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LETTER TO THE EDITOR

Sublattice order parameter in the BCSOS model: a finite-size Monte Carlo study

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Abstract. We introduce and investigate via Monte Carlo simulation the finite-size critical behaviour of the body-centred-solid-on-solid (BCSOS) model's sublattice order parameter and related (staggered) susceptibility. We confirm the scaling ansatz of Baxter for the susceptibility, a quantity which has remained hitherto unexplored. We also verify the Kosterlitz–Thouless universality class in the temperature dependence of both these equilibrium properties. Our extrapolation for the location of the infinite system roughening transition temperature is in good agreement with the exact value.

Surface roughening phenomena are often studied within solid-on-solid (SOS) models. The simplest of such models, such as the discrete Gaussian or the absolute SOS models, have no sublattice structure and therefore roughening takes place without any accompanying change of symmetry. Real surfaces, however, commonly exhibit two, and sometimes three or more, sublattices. For example: FCC (100) and (110), as well as BCC (100) and (111), have two sublattices, FCC (111) and BCC (110) have three, and so on. Their ground states are accordingly n-fold degenerate, corresponding to the equivalent possibilities of the topmost layer belonging to one of the n sublattices. At finite temperatures, one can therefore associate any thermodynamic state of the surface with a well defined *sublattice order parameter* $\mathcal{P}$. Moreover, we expect this order parameter to vanish identically in the rough state (where all sublattices must enter with equal weight). It follows that a sublattice disordering phase transition is expected to take place, either below the roughening temperature T_R, or at T_R itself. It should be stressed that, apart from this constraint, the two phenomena, sublattice disordering and roughening, are distinct. They will in general occur at different temperatures, and belong to different universality classes. den Nijs [1], as well as our group [2, 3], have introduced models which address this type of situation. Sublattice disordering is indeed analogous to the 'pre-roughening' of den Nijs, who calls the ensuing phase 'disordered flat'. This class of models is presently the subject of numerical investigations [4]; yet, it is highly desirable to understand sublattice disordering, if present, in simpler models, where a good deal of experience has accumulated over the years.

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The simplest surface model which is of the SOS type, but does embody the presence of two sublattices, is van Beijeren's well-known BCSOS model [5]. It is mapped onto the F version of the six-vertex model, for which many properties are known exactly. It is therefore of interest to enquire about sublattice disordering within the BCSOS model. The results of this enquiry form the main subject of this letter. In short, we first define the sublattice order parameter $\mathcal{P}$ and find its exact expression within the BCSOS model. We verify that it coincides with the Legendre conjugate to Baxter's staggered field in the F-model [6, 7]. We find that $\mathcal{P}$ vanishes continuously at T_R, so that sublattice disordering and roughening do coincide in the BCSOS model. For other relevant quantities, such as the sublattice susceptibility, there is no exact expression and we therefore perform a Monte Carlo finite size scaling study, similar to that needed for more realistic models [3, 4]. The results are very instructive, both for the BCSOS model, where an early conjecture by Baxter is checked, and in establishing a viable method for qualifying separately sublattice disordering and roughening phenomena.

A natural definition, within the BCSOS model, for the sublattice order parameter of (unreconstructed) BCC (100) and FCC (110) surfaces is as follows. Denote the two interpenetrating sublattices which make up the surface as B (black) and W (white). The ground state is doubly-degenerate and consists of the B sites at height $+1$ with respect to the W sites at height 0 (and vice versa: the ± 1 near-neighbour height difference restriction is implicit in the model). For a thermally excited configuration define probabilities of stepping up and stepping down from a given B site to one of its W nearest neighbours, $P_B^+ = 1 - P_B^-$ and P_B^-, where

$$P_B^- = \sum_{\text{odd}\ m=-\infty}^{+\infty} p_m b_m \tag{1}$$

and the sum extends over all the odd B site heights m. The analogous definition holds for P_W^-, where the sum runs over all even heights. Here p_m is the probability of finding a surface atom at height m (fixing the flat surface reference height at $m = \frac{1}{2}$), while b_m is the probability of stepping down from an atom at level m. For the F model we define, in Lieb's notation [8]

$$\Delta = -\cosh \lambda = \frac{a^2 + b^2 - c^2}{2ab} \tag{2}$$

with $a = b = \exp(-\epsilon/k_B T)$ and $c = 1$ the Boltzmann weights associated with the vertices of the F model. Then, the above probabilities read [9]

$$p_m = \text{constant} \times \exp\left[-\lambda(m - \tfrac{1}{2})^2\right] \tag{3}$$

and [10]

$$b_m = \begin{cases} \sum_{n=0}^{\infty} (-1)^n \exp[-\lambda n(n + 2m - 1)] & \text{for } m > 0 \\ 1 - b_{-m+1} & \text{for } m \leqslant 0. \end{cases} \tag{4}$$

The order parameter is then defined through

$$\mathcal{P}_1 = \frac{P_B^- - P_W^-}{P_B^- + P_W^-} \tag{5}$$

and takes values $+1$ (or -1) in the ground state and 0 in the disordered rough phase. At intermediate temperatures this quantity singles out which of the two sublattices' atoms are predominant in the surface top layer. The special feature of this quantity is that it vanishes with all its temperature derivatives at the roughening temperature T_R given by

$$k_B T_R = 4J/\ln 2 \simeq 5.771J \tag{6}$$

with $J = \epsilon/4$ the BCSOS coupling constant (throughout the paper temperatures are measured in units of J). This behaviour characterizes the sublattice order parameter of the infinite-order roughening transition.

Another definition of the order parameter was given by Baxter for the F model [6,7]. In the notation of Baxter, after partitioning the (dual) vertex lattice in two sublattices A and B, an energy $-s$ $(+s)$ is associated with every horizontal (vertical) arrow pointing from an A vertex to a B vertex and $+s$ $(-s)$ if it points from B to A. In this way s has the character of a staggered external field and is the equivalent of the magnetic field of the Ising model as it is able to lift the degeneracy of the ground state. Thus the order parameter which corresponds to this field is simply

$$\mathcal{P}_2 = -(\partial f/\partial s)_T \tag{7}$$

where f is the free energy per vertex. With the introduction of the field, the F model becomes insolvable, except for $T = 2T_R$ [6]. However, the order parameter $\mathcal{P}_2$ in zero field is known exactly at all temperatures and is given by [7]

$$\begin{aligned}\mathcal{P}_2(s\to 0^+) &= \left[\prod_{n=1}^{\infty}\tanh(n\lambda)\right]^2 \\ &= \left[1 + 2\sum_{n=1}^{\infty}(-1)^n \exp(-2n^2\lambda)\right]^2.\end{aligned} \tag{8}$$

It can be shown at this point that the series expansions for $\mathcal{P}_1$ and $\mathcal{P}_2$ are identical, so that the two order parameters are taken to be one and the same $\mathcal{P}$. No information is available, however, on the behaviour of the staggered field susceptibility, $\chi = -(\partial^2 f/\partial s^2)_T$, except again at $T = 2T_R$ and $s\to 0^+$ where it diverges as $\ln s$. Nevertheless, Baxter [7] has proposed that for $s = 0$ and in the neighbourhood of T_R this susceptibility should obey the scaling ansatz

$$\chi \sim \mathcal{P}^2/f_{\text{sing}} \tag{9}$$

where f_{sing} is the singular part of the free energy. If one considers that $f_{\text{sing}} \sim \exp(-\pi^2/\lambda)$ and that

$$\mathcal{P} \sim \lambda^{-1}\exp(-\pi^2/4\lambda) \tag{10}$$

one arrives at

$$\chi \sim \lambda^{-2}\exp(\pi^2/2\lambda) \tag{11}$$

which implies an extremely strong divergence at T_R, since, near T_R, $\lambda \sim (T_R - T)^{1/2}$.

In this letter we examine the general temperature behaviour of both $\mathcal{P}$ and χ by means of Monte Carlo simulation of the BCSOS model. In a finite size lattice, the operative definition of the order parameter $\mathcal{P}_1$ has to be modified as follows. Since for the BCSOS model lattice topology implies $P_B^- + P_W^- = \frac{1}{2}$, we have

$$\mathcal{P} = 4P_B^- - 1. \tag{12}$$

The stepping down probability P_B^- can be evaluated from the thermal and site average of the local $p_B^-(R_i)$ which, for a given configuration and B site i, is given by

$$p_B^-(R_i) = \tfrac{1}{2}\left[1 + m_B(R_i) - \tfrac{1}{4}\sum_D m_W(R_i + D)\right] \tag{13}$$

where D runs over the four neighbouring W sites. Taking the site average, $\mathcal{P}$ reads (the absolute value ensuring a meaningful averaging procedure)

$$\mathcal{P} = \left\langle \frac{1}{N}\left| \sum_B m_B - \sum_W m_W \right| \right\rangle = \langle P \rangle \tag{14}$$

where N is the number of B (or W) sites and the angular brackets denote thermal averaging. The related susceptibility is given by

$$\chi = \frac{N}{k_B T}\left[\langle P^2 \rangle - \langle P \rangle^2\right]. \tag{15}$$

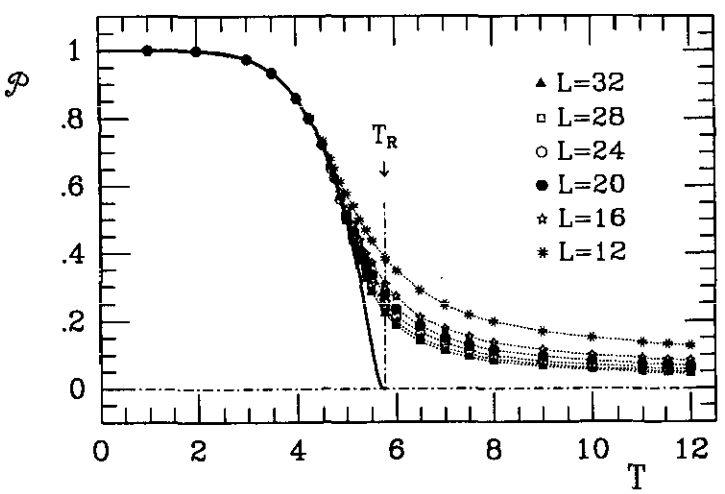

Figure 1. BCSOS order parameter temperature behaviour for different system sizes, compared with the infinite system exact behaviour (full curve). In this and all subsequent figures temperatures are expressed in units of J; no error bar is plotted if smaller than the point size.

In figure 1 we report our Monte Carlo results for the temperature dependence of the order parameter $\mathcal{P}$ for different linear lattice sizes $L=10$, 16, 20, 24, 28, and 32. Periodic boundary conditions are employed. A single Monte Carlo step consists of the random addition or removal of an 'atom', so surface height is not conserved. The infinite system critical behaviour (also reported for convenience) is approached slowly, like $L^{-1/2}$ at T_R as finite-size scaling would suggest, as the size L is increased. Below T_R however, one may attempt to fit the largest size data with the infinite-system asymptotic form, equation (10). We select a temperature window $0.70 < T/T_R < 0.88$ in order to avoid finite-size effects in the immediate neighbourhood of T_R, yet capturing the critical region temperature dependence. Our fitting is consistent with the form (10), yielding an exponential $\exp(-A/(T_R - T)^{1/2})$ having $A = 2.50\pm0.15$, which compares well with the exact value $A = \pi^2/2\sqrt{2}\ln 2 = 2.517\ldots$. Moreover, the same fitting yields a value of $T_R = 5.73\pm0.08$, to be compared with 5.771 of equation (6). The standard procedure for determining T_R has been the study of the interfacial width divergence at and above roughening within finite-size scaling [3]. The square of this width behaves as $\langle \delta h^2 \rangle \sim K(T) \ln L$ for $T > T_R$ with the universal behaviour $K(T) = 1/\pi^2 + C\sqrt{T - T_R}$ for $T \to T_R^+$, as clearly shown by our Monte Carlo data reported in figure 2. This procedure also yields an accurate estimate of $T_R = 5.66\pm0.11$.

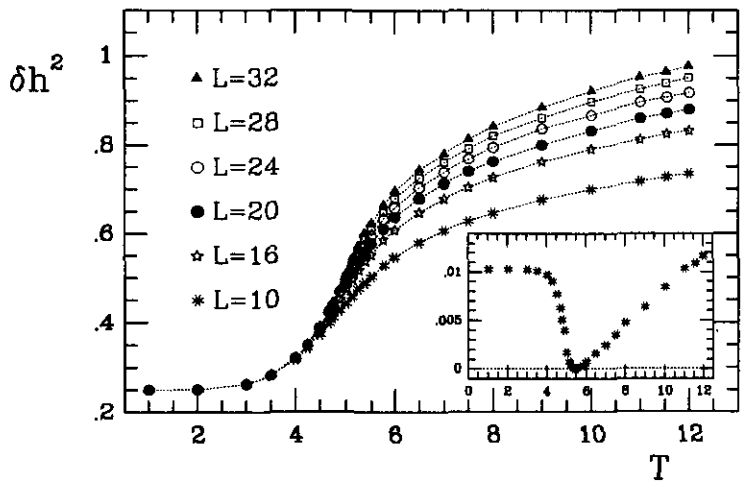

Figure 2. Finite-size behaviour of the average square interfacial width. In the inset, the behaviour of $[K(T) - 1/\pi^2]^2$ is reported in order to determine T_R from extrapolation of the linear temperature dependence (see text).

Having checked the method against exact results, the main purpose of this work consists in reporting novel data for the staggered field susceptibility χ, as shown in figure 3. In the infinite system, χ diverges at T_R remaining infinite above. For a finite lattice, we find a divergence with the size of the lattice typical of infinite-order transitions of the form

$$\chi(L, T) \sim L^{\omega(T)} \tag{16}$$

with an unknown temperature-dependent exponent ω. Exactly at T_R, Baxter's ansatz, equation (11), would imply (barring logarithmic corrections)

$$\omega(T_R) = 1. \tag{17}$$

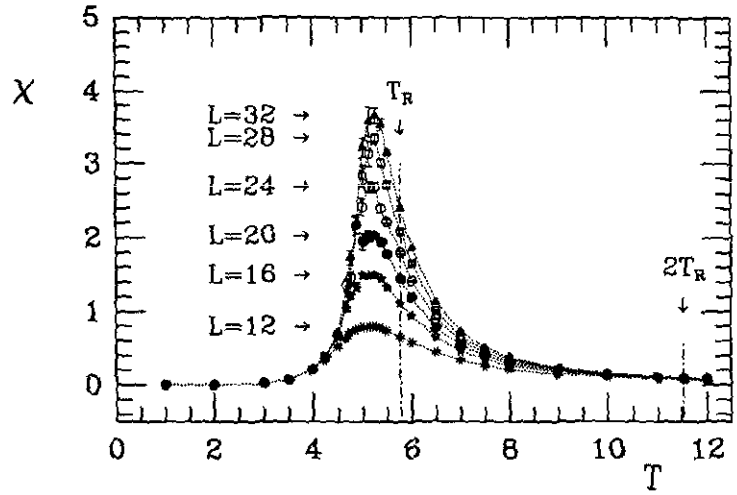

Figure 3. BCSOS staggered susceptibility for different system sizes. Notice the markedly different divergence with size at T_R and $2T_R$, respectively.

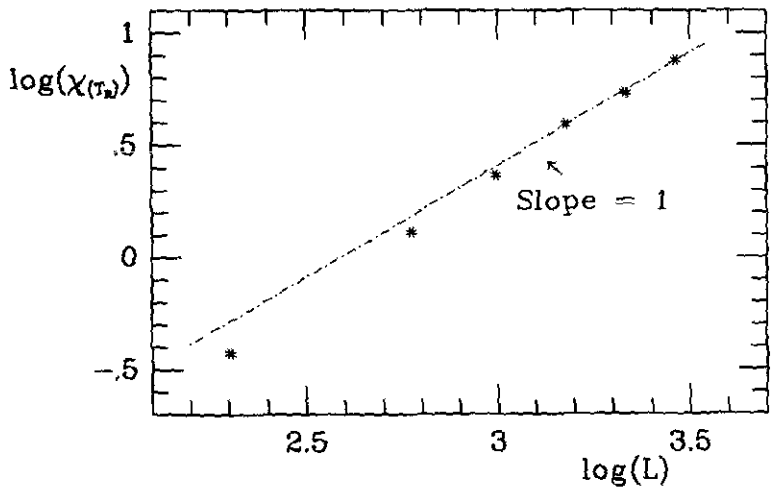

Figure 4. *Divergence of staggered susceptibility $\chi(L, T_R)$ with size L consistent with an exponent $\omega(T_R) = 1$ for the largest sizes available.*

This follows from the asymptotic form $\xi \sim \exp(\pi^2/2\lambda)$ for the correlation length which becomes of the order of L in a finite system at T_R. Our data are compatible with $\omega = 1$ (see figure 4); we can exploit our knowledge of the infinite-system T_R in order to get $\omega(T_R) = 0.98 \pm 0.06$ as obtained from fitting our largest sizes data. Furthermore we observe that the peak in $\chi(L, T)$ (which might be taken as a measure of T_R) shifts very slowly towards T_R, like $(\ln L)^{-2}$ to be precise, as L is increased. In turn, this whole procedure might represent a way of determining the sublattice disordering temperature in models of the BCSOS type where the transition point is unknown. Indeed, χ is the only sensible diverging quantity in an otherwise smooth phase transition. We point out that for the associated 2D XY magnetic model (where temperature scales inversely with respect to the SOS model) the direct field susceptibility is known to diverge at and below T_c as $L^{2-\eta(T)}$, where η is $\frac{1}{4}$ at T_c and decreases below. This leads to a stronger divergence in the critical phase,

contrary to the case of the staggered susceptibility where $\omega(T)$ is expected to vanish at $2T_R$. The latter result follows from the large-distance form $G(r, 2T_R) \sim r^{-2}$ of the staggered vertex correlation [6] and the usual fluctuation–dissipation formula

$$\chi(L, 2T_R) \sim \int_a^L d^2 r\, G(r, 2T_R) \sim \ln L$$

where a is the lattice spacing acting as a small-distance cutoff. Our data for $\chi(2T_R)$ are consistent with $\omega = 0$ and a $\ln L$ divergence. However, it is lamentable that no exact knowledge of the relation between $\omega(T)$ and $\eta(T)$ is as yet known. Were we to take a linear dependence, the conjecture $\omega = 8\eta - 1 = 2T_R/T - 1$ would reasonably fit our Monte Carlo data.

In conclusion, we have studied (for the first time to our knowledge) the exact and finite-size behaviour of the sublattice order parameter and related staggered susceptibility of the BCSOS model. The validity of Baxter's conjecture for the asymptotic diverging behaviour of χ at T_R has been verified. Sublattice disordering and roughening occur together at $T = T_R$, and with the same Kosterlitz–Thouless behaviour, in this model. Thus, sublattice disordering in the BCSOS model is driven by the thermal excitation of steps which are responsible for roughening. However, our definition of the sublattice order parameter and susceptibility, as well as the Monte Carlo finite size scaling method which allows for a separate study of sublattice disordering and of roughening, can now be taken over to more realistic surface models. For many of these models the two phenomena should become totally distinct.

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