

High Precision Verification of the Kosterlitz Thouless Scenario*

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Abstract

We verify the Kosterlitz Thouless scenario for three different SOS (solid-on-solid) models, including the dual transforms of XY-models with Villain and with cosine action. The method is based on a matching of the renormalization group (RG) flow of the candidate models with the flow of a bona fide KT model, the exactly solvable BCSOS model. We obtain high precision estimates for the critical couplings and other non-universal quantities.

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For a large class of two-dimensional statistical models, the unambiguous verification of the Kosterlitz Thouless (KT) scenario is still an open problem. The most recent large scale Monte Carlo studies of the XY model [1, 2] clearly favor a KT against a second order transition. However, systematic errors are not yet under control. Here we present an alternative approach. Our method exploits the fact that the BCSOS (body centered solid-on-solid) model can be solved exactly and has been *proven* to exhibit a KT transition [3]. The idea is to verify the KT scenario for an SOS model by demonstrating that its asymptotic RG flow at criticality matches with the flow of the critical BCSOS model.

The models. References for reviews on SOS models can be found in [4]. The models to be defined below live on two-dimensional square lattices with periodic boundary conditions. The discrete Gaussian model (DG) is dual to the XY model with Villain action. The spins h_i take integer values. The partition function is

$$Z = \sum_h \exp(-K^{DG} \sum_{\langle i,j \rangle} (h_i - h_j)^2),$$

where i and j are nearest neighbor points. The dual of the XY model with cosine action also has integer valued spins h_i , and partition function

$$Z = \sum_h \prod_{\langle i,j \rangle} I_{|h_i - h_j|}(\beta^{XY}),$$

where the I_n are modified Bessel functions. The ASOS model is defined by the partition function

$$Z = \sum_h \exp(-K^{ASOS} \sum_{\langle i,j \rangle} |h_i - h_j|).$$

The BCSOS model was introduced by van Beijeren [5]. The lattice is divided in even and odd sites, like a checker board. Spins on odd sites take values of the form $2n + 1/2$, spins on even sites are of the form $2n - 1/2$, n integer. The partition function can be written as

$$Z = \sum_h \exp(-K^{BCSOS} \sum_{[i,k]} |h_i - h_k|),$$

where i and k are next to nearest (i.e. diagonal) neighbors. Nearest neighbor spins h_i and h_j obey the constraint $|h_i - h_j| = 1$. The critical (roughening) coupling is $K_R^{BCSOS} = \frac{1}{2} \ln 2$. The BCSOS model is equivalent to a special case of the six vertex model. The critical behavior of several quantities is exactly known and follows the predictions of KT theory [3].

Matching. Universality, first introduced as the coincidence of the critical indices, can be understood as a convergence of the RG flow to a universal (model independent) flow as $K \rightarrow K_c$ and the number of block spin transformations goes to infinity. The RG flow can be monitored by studying correlations functions of block spins $\phi_i = B^{-2} \sum_{j \in i} h_j$ with increasing block size B .

We simulated the BCSOS model at the roughening coupling K_R^{BCSOS} on $L \times L$ lattices, with $L = 12, 16, 24, 32, 48, 64, 96, 128$. We measured block spin functions on block systems of size $l \times l$, with $l = 1, 2, 4$ ($L = lB$). The statistics was typically a few million single cluster updates (see the brief algorithm discussion at the end).

Motivated by KT theory, we chose as a monitor for the flow of the kinetic term the quantities $A_n = \langle (\phi_i - \phi_j)^2 \rangle$, $n = 1, 2$, where i and j are nearest neighbors on the block lattice for $n = 1$, and next to nearest neighbors for $n = 2$. As a monitor for the “fugacity” (periodic perturbation of a massless free field) we chose $A_{n+2} = \langle \cos(2\pi n \phi_i) \rangle$, $n = 1, 2, 3$.

There are two parameters to be adjusted in order to match the RG flow of one of the SOS models with that of the critical BCSOS model. First, matching can only occur if $K^{SOS} = K_R^{SOS}$ (the roughening coupling of the SOS model). Secondly, one has to adjust the ratio of the block sizes $b_m^{SOS} = B^{SOS}/B^{BCSOS}$. The freedom to set $b_m^{SOS} \neq 1$ is necessary in order to compensate for the different positions of the “bare” actions in the Kosterlitz-Thouless flow diagram. Matching occurs if the following condition holds: There exists a b_m^{SOS} and a K_R^{BCSOS} such that for all i and for all l

$$A_{i,l}^{SOS}(b_m^{SOS} B^{BCSOS}, K_R^{SOS}) \rightarrow A_{i,l}^{BCSOS}(B^{BCSOS}, K_R^{BCSOS})$$

in the limit of large B^{BCSOS} (moderate B 's are sufficient in practice). Here $A_{i,l}^{SOS}(B, K)$ denotes the observable A_i evaluated in the SOS model at coupling K on a block system of size $l \times l$, each block being of size $B \times B$. Notice that no additional wave function renormalization factors are expected, since the minima of the effective potential of the blocked system are fixed. This is due to the fact that, at all blocking levels, the models maintain the global symmetry of shifting all spins by an integer.

Finite size effects are exactly cancelled since the block systems to be compared always have the same number of blocks. Furthermore, since the blocks themselves are already large, we expect the matching values of K_R^{SOS} and b_m^{SOS} to stabilize for small l already.

In order to determine K_R^{SOS} we considered, for fixed L^{SOS} and l , the following two equations:

$$A_{i,l}^{SOS}(B^{SOS}, K_i^{SOS}) = A_{i,l}^{BCSOS}(B^{BCSOS}, K_R^{BCSOS}), \quad i = 1, 3.$$

For each of the available values of B^{BCSOS} we solved these equations numerically for K_i^{SOS} . The $A_{i,l}^{SOS}$ could be computed for a whole range of couplings with the help of the Swendsen-Ferrenberg method [6]. Thus we got two values K_1^{SOS} and K_3^{SOS} , which were in general not identical (matching occurs only for a specific choice of b_m^{SOS}). In a second step we plotted the values of K_1^{SOS} and K_3^{SOS} as function of B^{BCSOS} . To obtain continuous curves, we interpolated linearly in $\log B^{BCSOS}$. The intersection of the two curves $K_1^{SOS}(\log B^{BCSOS})$ and $K_3^{SOS}(\log B^{BCSOS})$ then uniquely determined an estimate for the roughening coupling K_R^{SOS} , and, in addition, for b_m^{SOS} . This completes the matching of the SOS and BCSOS flows at the

Table 1: β_R and $b_m = B^{XY}/B^{BCSOS}$ for the dual of the XY model with cosine action as obtained from the matching of A_1 and A_3

L^{XY}	l	β_R	L^{BCSOS}	b_m
16	2	1.1220(12)	19.0(1.1)	0.84(5)
16	4	1.1257(8)	21.3(4)	0.75(1)
24	2	1.1214(13)	26.5(2.3)	0.91(7)
24	4	1.1225(8)	28.6(8)	0.84(2)
32	2	1.1211(12)	34.5(4.3)	0.93(10)
32	4	1.1214(8)	37.4(1.5)	0.85(3)
48	2	1.1199(11)	54.1(9.6)	0.89(13)
48	4	1.1205(7)	53.6(2.1)	0.89(3)
64	2	1.1212(11)	78.(14.)	0.82(12)
64	4	1.1201(7)	72.1(3.9)	0.89(5)
96	2	1.1189(11)	108.(17.)	0.89(12)
96	4	1.1194(7)	100.9(8.0)	0.95(7)

roughening transition for given L^{SOS} and l . As an example we show in table 1 the results for the dual of the XY model with cosine action.

For all the three SOS models considered, the results for the roughening coupling K_R obtained for the various lattice sizes L and sizes l of the blocked system are consistent with one another within statistical errors. Only the couplings for $l = 4$ on the smallest two lattices sizes and for $l = 2$ on the smallest lattices slightly deviate from the rest. The same is true for the b_m . This indicates an extremely fast convergence to a universal RG flow of the models. To estimate K_R for the three models we averaged the values obtained from the largest L^{SOS} we considered both for $l = 2$ and $l = 4$, and from the second largest L^{SOS} for $l = 2$ only. We arrive at the following results:

$$\begin{aligned}
\beta_R^{XY} &= 1.1197(5), & b_m^{XY} &= 0.89(5) \\
K_R^{DG} &= 0.6645(6), & b_m^{DG} &= 0.31(2) \\
K_R^{ASOS} &= 0.8061(3), & b_m^{ASOS} &= 2.8(3)
\end{aligned}$$

The errors are statistical errors. Systematic errors due to deviations from the universal flow should be much smaller.

In order to check the universality of the matching we evaluated the observables A_2 , A_4 and A_5 at the critical couplings K_R determined above from A_1 and A_3 alone. The results show that (within errors) matching occurs for all observables.

Other non-universal constants. The method allows to determine other non-universal constants appearing in the formulas for the divergence of observables near the roughening transition [7]. For the constants in the asymptotic formula $\xi =$

$A \exp \left(C \left| \frac{K-K_R}{K_R} \right|^{1/2} \right)$ we find:

$$\begin{array}{ll} A^{XY} &= 0.223(13), & C^{XY} &= 1.78(2) \\ A^{DG} &= 0.078(5), & C^{DG} &= 2.44(3) \\ A^{ASOS} &= 0.70(8), & C^{ASOS} &= 1.14(2) \end{array}$$

(for the XY model we used $|\frac{\beta-\beta_R}{\beta_R}|$ in place of $|\frac{K-K_R}{K_R}|$).

Our results compare quite well with results from other Monte Carlo simulations [1, 2] if the systematic errors in these studies are taken into account. Actually, our statistical errors are considerably smaller.

Algorithms. For the algorithms used in the simulation of the DG, the dual XY and the ASOS models we used algorithms as described in [4]. Details of the BCSOS algorithm, which is also based on the ideas developed in [4], will be described elsewhere [8]. Our BCSOS algorithm has a critical dynamical exponent ≈ 1 . Therefore more than two thirds of the CPU time we used for this study were spent for the BCSOS simulations. With a recently developed new algorithm for the six vertex model, the necessary resources would have been considerably smaller [9].

The matching method was also applied to the Ising interface, for which also a cluster algorithm was developed [10]. Results on this work will be reported elsewhere [11].

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