality mapping, leading to the Coulomb gas and solid-on-solid (SOS) pictures, is very well established (see, for instance, Ref. 8 and 9, in general, and 4 and 5 for the case we are considering), however we think it is very useful to focus on the main points in order to better describe the outcomes of our simulations in comparison with the results of Korshunov. Then we will present the results of the simulations and finally the conclusions.

II. THE VILLAIN TRANSFORMATION

In order to get the Coulomb gas and roughening pictures in the space time, we start from the Villain approximation of the Hamiltonian defined in Eq. (1) which consists of substituting

$$\exp[\lambda \cos(u)] \rightarrow \sum_{m=-\infty}^{\infty} \exp\left[-\frac{1}{2\lambda} m^2 - imu\right]$$

for each bond on the space time. The partition function therefore reads

$$Z_V = \text{Tr} \exp \left[- \sum_{i\tau} \left[\frac{\epsilon U}{2} (\nabla_x n_{i,\tau})^2 + \frac{1}{2\epsilon Y} m_{i,\tau}^2 + i (\nabla_\tau n_{i,\tau} + \nabla_x m_{i,\tau}) \varphi_{i,\tau} \right] \right], \quad (2)$$

where the trace is defined $\text{Tr} \equiv \sum_{\{n\}} \sum_{\{m\}} \int_0^{2\pi} \prod_{i\tau} d\varphi_{i,\tau}$ and ∇ is the lattice derivative. The time slices are spaced by the quantity ϵ and the number of sites in the time direction is given by $\beta = N_\tau \epsilon$. The phase can be integrated out and as a result of this a δ function is produced at each lattice point

$$\nabla_\tau n_{i,\tau} + \nabla_x m_{i,\tau} = 0.$$

The constraint can be solved by introducing an integer valued scalar field $h_{i,\tau}$ such that

$$n_{i,\tau} = \nabla_x h_{i,\tau}, \quad m_{i,\tau} = -\nabla_\tau h_{i,\tau}. \quad (3)$$

By substituting Eq. (3) and performing the standard rescaling in the time direction (see, for instance, Ref. 4), it is possible to express the partition function as a classical roughening problem in 1+1 dimensions.

$$Z_V = \sum_{\{h\}} \exp \left[-J \sum_{i,\tau} [(\nabla_x^2 h_{i,\tau})^2 + (\nabla_\tau h_{i,\tau})^2] \right], \quad (4)$$

where

$$J = \frac{1}{2} \sqrt{U/Y}. \quad (5)$$

The model defined by the effective action (4) is a type of generalized SOS model (GSOS); it has a very strong anisotropy in the space time. We stress at this point that the GSOS model cannot be reduced to an XY model in 1+1 dimensions; due to the second-order lattice derivative in the space direction each lattice site is connected to both nearest neighbors along the chain and the derivation discussed by Knops⁹ cannot be applied.

All the simulations which we carried on were performed using the GSOS model defined by Eq. (4); as already stressed in the Introduction, the most transparent physical picture of the transition is given in the Coulomb gas language so it is useful to establish the connection between these two different representations. The method

discussed by Chui and Weeks allows us to map the problem onto a generalized Coulomb gas model in 1+1 dimensions; by means of the Poisson resummation formula

$$\sum_{h=-\infty}^{\infty} f(h) = \int_{-\infty}^{\infty} dh f(h) e^{2\pi i p h}$$

it is possible to integrate out the h field and the resulting Hamiltonian reads

$$H = -\pi^2 J^{-1} \sum_{i,i',\tau,\tau'} p_{i,\tau} G(i-i', \tau-\tau') p_{i',\tau'}. \quad (6)$$

$p_{i,\tau}$ are the charges of the Coulomb gas and are related to the topological excitations (in the space time) of the original phase field defined in Eq. (1). By means of the last duality transformation the strong and weak coupling limits of the two representations (4) and (6) are reversed. The interaction potential for the Coulomb charges is

$$G(i,\tau) = \frac{1}{N_x N_\tau} \sum_{k,\omega} \frac{1 - \cos(kx_i + \omega\tau)}{4(1 - \cos k)^2 - 2(1 - \cos \omega)}. \quad (7)$$

The summation is extended to the first Brillouin zone. As usual the subtraction of the zero momentum and frequency contributions is related to the overall neutrality condition for the $p_{i,\tau}$ charges. The interaction potential defined in Eq. (5) is very anisotropic; it increases faster than a logarithm in both directions

$$G(i,\tau) \propto \begin{cases} i & i \gg 1; \tau = 0, \\ \sqrt{\tau} & \tau \gg 1; i = 0. \end{cases} \quad (8)$$

This observation could induce one to conclude that no phase transition of the KTB type can be present in such a system. The charge-anticharge pairs will be always tightly bound in the whole phase diagram; in terms of the roughening model defined in Eq. (4) this means that the interface (in the space time) should be rough. It is, however, well known that the pairs will feel a screening effect

due to dipoles of smaller separation; as a result the interaction will be renormalized. This effect has been included in a low fugacity expansion in Ref. 6 where it was shown that the first-order correction in the concentration of dipoles leads to an effective interaction between vortices of the type $G_{\text{eff}}(i, \tau) \approx \ln(i^2 + \tau^2)$, the effective coupling constant depending on the fugacity. In this way a transition takes place in the system at a certain critical value of J which should be determined self-consistently.

Similar duality transformations can be performed also for the correlation functions. Of particular relevance is the height-height correlations function of the model (4)

$$g_{hh}(i, \tau) = \langle [h_{i, \tau} - h_{0,0}]^2 \rangle = -Z_V^{-1} \frac{\partial^2}{\partial a^2} Z_V[S, a] \big|_{a=0}, \quad (9)$$

where the generating functional is defined as

$$Z_V[S, a] = \sum_{\{h\}} \exp \left[-J \sum_{1, \sigma} [(\nabla_x^2 h_{1, \sigma})^2 + (\nabla_\tau h_{1, \sigma})^2 + ia S_{1, \sigma} h_{1, \sigma}] \right] \quad (10)$$

and

$$S_{1, \sigma} = \delta_{(i, j), (1, \sigma)} - \delta_{(0, 0), (1, \sigma)}.$$

In the Coulomb gas language this correlator is related to the effective interaction potential between the charges, in the Fourier space

$$g_{hh}(k, \omega) = J^{-1} G(k, \omega) [1 - 2\pi^2 J^{-1} G(k, \omega) \langle p(k, \omega) p(-k, -\omega) \rangle_{\text{CG}}], \quad (11)$$

where the subscript CG means that the average is performed over the Coulomb gas partition function. The expression in brackets in the right-hand side (rhs) of Eq. (11) is related to the dielectric function $\epsilon(k, \omega)$ of the Coulomb gas, therefore the renormalization effect, which is responsible for the transition, will show up in the asymptotic form of the height-height correlation function. In the weak coupling region ($J < 1$) the interface will be (surely) rough; $g(i, \tau)$ will then increase with the distance (in the space time). If the renormalization effect were absent we should expect a behavior like in Eq. (8) and moreover the interface being rough at all values of the coupling constant J . Moreover near the transition region the height-height correlation should be “fairly isotropic” despite the strong anisotropic bare interaction [see Eq. (8)] and will increase as a logarithm. We stress once more that from now on when we talk about rough interface we refer to the rough phase of the classical GSOS model in 1+1 dimensions.

III. THE SIMULATIONS

We performed the Monte Carlo simulations using the standard Metropolis algorithm using the effective classical roughening model in (1+1) dimensions defined in Eq. (2). The averages were done over 2×10^6 configurations; the first 10^4 were used for thermalization. Starting from the strong coupling limit ($J \gg 1$) the initial configuration was chosen with all the integer variables $h_{i, \tau}$ equal to zero. Independent runs were done heating and cooling the system and no hysteresis was detected. In all the samples considered periodic-boundary conditions were applied both in space and time directions. The boundary condition in time direction comes directly from the definition of the partition function. We proceed in an analogous way of simulations performed on other types of roughening models in two dimensions.^{10–12} First of all we present the results for the energy per site and the specific heat of the system; the specific heat per site is cal-

culated from the fluctuation dissipation theorem and is defined as

$$C_V / N^2 = (\langle E^2 \rangle - \langle E \rangle^2) / N^2, \quad (12)$$

where $N^2 = N_x N_\tau$ (in the cases we consider $N_x = N_\tau = N$) is the total number of sites in the space-time lattice. In Fig. 1 it is shown the energy per site; it is weakly independent on the lattice size up to systems large as 32×32 (in units of the lattice spacing). This is typical of the KTB transition. In the same way the specific heat calculated from (12) develops a maximum when the coupling constant is of the order of one; the height of the maximum is nearly independent on the lattice size; we checked the scaling behavior of the peak and we observed

FIG. 1. The energy per site of the system is plotted against the effective coupling constant J for various lattice size (10×10 , 16×16 , and 32×32); it is practically independent on the lattice dimensions and its behavior is typical for the KTB transition. The change in the slope is related to the peak of the specific heat.

FIG. 2. It is shown the specific heat per site vs the coupling constant J as obtained from the fluctuation dissipation theorem.

a saturation for lattices larger than 32×32 up to 56×56 (similar results can be obtained taking the derivative of the energy in Fig. 1). As it is well known the peak of c_v does not coincide with the transition point; it is simply related to the increase of entropy after all the charges (in the Coulomb gas language) had dissociated. Although it is not related to any critical property, it furnishes a useful upper bound for the location of the transition point (Fig. 2).

A better understanding of the properties of the transition comes from the analysis of the height-height correlation function which we defined above. For the correlation functions we were mostly concerned with a 32×32 lattice. In Figs. 3 and 4 we show our results for the correlator along the x and τ directions respectively. The curves are calculated for different values of J ; starting from the lowest at $(1/J)=1.4$ up to $(1/J)=1.9$. In the strong coupling regime $g_{hh}(i, \tau)$ should saturate approaching a finite value; this means that the screening length is finite; correspondingly in the dual Coulomb gas model the charges are in the plasma phase. The error

FIG. 3. It is shown the height-height correlation function in the x direction for different values of J ; starting from the lowest curve, the values of J^{-1} are 1.4, 1.5, 1.55, 1.60, 1.65, 1.7, 1.8, and 1.9.

FIG. 4. The same as in Fig. 3 but along the τ direction.

bars are of the same order of the size of the symbols. As discussed extensively in the paper of Saito and Müller-Krumbhaar,¹³ in order to minimize the rounding effect due to the periodic-boundary conditions and to show the divergence of the correlator in the massless phase it is useful to plot $g_{hh}(i, \tau)$ against the two-dimensional lattice Green's function

$$V_{2D}(i, \tau) = \frac{1}{4N^2} \sum_{k, \omega} \frac{1 - \cos(kx_i + \omega\tau)}{2 - \cos k - \cos \omega}. \quad (13)$$

$V_{2D}(i, \tau)$ is proportional to $\ln(i^2 + \tau^2)$ for a certain range of the distance (in the space time) between the charges but when the distance becomes comparable to half of the size of the sample, V_{2D} takes correctly into account the effects of the periodic-boundary conditions. Figures 5 and 6 show how the correlator scales with the 2D logarithmic Green's function in both the directions. The values of the coupling constants at which the correlation

FIG. 5. The height-height correlation functions along the x direction is plotted against the two-dimensional lattice Green's function defined in Eq. (13). The curves are parameterized by the same values of J as in the Figs. 3 and 4. Above the curve at $J^{-1}=1.7$ no saturation effect is observed and the correlator diverges as $V_{2D}(i, 0)$ while far in the rough phase it diverges stronger.

FIG. 6. The same as in Fig. 5 but along the τ direction. The curves are parametrized by the same values of the coupling constant J as in the previous figures. The behavior of the height-height correlation function is logarithmic in the critical region; far in the rough phase it diverges stronger but it is smaller in magnitude than the correspondent curve in the x direction.

function are calculated are the same as those considered in Figs. 3 and 4. As a general feature concerning Figs. 5 and 6 we can state that at a critical value

$$J_{\text{cr}} \approx 0.6 \quad (14)$$

the KTB phase transition takes place. In both the plotted correlators the correlation function saturate in the strong coupling regime while above the critical value is unbounded. In the critical region the renormalization effect discussed in Ref. 6 is evident; the height correlation diverges logarithmically. Far in the weak coupling regime g_{hh} diverges more rapidly and eventually will behave as the interaction defined in Eq. (7).

In the next plot we present Fig. 7, a comparison of the height-height correlation function along the space and time directions. This is done in order to check the effective isotropy of the interaction because of the screening effect of small distance pairs. The values of the coupling that we consider are that near the phase transition. Despite the strong anisotropy the correlations, in practice, overlap in both directions below and in the critical region. For higher values of J^{-1} g_{hh} starts diverging stronger along the space direction as can be guessed from the bare interaction. Again in the Coulomb gas language this effect can be explained more easily; in this range of coupling constants the density of pairs is very low (their activity is proportional to $\exp\{-cJ\}$ with c a numerical factor) so that the screening of the interaction is less effective and the anisotropy of the bare interaction can appear. Of course we cannot rule out that the anisotropy just above the transition can also be simply related to the finite size of the system, in this case the small distance pairs which contribute to the renormalization of the interaction feel the very anisotropic interaction so that the overall effective interaction in the “real” case can be more complicated than a logarithmic. At the transition the scale invariance related to the algebraic quasi-long-

FIG. 7. In this figure we show the correlation function on both axes against the 2D Green function for $J^{-1} = 1.55, 1.6, 1.65$, and 1.7 ; the correlators in the τ direction are indicated with the crosses while in the space direction with squares. We see that the correlators (although the original model is highly anisotropic) overlap up to the critical region. For higher values the correlator in the x direction increases faster than that in the τ direction.

range order is preserved also in the time correlations. Therefore these discrepancies that we detect in the simulation can be related to the noncritical feature that are not (of course) included in the treatment of Korshunov. The distinction between a massless (algebraic quasi-long-range order) and a massive (finite screening length) phase is nevertheless neat.

On the contrary if one studies, in the critical region, the height-height correlation function against the $G(i, \tau)$, that is the bare interaction potential between the Coulomb charges, one does observe a saturation indicating that the correlation does not follow what the weak coupling expansion for the height-height correlation function would give

FIG. 8. The correlator g_{hh} in the space direction is plotted against the 2D lattice Green function for a system of 56×56 . The curves are calculated at values of J^{-1} of $1.5, 1.6, 1.7$, and 1.8 .

FIG. 9. The same as in Fig. 9 but for the time direction.

$$g_{wc}(i, \tau) = \frac{1}{J} \frac{1}{N_x N_\tau} \sum_{k, \omega} G(k, \omega) \{1 - \exp[i(kx_i + \omega\tau)]\}. \quad (15)$$

Up until now all the results that we discussed were exclusively for a lattice of 32×32 . In order to support, we believe, the previous analysis, we present the same plot as in Figs. 3 and 4 but for a system of 56×56 . The behavior is the one expected; both in the space (Fig. 8) and in time (Fig. 9) directions the correlation function diverge logarithmically in the critical region and more rapidly for smaller values of the coupling constant J . In both figures the curve at $J^{-1} = 1.7$ is in the critical region (in the time direction the divergence is a bit stronger). A more detailed analysis for this large array seems to be in order to pin the value of the critical point. However we believe that these results for the large array together with the more detailed analysis for the 32×32 system is sufficiently convincing to ascertain the existence of a phase transition in the quantum roughening model

FIG. 10. The quantity r_{asym} defined in the text is plotted vs the coupling constant for the space (solid line) and time (dashed line) directions. The increase of r_{asym} is a signal of the roughening transition.

defined by the Hamiltonian of Eq. (1).

In principle the transition point should be determined by finding the coupling constant at which the correlation function starts to diverge (which of course is not possible for a finite sample). A good evidence for the occurrence of the roughening transition is to study, as in Fig. 10, the dependence on the coupling constant of the scale at which the g_{hh} saturate (we follow the notation of Ref. 11). As in Ref. 12 we defined r_{asym} as the smallest site for which the correlator is within 1% of its value at the 12th site for the 32×32 and at the 21st for the 56×56 lattices. Although we cannot get rid of finite-size effects the parameter defined above is essentially a measure of the correlation length. The rapid increase of r_{asym} is a signal of the roughening transition; in Fig. 10 the curves refer to the space (solid line) and the time (dashed line) direction. The results seem to confirm the existence of the transition around the above-mentioned critical value.

IV. CONCLUSIONS

In this work we presented our numerical simulations of the one-dimensional quantum roughening model. The Monte Carlo simulations were performed on the equivalent representations in the $1+1$ space-time defined in Eq. (4). The simulations aimed to the calculation of the energy, of the specific heat, and of the relevant correlation functions. We showed that the system undergoes a $T=0$ phase transition of the KTB type when the ratio J is varied. In terms of the roughening model in the space time, the system's interface is smooth (the height-height correlation function is bounded) up to $J^{-1} \approx 1.7$; above this value there is a transition to a rough phase (and the height-height correlation function is unbounded). In the transition region the correlator diverges as the logarithm of the distance between the sites (both in space and in time). Going far in the rough phase the correlator becomes more anisotropic (see Fig. 7). We remind that g_{hh} is related to the screened interaction potential in the Coulomb gas representation. Korshunov has extensively discussed the mechanism responsible for the transition. A *charge* in the Coulomb gas description is related to the occurrence of phase slips in the roughening model. These *charges* interact via the highly anisotropic potential defined in Eq. (7). The small distance dipoles present in the system screen the interaction so that it becomes effectively logarithmic and, as a consequence, a KTB transition takes place. The Monte Carlo simulations performed in this paper confirm this picture showing the corresponding phase transition from a rough to a smooth phase.

By means of the same duality transformations that were described in the preceding sections, it is possible to relate the correlator to the phase-phase correlation functions both in the space and in the imaginary time direction. As discussed in Refs. 3, 4 and 6, the mobility of the steps can be expressed in terms of the g_{hh} or in terms of the *charge-charge* correlation in the Coulomb gas language. Therefore a calculation of g_{hh} directly relates to the frequency and wave-vector dependence of the mobility; in terms of the original quantum roughening model

the results obtained in this work can be stated as follows. When the hopping strength is increased above a certain value, the linear friction (see Ref. 6) vanishes in the superfluid state while at finite temperature, although non zero, it is exponentially small. The superfluid phase corresponds to values of J larger than the critical value where the calculated g_{hh} is bounded (both in space and in time).

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