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Monte Carlo simulation of the 1D-Quantum Roughening Model - evidence of a KTB transition -

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Abstract. In this contribution we describe the results of a Monte Carlo simulation on the 1D Quantum Roughening Model (QSOS). We show that the model has a phase transition of the Kosterlitz-Thouless-Berezinskii type.

Introduction

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:

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

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 system can undergo a transition to a superfluid state due to the breaking of the gauge symmetry. In this contest the superfluidity is related to the possibility of non dissipative mass transfer.

Very recently Korshunov [1] studied the model defined in eq.(1) in the equivalent Coulomb gas representation in 1+1 dimension and showed the very important role of the *charge-anticharge* pairs of small separation. These dipoles renormalize the interaction between the pairs of larger dimensions and the resultant screened potential is logarithmic, therefore at a certain strength of the coupling constant the dipoles dissociate and the KTB transition takes place.

The Monte Carlo simulation

We performed the Monte Carlo simulations using the standard Metropolis algorithm using the effective classical roughening model in the space-time which can be obtained by standard duality mapping [2] from (1) and which is defined:

$$H = J \sum_{i,\tau} [(\nabla_x^2 h_{i,\tau})^2 + (\nabla_\tau h_{i,\tau})^2)] \qquad (2)$$

where h is integer valued and $J = (U/2Y)^{1/2}$. The averages were done over 2×10^6 configurations; the first 10^4 were used for thermalization. Starting form the strong coupling limit ($J \gg 1$) the initial

configuration was chosen with all the integer variables equal to zero. In all the samples considered periodic boundary conditions were applied both in space and time directions. In fig.1 we show the outcomes for the height-height correlation function $\langle [h_{i,\tau} - h_{0,0}]^2 \rangle$ (a more detailed analysis will be given elsewhere [3]).

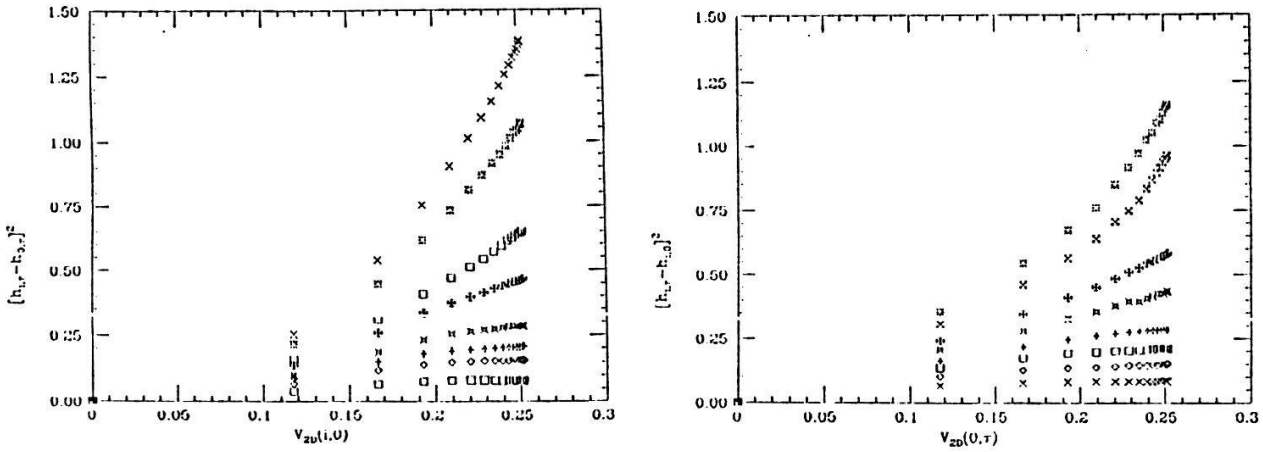

Fig.1 The height-height correlation functions along the x and direction is plotted against the 2-dimensional lattice Green's function $V_{2D}(i, 0)$ (proportional to $\ln(i^2 + \tau^2)$). The values of J^{-1} are 1.4; 1.5; 1.55; 1.60; 1.65; 1.7; 1.8 and 1.9.

In the strong coupling regime the correlation function saturates approaching approach a finite value; this means that the screening length is finite. At a critical value $J_{cr} \approx 0.6$ 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.Finally we want to go back to the original quantum roughening model and describe the obtained results in this context: when the hopping strength for the step on the surface of the crystal Y is increased above a certain value, a non dissipative mass transfer is possible in the system.

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