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SCUOLA INTERNAZIONALE SUPERIORE DI STUDI AVANZATI
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Order Parameters of SOS Models in Disordered Flat Surfaces

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1 Introduction

Surfaces of fcc metals, in particular (110) faces, display a variety of phase transitions which have been the subject of considerable experimental and theoretical work.

Experimentally, (110) faces of some fcc metals - like Au or Pt - do reconstruct at low temperature into a (2×1) missing-row or related structures, whereas other metals - like Ag, Ni, and Pd - retain their bulk structure. As the temperature is raised, reconstructed surfaces tend to show two separate transitions: a critical deconstruction transition followed - generally at a measurably higher temperature - by a roughening transition.[1] Unreconstructed surfaces have failed, so far, to reveal a similar two-transition scenario, i.e., some critical disordering occurring below the actual roughening. Only the latter is well documented in this case.

From the theoretical side many studies have been devoted to the problem.[2, 3, 4, 5] The situation is somewhat different for the two cases, the unreconstructed and the missing-row reconstructed. The structure of a fcc (110) surface, see Fig. 1, is such that one can identify two interpenetrating anisotropic sublattices, call it white (W) and black (B). The unreconstructed (ideal) surface has *two* $T = 0$ ground states, differing for the sublattice which occupies the top layer. The problem has been considered by den Nijs, who argued that the phase diagram for an unreconstructed fcc (110) surface should be qualitatively the same as that of a simple cubic (110) surface.[6] In particular, he argues that Ag and Pd (which do not reconstruct) are good candidates for realizations of the *preroughening*, a non-universal critical transition from a low temperature ordered phase to an intermediate temperature *disordered flat* phase, previously identified in the context of restricted solid-on-solid (RSOS) models for simple cubic (110) surfaces.[7] In terms of the two ground states of the unreconstructed surface, the preroughening transition can be viewed as a loss of order for the surface due to the proliferation of step-like defects which separate regions in which the B sublattice dominates in the top layer and regions in which the W sublattice dominates. Such steps mantain, however, a form of long range up-down order - stabilized by a combination of up-up (down-down) step repulsion and entropy - which prevents the surface from being rough.

The situation is somewhat different for the (2×1) missing-row reconstructed phase. Due to half "coverage" of missing rows running in the y-direction, the periodicity in the x-direction is doubled, and one has four sublattices to deal with. The surface has therefore *four* degenerate $T = 0$ ground states, which can be classified by a clock variable $\theta = 0, \pi/2, \pi, 3\pi/2$, according to the "colour" and the position of the missing-row in the doubled unit cell, i.e. according to which of the four sublattices sits in the top layer. Fig. 4 shows a schematic height profile of the four missing-row ground states. The most elementary extended defects which one can consider are illustrated in Fig. 3. These are a) *steps*, which simultaneously change the average height by $\Delta h = \pm 1$, and the reconstruction variable by $\Delta\theta = \pi/2$ (*clockwise* or (3×1) steps) or $\Delta\theta = -\pi/2$ (*anticlockwise* or (1×1) steps), b) *Ising wall defects* which do not

change the average height, and change the reconstruction variable by $\Delta\theta = \pi$. They can be seen as a bound state between two steps of opposite sign (up and down), but *same* $\Delta\theta$. In this framework, den Nijs has introduced a four state clock-step model to describe the interplay between reconstruction and roughening degrees of freedom.[3] The model is formulated on a length scale somewhat larger than the microscopic one, through the introduction of a lattice of cells in which a integer variable $h_{\mathbf{r}}$, representing the average height in the cell, and a clock reconstruction variable $\theta_{\mathbf{r}}$ are defined. A bond in the lattice can be either empty (no defect), or occupied by an up or down step of either kind, or doubly occupied by an up and down step of the same kind (equivalent to an Ising wall). den Nijs found that when 1×1 and 3×1 steps have the same energy - the so-called *zero chirality limit* - the model displays two possible scenarios: *(i)* If the parameters are such that the energy of an Ising wall E_w is less than roughly twice the energy of a step E_s, by increasing the temperature the system goes from the ordered phase to a disordered flat phase with an Ising transition, and then to a rough phase with a conventional Kosterlitz-Thouless (KT) transition; *(ii)* When steps are instead energetically favoured - $E_w > 2E_s$ - the system undergoes a single roughening-assisted deconstruction transition, which is Ising-like for the reconstruction degrees of freedom and KT-like for the height degrees of freedom. The disordered flat phase present for $E_w/E_s < 2$ is quite clearly characterized by the proliferation of Ising wall defects (their free energy per unit length goes to zero at the deconstruction). Accordingly, the surface shows a prevalence of $\theta = 0$ and $\theta = \pi$ terraces, say, over $\theta = \pi/2$ and $\theta = 3\pi/2$ ones. Using the terminology introduced in Ref. [8], such a phase could be called Disordered Even Flat (DEF). It has an obvious non-zero order parameter which counts the difference in the abundance of $\theta = 0, \pi$ terraces over that of $\theta = \pi/2, 3\pi/2$ ones, and vanishes only in the rough phase. By contrast, when single steps dominate - i.e., $2E_s < E_w$ - there is apparently no mechanism in this simple model which may stabilize the up-down long range order for steps, typical of disordered fla phases. It has been argued that suitable interactions penalizing the crossing of two up-up or two down-down steps - not considered by den Nijs - should stabilize such a hypothetical step-dominated disordered flat phase.[8] A disordered flat phase of this kind - termed DOF in Ref. [8] after den Nijs - should be characterized by an equal abundance of all types of cells $\theta = 0, \pi/2, \pi, 3\pi/2$, i.e., by *a vanishing of the order parameter characterizing the DEF phase*.[8] If such a scenario is realized a critical line of some kind, separating a DEF from a DOF phase, should appear in the phase diagram, see Fig. 15 in Ref. [8].

Quite interestingly, the situation does not change much in the so-called *strong chirality limit* considered by den Nijs, i.e., when anti-clockwise steps (say, of 1×1 type) are very costly and thus completely neglected. In such a case the problem is mapped into a fermionic model containing a Hubbard type on-site interaction U which allows to parametrize the energy of a Ising wall configuration (doubly occupied site) as $E_w = 2E_s + U$. For $U < 0$, the physics is the same as in the zero chirality limit case, i.e., a DEF phase is obtained. When steps dominate - i.e., for $U > 0$ - there are two distinct rough phases appearing), and the deconstruction transition is

no longer of the Ising type. However there is again no disordered flat phase , eithr DEF or DOF. Balents and Kardar have independently analized the fermionic problem obtaining a completely similar phase diagram.[4] Quite disappointingly, DOF phases seem to be absent in the four state clock-step model of a (2×1) reconstructed surface. Although the question of stabilizing them by turning on suitable interactions has to be further analyzed. We will comment further on this point in the final section of this thesis.

Do *microscopic* models display different features, one might ask? The question has been considered by Mazzeo *et al.*, who have introduced, and studied by Monte Carlo technique, a microscopic solid-on-solid (SOS) model which is able to deal with both unreconstructed and reconstructed situations.[5] Their model is a simple modification of the exactly solvable body-centered solid-on-solid model (BCSOS) [9] obtained by adding a further neighbor interaction in order to stabilize the (2×1) missing-row reconstruction. For a reconstructed case, a two-transition scenario is confirmed, with an Ising deconstruction to a disordered flat phase followed by a conventional KT roughening. Quite interestingly, the unreconstructed case studied also shows *two transitions*, with a non universal critical transition to a disordered flat phase followed by a KT roughening.[5]

In the light of the previous discussion about DEF (Ising wall dominated) as opposed to DOF (step dominated) phases, the question naturally arises as to what kind of disordered flat phase (or phases) is realized in such a simple modification of the BCSOS model. (Note that, by tuning the parameters of the model, the $T = 0$ defect energies can be substantially modified.) The first problem to deal with is how to define a suitable order parameter P_{BW} to distinguish between a DEF and a DOF. This definition turns out to be not completely straightforward. Mazzeo *et al.* have discussed different order parameters in the (1×1) and in the (2×1) cases. The finite size scaling behaviour of P_{BW} was not definitive in their work because of size limitations.[5]

In the same spirit of investigating simple microscopic models as in Mazzeo's work, Santoro *et al.* have considered yet another simple modification of the BCSOS model, similar but not identical to the one of Ref. [5], with the additional virtue of being easy to map into a quantum spin-1/2 chain problem of the Heisenberg type with further neighbor interactions.[10] They find a phase diagram with two ordered phases - (1×1) and (2×1) - one disordered rough phase and one disordered flat phase. They also show that the physics of the disordered flat phase occurring in their model is likely to be the same as that of the dimer quantum spin phase studied by Haldane, [11] i.e., a doubly degenerate state which breaks translational invariance and in which dimer-dimer correlation functions acquire long range order (LRO). In particular, they show that the long-range dimer order implies LRO for the correlation function between local surface maxima, which in turn leads to a new, more physical definition of the order parameter P_{BW} for the surface problem.[10] However, it proved once again difficult to verify explicitly these theoretical guess using exact diagonalization data

for chains up to 28 sites only.

The aim of the present work is to clarify some of these open problems, particularly concerning the nature of disordered flat phase in simple BCSOS-like microscopic hamiltonians of fcc (110) surfaces. We have pursued this goal by setting up a classical Monte Carlo code which allows studying larger lattice sizes, and to perform a more reliable finite size scaling analysis of the interesting quantities. In particular, we ask ourselves the following question: *Is P_{BW} vanishing or different from zero for the disordered flat phases of BCSOS hamiltonians studied so far*? The answer to this question is that P_{BW} is *different from zero* in all the cases so far studied, i.e. in both the models of Ref. [5] and of Ref. [10]. Moreover, the dimer phase scenario found by a mapping on a quantum spin chain, is quite well reproduced by our Monte Carlo study. Open questions do nevertheless remain on the nature of the disordered flat phase we are dealing with, and a discussion of these points is deferred to the final section of this thesis.

The thesis is organized as follows. Section 2 introduces the BCSOS models that have been considered and discusses in more depth the questions we are trying to answer. In Section 3 we discuss the relevant order parameter to be calculated in order to characterize the phases under investigation. In Section 4 we present and discuss our results. Section 5, finally, contains some concluding remarks as well as a discussion of open problems.

2 Solid on solid models for an fcc (110) surface

The (110) surface of an fcc metal, shown in Fig. 1, is comprised of two interpenetrating rectangular sublattices in a plane of lattice constants $a_x = \sqrt{2}a_y$, which we will conventionally refer to as the white (W) and the black (B) sublattice. In the ideal unreconstructed (110) surface, one of the two sublattices - the B one, say, - lies above the other sublattice at a distance $a_z = a_y/2$. Within a solid-on-solid (SOS) framework,[13] one associates to each site of the lattice a height variable h_{r} which can take only *integer* values (take $a_z = 1$). In doing so one neglects overhangs as well as deformations from the ideal lattice structure. A further assumption of an SOS model is that the energy of a surface configuration $\{h_{\mathrm{r}}\}$ depends in some simple way on height differences between neighbour atoms. The models we are going to study have an additional restriction, in that the the height difference between each site and its nearest neighbours (belonging to the other sublattice) are forced to be $\Delta h = \pm 1$. This is the restriction typical of the so-called BCSOS, a very popular model which can be solved exactly.[9] A height difference of 0 is excluded in order to describe an fcc (110) surface, whereas larger values of Δh are excluded since they are in practice much more costly energetically. As a consequence of this height restriction, the values of h_{r} are forced to have opposite parity on the two sublattices, even on W and odd on B, say.

Our general hamiltonian is written as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \ ,$$

where $\mathcal{H}_0$ describes interactions between sublattice nearest neighbours, and $\mathcal{H}_1$ takes into account further neighbour interactions which will favour or disfavour reconstructed phases. More specifically, we take

$$\mathcal{H}_0 = K_{2y} \sum_{\mathrm{r}\in B+\mathrm{W}} (h_{\mathrm{r}} - h_{\mathrm{r+y}})^2 \ + \ K_{2x} \sum_{\mathrm{r}\in B+\mathrm{W}} (h_{\mathrm{r}} - h_{\mathrm{r+x}})^2 \ , \qquad (1)$$

with different coupling strenghts in the two directions to take into account the anisotropy of the surface. Here $\mathrm{x} = a_x\hat{\mathrm{x}}$ and $\mathrm{y} = a_y\hat{\mathrm{y}}$ are the surface lattice basis vectors, $\hat{\mathrm{x}} = (001)$, $\hat{\mathrm{y}} = (1\bar{1}0)$. K_{2y} will be always assumed to be *positive* and is generally the largest energy in the problem. The correspondent physics is that it is very costly to create a kink on a tighly packed $(1\bar{1}0)$ row. The absolute value of K_{2x}, i.e. of the coupling between rows, is instead much smaller. Moreover, for $K_{2x} > 0$, the (110) surface is stable in its (1×1) unreconstructed form, while for $K_{2x} < 0$, it becomes unstable against $(1\bar{1}0)$ step formation. In this case the final stable state is determined by $\mathcal{H}_1$. As for $\mathcal{H}_1$, two possible simple choices can be made, giving rise to two possible models, which we will name the K_3–model and the K_4–model. The K_3–model has been introduced by Mazzeo *et al.* in Ref. [5], and is defined by

$$\mathcal{H}_1 = \frac{1}{2} K_3 \sum_{\mathrm{r}\in B+\mathrm{W}} \left[(h_{\mathrm{r}} - h_{\mathrm{r+x+b}})^2 \ + \ (h_{\mathrm{r}} - h_{\mathrm{r+x-y+b}})^2 \right] \ , \qquad (2)$$

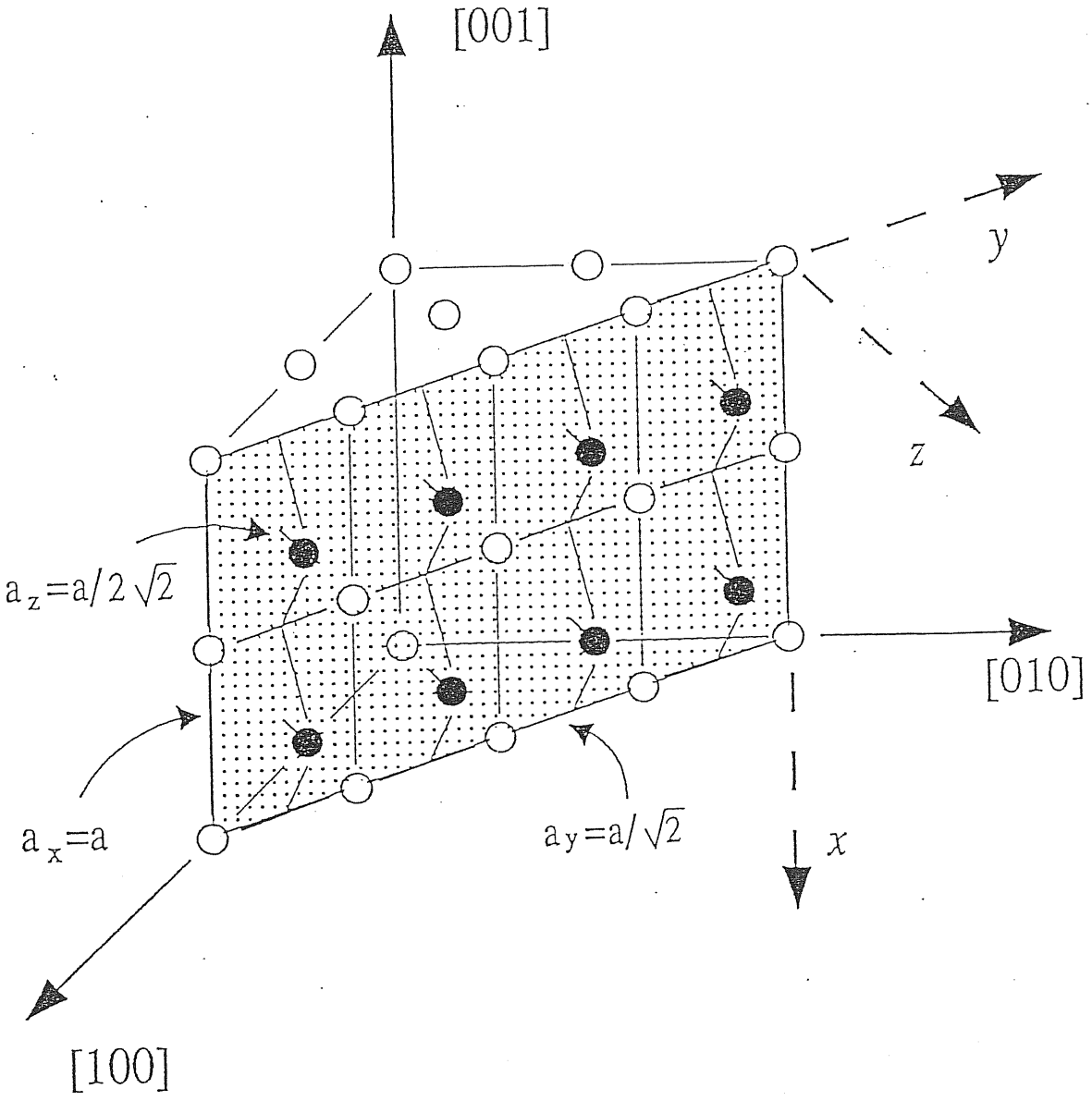


Figure 1: (110) surface of a fcc lattice. The surface reference system xyz and the interatomic spacings are also shown

with $K_3 \geq 0$, and $\mathbf{b} = (\mathbf{x}+\mathbf{y})/2$. The introduction of this further neighbour interaction one stabilizes the missing-row (2×1) reconstructed phase.[5] In fact, it is very easy to check that, for $K_{2x} < 0$, $K_3 > 0$ stabilizes an ordered succession of up and down $(1\bar{1}0)$ steps, which is precisely the (2×1) missing-row state.

An alternative way of stabilizing the same (2×1) missing row state against (111) faceting is realized with the K_4–model, whose $\mathcal{H}_1$ reads

$$\mathcal{H}_1 = K_4 \sum_{\mathbf{r} \in B+W} (h_{\mathbf{r}} - h_{\mathbf{r}+2\mathbf{x}})^2 \,, \tag{3}$$

with $K_4 \geq 0$. The fourth neighbour interaction in the x direction has the effect, once again, of increasing the energy of configurations with $|h_{\mathbf{r}} - h_{\mathbf{r}+2\mathbf{x}}| = 4$. This model was originally proposed by Kohanoff and Tosatti,[12] and has been studied recently in detail by Santoro *et al.*.[10] The two models should contain the same physics, with only quantitative differences. The K_3–model was preferred by Mazzeo *et al*,[5] because the interactions are shorter ranged. The K_4–model is instead more suitable for a mapping on a quantum spin chain, whence it was preferred by Santoro *et al.*[10]

The lattice is taken to have $N_c = N_x \times N_y$ cells (i.e., $N = 2N_c$ atoms), and periodic boundary conditions are always assumed in both directions. A schematic diagram representing the lattice and the interactions is given in Fig. 2

The classical $T = 0$ ground states for both models are easy to work out as a function of the dimensionless ratio $\mathcal{K} = K_{2x}/K_3$ or $\mathcal{K} = K_{2x}/K_4$. For the K_3–model we have:[5]

1. $\mathcal{K} > 0$: The ground state is unreconstructed [or (1×1)]
2. $-4 < \mathcal{K} < 0$: The ground state is (2×1) missing-row reconstructed
3. $\mathcal{K} < -4$: The ground state is an infinite (111) facet.

For the K_4–model, the corresponding $T = 0$ phase diagram reads:[12, 10]

1. $\mathcal{K} > 0$: The ground state is unreconstructed
2. $-4 < \mathcal{K} < 0$: The ground state is (2×1) missing-row reconstructed
3. $(12 - 8n)/(n-1) < \mathcal{K} < (20 - 8n)/(n-2)$ with $n \geq 3$: The ground state is $(n \times 1)$ missing row reconstructed
4. $\mathcal{K} < -8$: The ground state is an infinite (111) facet.

When $K_{2x} > 0$ and $K_3 = K_4 = 0$ we recover the simple BCSOS model which can be exactly solved through a mapping to the six vertex model,[9] and shows a *single*

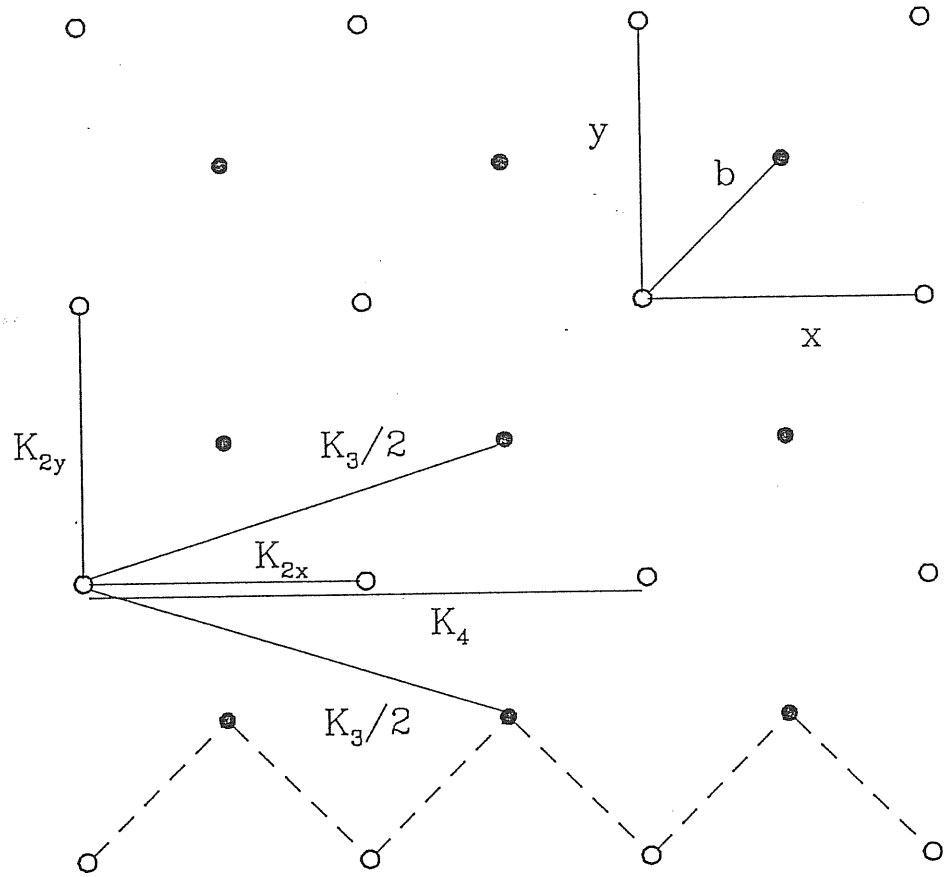


Figure 2: Schematic top view of the fcc (110) surface. The interactions considered in the two models are indicated together with lattice basis vectors. The dashed line represents a "time-slice" used in the spin-chain mapping.

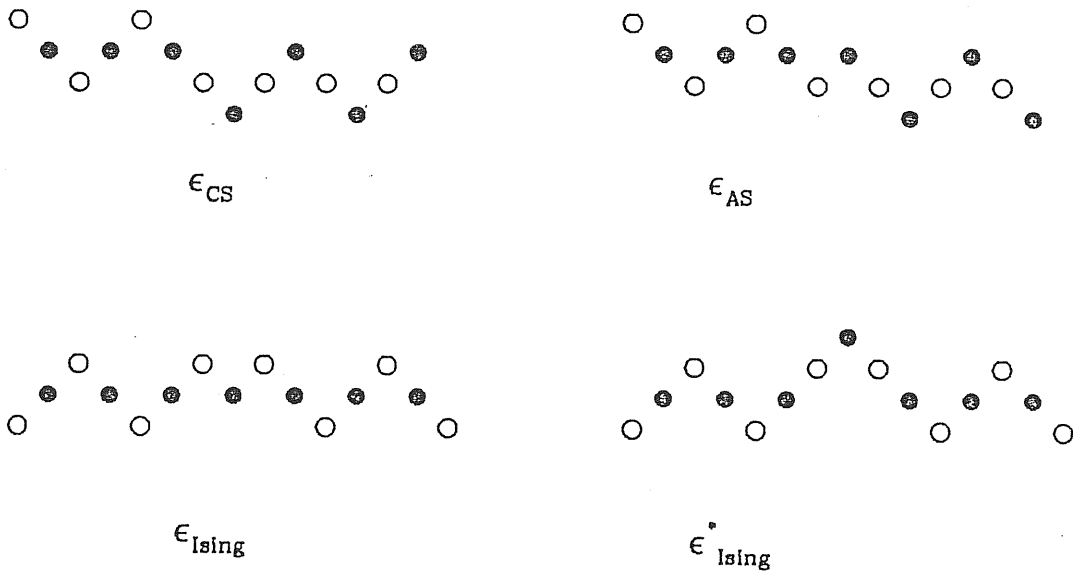
	K_3–model	K_4–model
$\epsilon_{2\times1}$	$-4K_{2x}$	$-4K_{2x}+8K_4$
$\epsilon^*_{2\times1}$	$-8K_{2x}$	$-8K_{2x}+8K_4$
ϵ_{CS}	$-2K_{2x}+8K_3$	$-2K_{2x}+8K_4$
ϵ_{AS}	$2K_{2x}$	$2K_{2x}+8K_4$
ϵ_{Ising}	$4K_{2x}$	$4K_{2x}+8K_4$
ϵ^*_{Ising}	$-4K_{2x}+16K_3$	$-4K_{2x}+16K_4$

Table 1: Ground state energy of the defects shown in Fig. 3 for the K_3 and K_4–models

transition, of the Kosterlitz-Thouless (KT) type, between a low temperature ordered (unreconstructed) flat phase and a high temperature disordered rough phase.

Neglecting adatoms, vacancies and overhangs, the defects which play a role in the disordering and roughening transitions are both unbound steps and (for the reconstructed case) bound pairs of steps, i.e."Ising" domain walls. Fig. 3 illustrates the most relevant defects for both a (1×1) and a (2×1) surface. The ground state energies of these defects are given, for both the K_3 and the K_4–model, in table 2. Notice that periodic boundary conditions impose constraints on the possible combinations of defects which are allowed. (In the (1×1) case, for instance, the same number of up and down (2×1)–steps must be present.) For the unreconstructed case, (2×1)–steps are the cheapest defects. We note that an up and a down (2×1)–step attract each other at very short range for the K_4–model but not in the K_3–model, see table 2. The K_3–model always has two different defects whose energy goes to zero as $K_{2x}\to0$. They are the (2×1)–step and the $(2\times1)^*$–wall in the (1×1) case, or the AS–step and the Ising wall in the (2×1) reconstructed case. The $K_{2x}\approx0$ region is therefore slightly unphysical for this model, and one might expect disorder to occur at very small temperatures. As a second point, observe that in the K_3–model the *Ising** walls, which can be seen as a bound pair of up and down CS–steps, are never energetically stabilized with respect to two unbound steps and will therefore be disfavoured at finite T for entropic reasons. Third, there is a whole region of small values of $\mathcal{K}$ where CS–steps are energetically more costly than *Ising* walls and AS–steps. More precisely, for the K_3–model, a combination of four AS-steps (or two AS–steps and an *Ising* wall, or two *Ising* walls) is favoured with respect to the corresponding combinations involving CS–steps as soon as $\mathcal{K}=K_{2x}/K_3>-2$. Even more clear is the situation for the K_4–model, where a combination of two *Ising* walls wins against combinations involving CS–steps for $\mathcal{K}=K_{2x}/K_4>-1$, while it always wins against AS–steps. Therefore, a good candidate to a DEF (wall dominated) phase seems to be possible for $\mathcal{K}<1$ in the K_4–model. Later on we will present results obtained for $\mathcal{K}=.56$, which show how ground state defect energy considerations can be somewhat misleading: the phase obtained does not have the features of an ideal DEF.

(1x1) DEFECTS



(2x1) MISSING–ROW DEFECTS

Figure 3: The most relevant defects for a (1×1) and for a (2×1) reconstructed surface.

2.1 Known results on the K_3–model

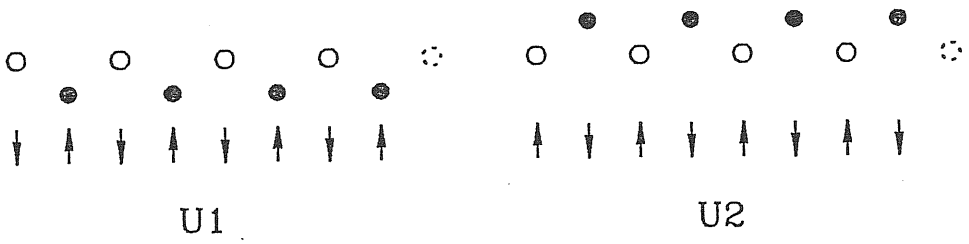
The K_3–model has been studied by Monte Carlo simulation in Ref. [5] for two values of the parameters. One set of parameters corresponds to $\mathcal{K} = -4$ and is intended to describe the situation of an unreconstruced surface like Ag (110). Two transitions are found. First a sublattice disordering transition takes place at $T_D \approx 1.81 K_{2y}$ with non-Ising critical exponents. Such a behaviour fits quite naturally into the realization of a preroughening transition proposed by den Nijs.[6] In particular, the critical exponents should be continously varying along the preroughening line separating the ordered flat phase from the disordered flat one.[6] At $T_R \approx 2.25 K_{2y}$ a Kosterlitz-Thouless (KT) roughening transition is detected from the logarithmic divergence of the height-height correlation function.

The second choice of parameters, for which $\mathcal{K} = K_{2x}/K_3 = -2.3$, describes a missing-row reconstructed surface, as is the case of Au (110) (2×1). Once again two transitions are seen, an Ising-like deconstruction at $T_D \approx 2.90 K_{2y}$, followed by a KT roughening at $T_R \approx 3.09 K_{2y}$.

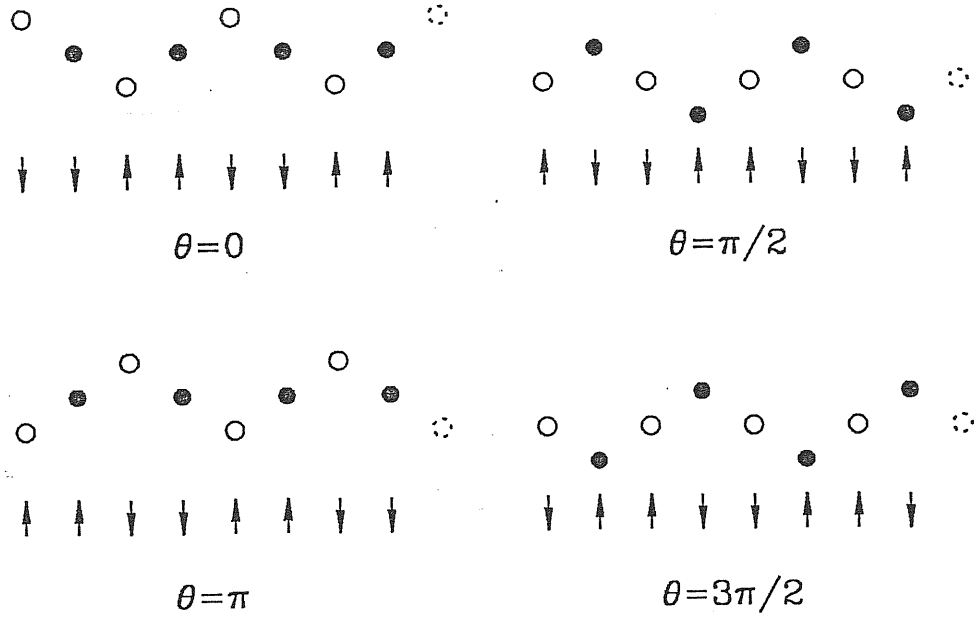
2.2 Known results on the K_4–model

The K_4–model has been studied by a mapping to a one-dimensional quantum spin chain in Ref. [10]. The method consists in viewing the y-direction of the lattice as the (imaginary) time direction of an appropriate 1D quantum problem, whose hamiltonian H_S is selected in such a way that the matrix elements of the imaginary-time evolution operator $e^{-\tau H_S}$ coincide, in the so-called *time-continuum limit*, with the matrix elements of the classical transfer matrix of the original problem. The crucial physical requirement is that the "time" direction must coincide with the hard direction of the classical problem, i.e. the coupling in the y direction has to be much stronger than the other couplings. Anisotropy is not expected to play a role in the qualitative phase diagram of the model. (As it turns out, the mapping allows to extract quantitative information on the classical phase diagram with transition lines determined to within a few percent.) The height restriction contraint between nearest neighbours suggests that the relevant degrees of freedom can be described by introducing a spin-1/2 Hilbert space, and mapping the z-component of the spin operator to the height difference between nearest-neighbours within the same "time-slice" (the dashed lines in Fig. 2), i.e., $S_i^z \longleftrightarrow (1/2)(h_{i+1,0} - h_{i,0})$. Fig. 4 illustrates the explicit mapping of the (1×1) and (2×1) ground states in terms of spin configurations along a time-slice. In terms of the usual spin-1/2 operators, the quantum hamiltonian reads

$$H_S = -\frac{J}{2}\sum_{i=1}^{N_s}[S_i^+ S_{i-1}^- + S_i^- S_{i-1}^+] + \sum_{i=1}^{N_s}[J_z S_i^z S_{i-1}^z + J_2 S_i^z S_{i-2}^z + \frac{J_2}{2} S_i^z S_{i-3}^z] \,, \quad (4)$$



(1x1) UNRECONSTRUCTED GROUND STATES



(2x1) MISSING–ROW GROUND STATES

Figure 4: Schematic height profiles of the two possible ground states of the unreconstructed surface, and of the four possible ground states of the (2×1) missing-row surface. The reconstruction variable is indicated. The spin representation of each state is explicitly given.

where the spin couplings are related to the original couplings as follows:

$$\begin{aligned} J &= 2\exp(-4\beta K_{2y}) \\ J_z &= 8\beta(K_{2x}+3K_4) \\ J_2 &= 16\beta K_4\,, \end{aligned} \tag{5}$$

and $\beta = 1/k_BT$. $N_s = 2N_x$ is the number of atoms in a time-slice. It is well known that the mapping is such that the free energy per site of the classical problem is related to the ground state energy per site of the one-dimensional quantum problem, i.e., $\beta f = \epsilon_{GS}$. [14] The temperature clearly enters through the spin couplings, see Eqs. 5, so that any temperature singularity of the classical free energy can be seen as a ground state energy singularity for the quantum problem as a function of the couplings J_z/J and J_2/J. Moreover, temperature averages for correlation functions of the classical problem can be likewise rewritten in the form of ground state averages for the corresponding quantum correlation function.[14] In summary, to obtain information about the temperature phase diagram of the classical model one studies the *ground state phase diagram* of the spin chain model.

The phase diagram of the spin model in Eq. 4, was obtained in Ref. [10] by finite size scaling analysis of exact diagonalization data for chains up to $N_s = 28$ sites. Its translation (using Eqs. 5) into a temperature phase diagram for the classical problem is shown in Fig. 5. Four phases are found in a region of parameters relevant to the unreconstructed and (2×1) recontructed case. Apart from the ordered phases present at low temperatures (large values of the spin couplings in the spin-chain problem), there is a rough phase at high temperatures, corresponding in the spin problem to the region close XY-point ($J_z = J_2 = 0$) in which the spin-spin correlation functions show power-law behaviour at large distance. The other phase appearing in Fig. 5 is a disordered flat phase. It corresponds, in the spin language, to the dimer phase - predicted analytically by Haldane [11] - where spin–spin correlations decay exponentially to zero, but four–spin correlation functions show long range order. More specifically

$$D_{ij} = \langle (S_i^z S_{i+1}^z)(S_j^z S_{j+1}^z)\rangle \approx \text{const}(-1)^{i-j} \qquad |i-j| \to \infty\,. \tag{6}$$

Such a phase has a *gap* in the excitation spectrum, and a doubly degenerate infinite volume ground state which *break translational symmetry*. As shown in Ref. [10] these features are enough to guarantee the existence of a non-zero order parameter, counting the difference in the number of local surface maxima in the W and B sublattice. Strictly speaking, therefore, the obvious disorder present in the dimer phase is not enough to prevent distinguishing wheter the W or the B sublattice prevails in the topmost layer. Numerically, however, it is extremely difficult to assess in a clear manner the presence of such a dimer-dimer long range order, even with chains up to 28 sites.[10] One of the motivation of the present study is therefore the check of this prediction directly on the classical K_4–model, where our Monte Carlo techniques allow us to deal with larger systems.

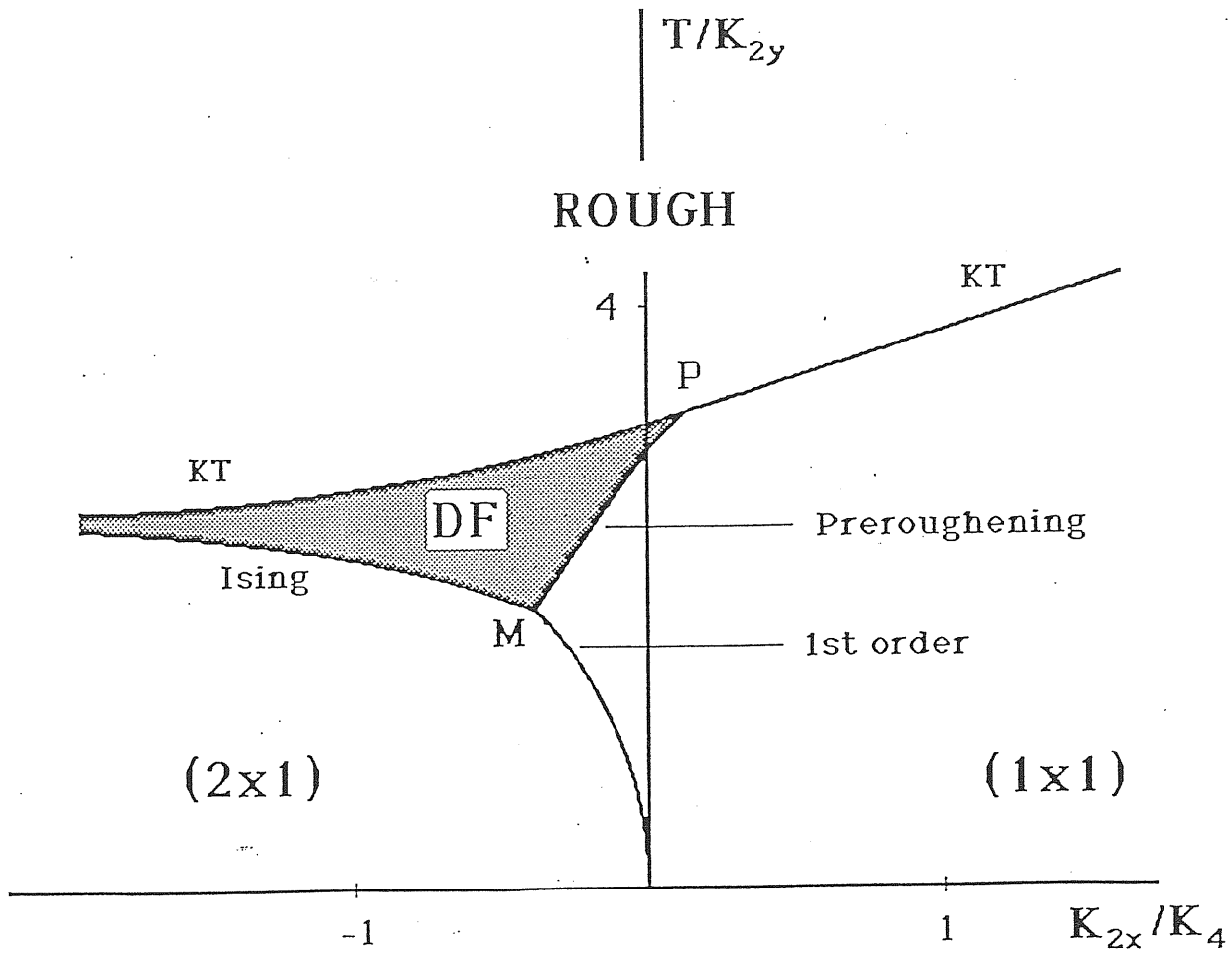


Figure 5: Phase diagram for the K_4–model, as obtained from the quantum spin-chain mapping.

3 Order parameters to look at

We define in this section the order parameters by means of which we try to characterize the different phases discussed previously.

For the (1×1) symmetry, the simplest order parameter is just the appropriate Fourier transform of the height configuration

$$P_{1\times 1} = \langle \frac{1}{N_c} \sum_{\mathbf{r}\in W,B} h_{\mathbf{r}} e^{i\mathbf{G}\cdot\mathbf{r}} \rangle \ , \tag{7}$$

where N_c is the number of cells in each sublattice, and $\mathbf{G} = (2\pi/a_x)\hat{\mathbf{x}}$. Splitting the sum over all sites in terms of a sum over primitive cells (denoted by $\mathbf{R}$), plus a sum over the two sublattice sites, we can easily rewrite

$$P_{1\times 1} = \langle \frac{1}{N_c} \sum_{\mathbf{R}} [h_{\mathbf{R},W} - h_{\mathbf{R},B}] \rangle \ , \tag{8}$$

where the last expression, introduced in Ref. [5], makes explicit the fact that $P_{1\times 1}$ distinguishes which sublattice prevails in the top layer.

For the case of a (2×1) missing-row reconstructed surface, a lattice order parameter can be once again written as the $\mathbf{G}/2$-component of the Fourier transform of the height profile:

$$P_{2\times 1} = \langle \frac{1}{2N_c} \sum_{\mathbf{r}\in W,B} h_{\mathbf{r}} e^{i\mathbf{G}\cdot\mathbf{r}/2} \rangle \ . \tag{9}$$

Notice now that $P_{2\times 1}$ takes the value $\pm 1, \pm i$ on the four possible ground states of a (2×1) surface. Assigning an index $\theta = 0, \pi/2, \pi, 3\pi/2$ to the four possible sublattices of a (2×1) structure - $0, \pi$ and $\pi/2, 3\pi/2$ being associated to W and B sublattices being on the top layer, respectively - we see $P_{2\times 1}$ takes the value $+1$ (-1) if the W sublattice with $\theta = 0$ $(\theta = \pi)$ is on the top layer, and the value $+i$ $(-i)$ if the B sublattice with $\theta = \pi/2$ $(\theta = 3\pi/2)$ is on the top layer. $P_{2\times 1}$, therefore, can be zero even if one of the two sublattices prevails in the top layer. For instance, an *Ising* wall, see Fig. 3, causes a change of sign in the order parameter, but the same sublattice sits on the top layer on both sides of such a defect. One can then hope to distinguish between a deconstructed surface ($P_{2\times 1} = 0$) which has some remnance of order in that one of the two sublattices (W or B) prevails in the top layer, and a completely disordered situation.[8] For this purpose the (2×1) order parameter 8 is not useful, since it vanishes even at $T = 0$ in the presence of a (2×1) reconstruction. A possible way of doing this is to define the local "peak" operator

$$O_{\mathbf{r}} = \frac{1}{16} \prod_{i=1,\cdots,4} [\Delta h_{\mathbf{r},i} - 1] \tag{10}$$

where $\Delta h_{\mathbf{r},i} = h_{\mathbf{r}+\mathbf{b}_i} - h_{\mathbf{r}}$ and $\mathbf{b}_i$ with $i = 1, \cdots, 4$ are the vectors connecting a chosen site to its four nearest neighbours (belonging to the opposite sublattice). $O_{\mathbf{r}}$ takes the

value 1 for the atoms lying above all their neighbours and zero otherwise. Summing over all the sites with a phase factor 1 for the W sites and -1 for the B ones, we get an extensive operator, measuring again which sublattice prevails in the top layer,

$$P_{BW} = \langle \frac{1}{N_c} \sum_{\mathbf{r}} e^{i\mathbf{G}\cdot\mathbf{r}} O_{\mathbf{r}} \rangle \,. \tag{11}$$

As defined, P_{BW} is normalized to 1 on the unreconstructed ground states, and to 1/2 on the reconstructed (2×1) ground states. P_{BW} coincides, apart from a factor 2, with the order parameter P_{EO} defined in Ref. [8].

Notice, in passing, that the peak operator $O_{\mathbf{r}}$ allows us to write another order parameter for the missing-row reconstructed phase which should contain the same information as $P_{2\times1}$ in the following way:

$$P'_{2\times1} = \langle \frac{2}{N_c} \sum_{\mathbf{r}} e^{i\mathbf{G}\cdot\mathbf{r}/2} O_{\mathbf{r}} \rangle \,. \tag{12}$$

(As written, $P'_{2\times1}$ coincides with the corresponding order parameter introduced in Ref. [8].)

A third alternative route to define a P_{BW} order parameter, closely related to the simmetry of the (2×1) ground state, was followed by Mazzeo *et al.* [5]. They take

$$P_{BW}^{(2\times1)} = \langle \frac{1}{4N_c} [\sum_{\mathbf{r}\in W} |S_{\mathbf{r}}| - \sum_{\mathbf{r}\in B} |S_{\mathbf{r}}|] \rangle \,, \tag{13}$$

where the "spin" variables $S_{\mathbf{r}}$ are defined in terms of the nearest neighbours height differences as

$$S_{\mathbf{r}} = \sum_{i=1,\cdots,4} \Delta h_{\mathbf{r},i}. \tag{14}$$

We note that $P_{BW}^{(2\times1)}$ so defined is not relevant for a surface which is not (2×1) reconstructed, since it vanishes, for instance, on the unreconstructed ground states.

4 Results and discussion

We have performed extensive Monte Carlo simulations in order to clarify the behaviour of the K_3 and K_4–models in the disordered flat phase. The question addressed is the following: What do order parameters do in this phase diagram, specifically, *Is the order parameter P_{BW} equal to zero or different from zero in the disordered flat phase?*

A classical grand canonical Monte Carlo code has been set up and used for lattices of linear size $L = N_x = N_y$ up to 100. Starting from a disordered surface, we randomly add or remove particles, by making sure that the BCSOS constraint is

fulfilled, and accept moves according to the standard Metropolis algorithm. $2L^2$ attempted moves (the number of sites in the lattice) are referred to as a *sweep* or a Monte Carlo step. The configurations resulting from consecutive sweeps are usually quite correlated, so that independent values for the various averages are obtained as a result of a sufficiently large number of Monte Carlo steps. It is on the basis of such "independent measurements" that the statistical errors are estimated. Tipically 20 to 50 such measurements are performed, each of which consists of $10^5 - 10^6$ sweeps, after a suitable equilibration of the system. Such a heavy request of uncorrelated random numbers calls for a good random number generator. We have adopted a recently tested random number generator, of the lagged Fibonacci type, with a period of 10^{21}.[15]

For the K_3–model, we started from the previously quoted results of Mazzeo *et al.* They consider a point in the reconstructed part of the phase diagram, with coupling parameters chosen so as to fit the glue model results of Ercolessi *et al.* for gold.[16] An Ising type deconstruction transition is detected to take place at $T_D \approx 2.90 K_{2y}$, while a Kosterlitz-Thouless roughening transition is found at $T_R \approx 3.09 K_{2y}$. Whereas below deconstruction, and above roughening, the knowledge of the thermodynamics of the system is quite satisfactory, the situation is much less clear at intermediate temperatures, where the nature of the disordered flat phase is not yet fully understood. Available numerical results on smaller systems ($L \leq 32$), while succesful in determining other quantities, such as the deconstruction and roughening temperatures and their related exponents, are as yet inadequate, as we shall see, in assessing the behaviour of the P_{BW} order parameter.[5] In the disordered flat portion of the phase diagram, at temperatures intermediate between deconstruction and roughening, the correlation length ξ_{BW} of peak-peak correlation function is in fact much bigger, (as will be found in this section), than the corresponding reconstruction length $\xi_{2\times1}$.

We decided to perform first a careful finite size scaling analysis of all the different order parameters in the disordered flat region, selecting the temperature to be $T = 3.0 K_{2y}$, in the K_3–model with the same parameter values used in Ref. [5] for the (2×1) reconstructed situation. The surface is still flat at this temperature, as demonstrated from the size dependence of the square mean width δh^2

$$\delta h^2 = \frac{1}{2N^2} \sum_{\mathbf{r},\mathbf{r}'} \langle (h_{\mathbf{r}} - h_{\mathbf{r}'})^2 \rangle \ , \tag{15}$$

which should diverge logarithmically in the rough phase - $\delta h^2 \approx K(T) \log L$ - with a coefficient $K(T)$ larger than the universal minimum value $K(T_R) = 1/\pi^2$ (attained at roughening). Fig. 6 shows that our data for δh^2 versus $\log L$ stay definitely below the universal critical value of $K(T_R)$, which implies that δh^2 will actually saturate to a costant as $L \to \infty$. Fig. 7 shows the results obtained for $P_{2\times1}$ (solid circles), P_{BW} (diamonds), and $P_{BW}^{(2\times1)}$ (squares). The order parameter $P_{2\times1}$ vanishes as the inverse of the linear size L of the system, see inset of Fig. 7, confirming that at $T = 3.0 K_{2y}$ we are above the deconstruction temperature T_D in agreement with Ref.

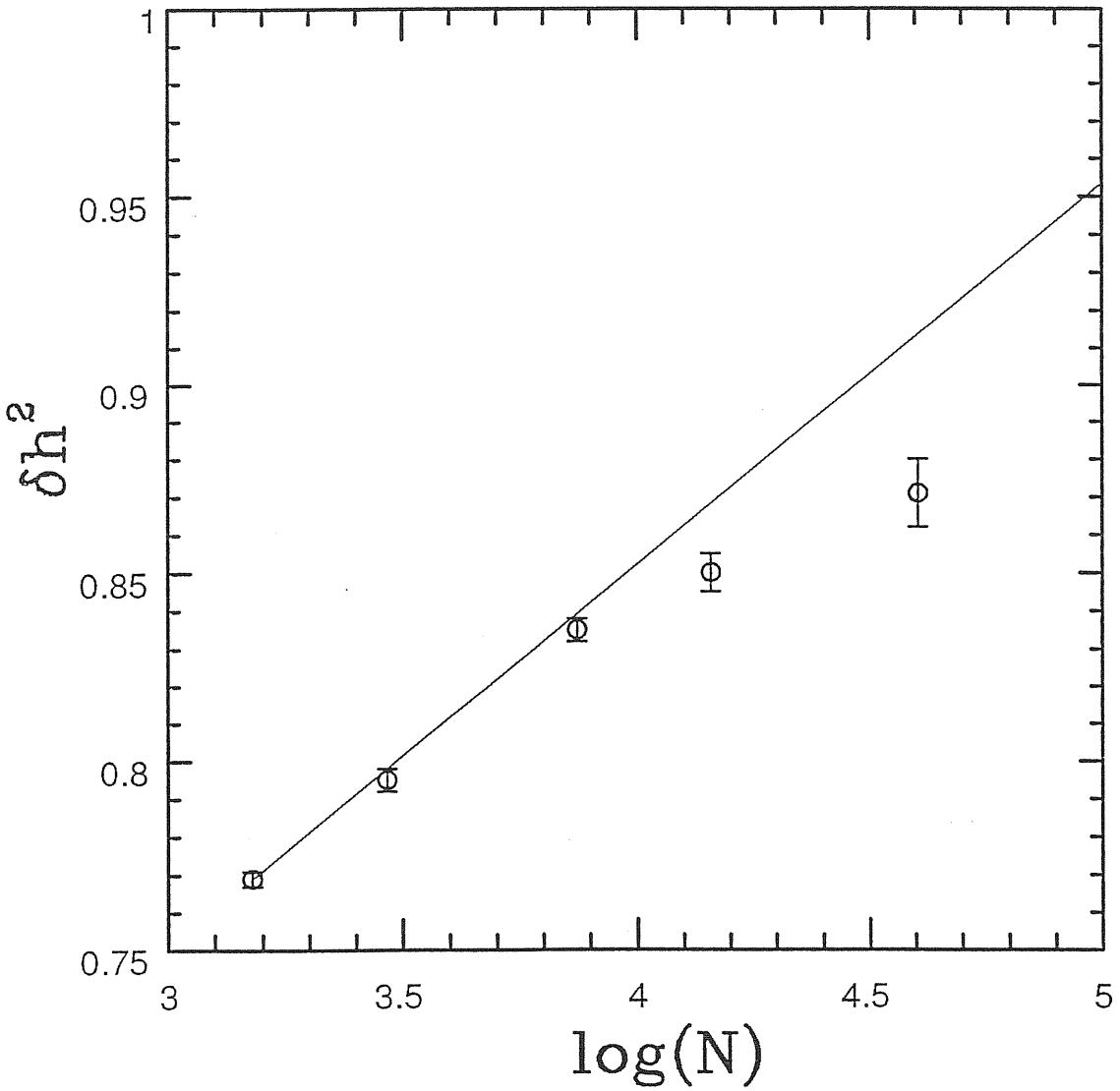


Figure 6: Finite size scaling of the height fluctuations for the K_3 point considered. A line having the critical slope $K(T_R) = 1/\pi^2$ is also shown.

[5]. This power law behaviour is readily understood in the following way. $P_{2\times1}$ is calculated as a lattice sum of the local operator $A_{\mathbf{r}} = h_{\mathbf{r}} e^{i\mathbf{G}\cdot\mathbf{r}/2}$. Its size dependence is therefore determined by the large distance behaviour of the corresponding AA correlation function

$$G_{AA}(\mathbf{r}) = \langle A_{\mathbf{0}} A_{\mathbf{r}} \rangle \ . \tag{16}$$

The L^{-1} dependence of $P_{2\times1}$ arises from an exponential, or otherwise integrable, decay at large r of the $G_{AA}(\mathbf{r})$. In particular, we expect exponential (2×1) correlations above deconstruction, consistent with $P_{2\times1} \sim L^{-1}$.

Instead a glance at Fig. 7 shows that *the same must not be true for the BW order parameters*. Both P_{BW} and $P_{BW}^{(2\times1)}$ decrease much slower than L^{-1}. This rules out an exponential decay to zero of the corresponding local operator correlation functions. A log-log plot helps clarifying the situation. Fig. 8 shows the logarithm of P_{BW} versus $\log L$. We observe that the data for small lattices - L up to 48 - can be fit with a power law $L^{-\omega}$ with $\omega \approx 0.37$. For larger values of L a crossover is seen to what is most probably an exponential convergence to *a non zero limit* for P_{BW}. In other words, systems up to $L = 48$ are still smaller than the actual value of ξ_{BW}, so that a fictitious power law behaviour is initially seen. A very similar behaviour is also found for $P_{BW}^{(2\times1)}$.

The corresponding results for a point inside the disordered flat phase of the K_4–model - $K_4/K_{2y} = 0.1$, $K_{2x}/K_{2y} = -0.0565$, and $T/K_{2y} = 2.3$ - are shown in Figs. 9-10. Entirely similar comments apply to this case.

The physics of the K_4–model is actually somewhat clearer than that of the K_3–model. The point considered in the K_4–model phase diagram is located close to the preroughening line which ends the unreconstructed phase. A typical snapshot of the way the surface looks like at this temperature is shown in Fig. 11. Although strictly speaking we are in a parameter region in which the classical ground state is (2×1) missing-row reconstructed and the most energetically favoured defects are *Ising* walls, we clearly see that there are large regions in which the surface looks unreconstructed (with either the W or the B sublattice on the top layer) and the most common defects are (2×1) steps.

The state of the system is indeed predicted to have the physics of a dimer spin state, which is a fluid of (2×1) steps with up-down order but without positional order.[10] Reconstructed regions can be seen as regions with (2×1) steps gaining positional order. (The (2×1) missing row ground state is nothing but a solid of such steps.) All this features are clearly seen in Fig. 11.

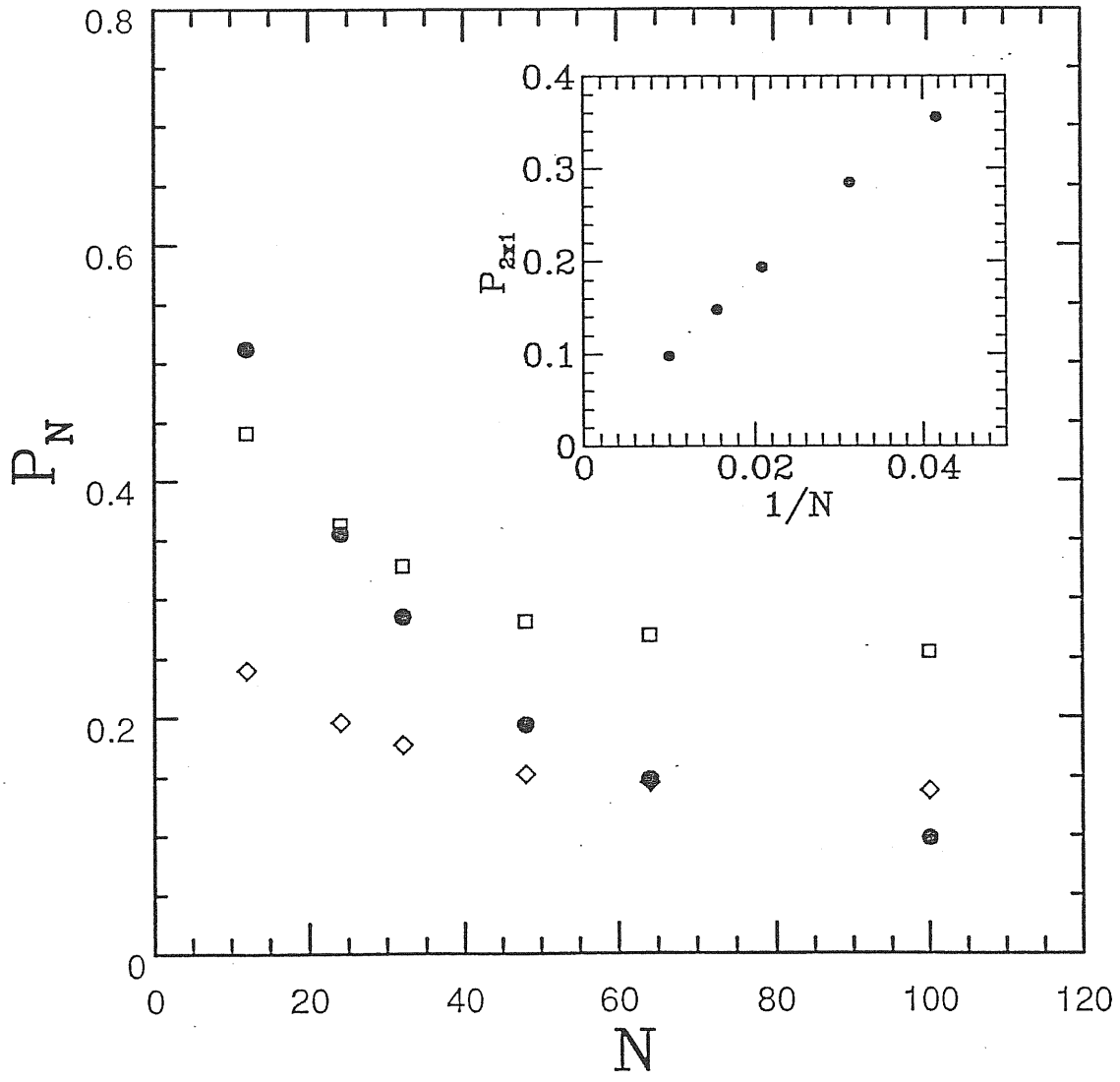


Figure 7: Finite size scaling of $P_{2\times1}$ (the reconstruction order parameter, full circles), $P_{B1\cdot}$ (open diamonds), and $P_{B1\cdot}^{(2\times1)}$ (open squares) for the K_3 point considered. The inset shows that $P_{2\times1}$ decays as the inverse of the linear size N of the lattice.

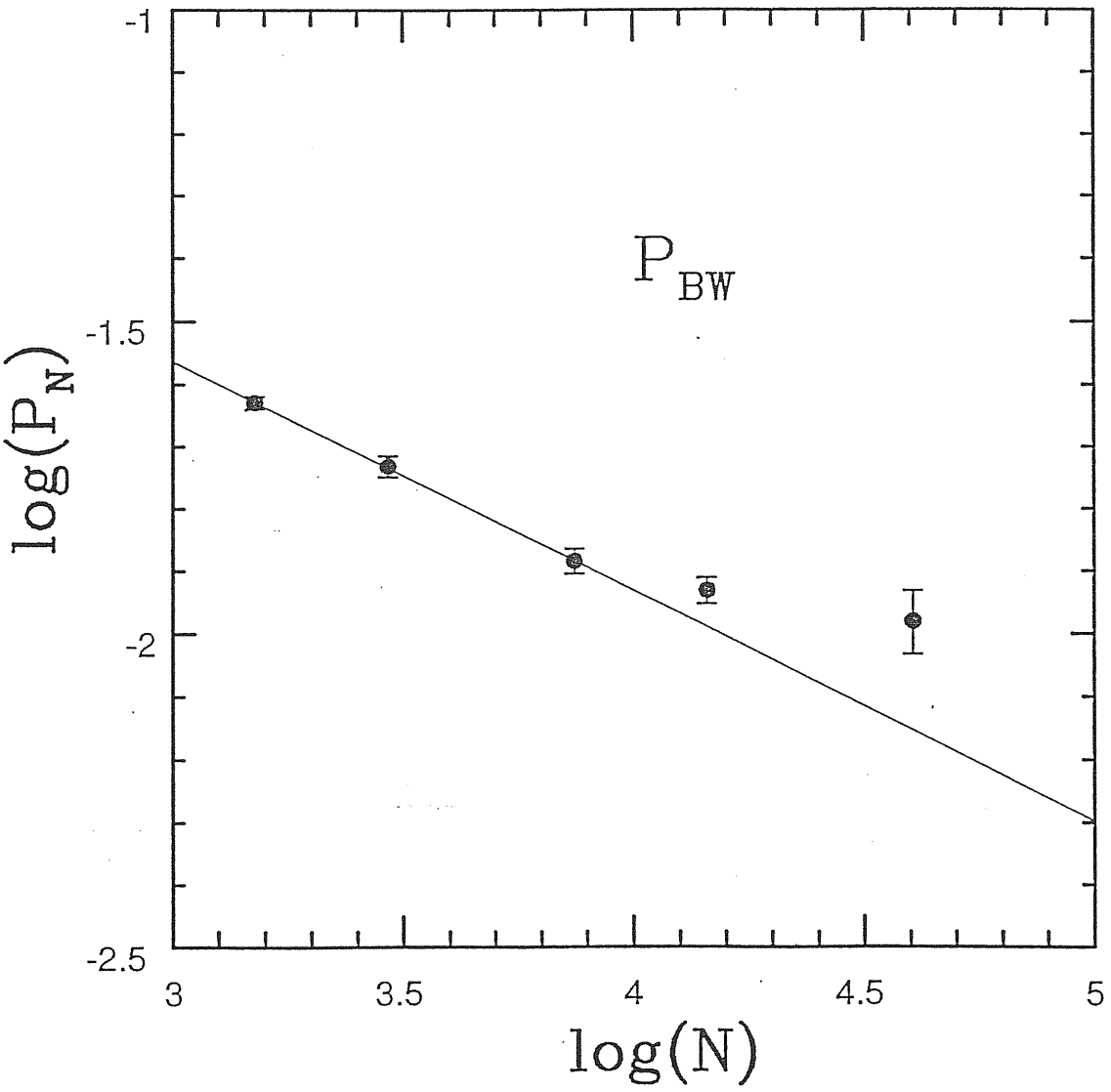


Figure 8: Log-log plot of the finite size behaviour of the P_{BII} order parameter for the K_3–model.

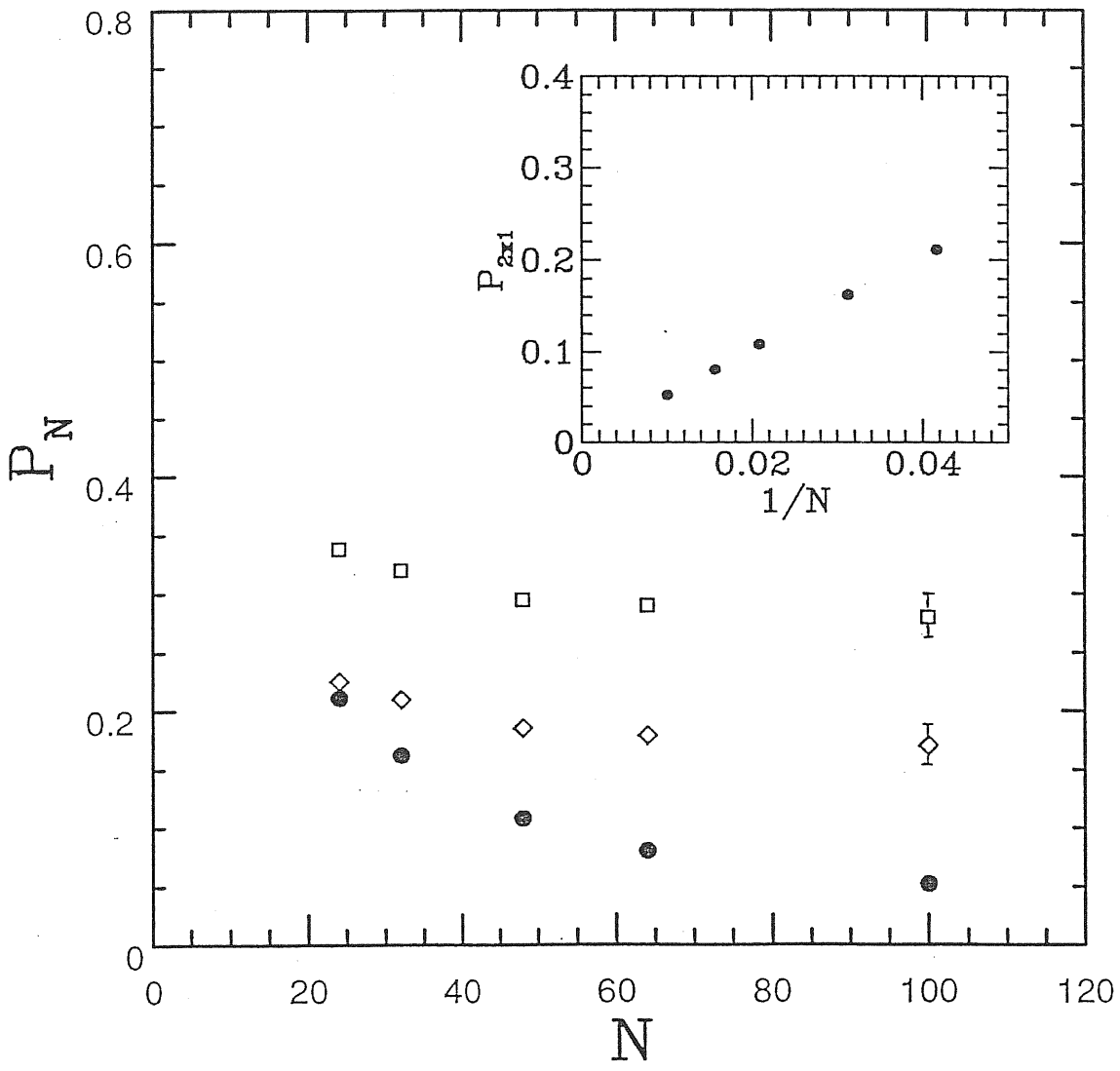


Figure 9: Finite size scaling of $P_{2\times1}$ (full dots), of $P_{BII'}$ (open diamonds), and of $P_{BII'}^{(2\times1)}$ (open squares) for the K_4 point considered.

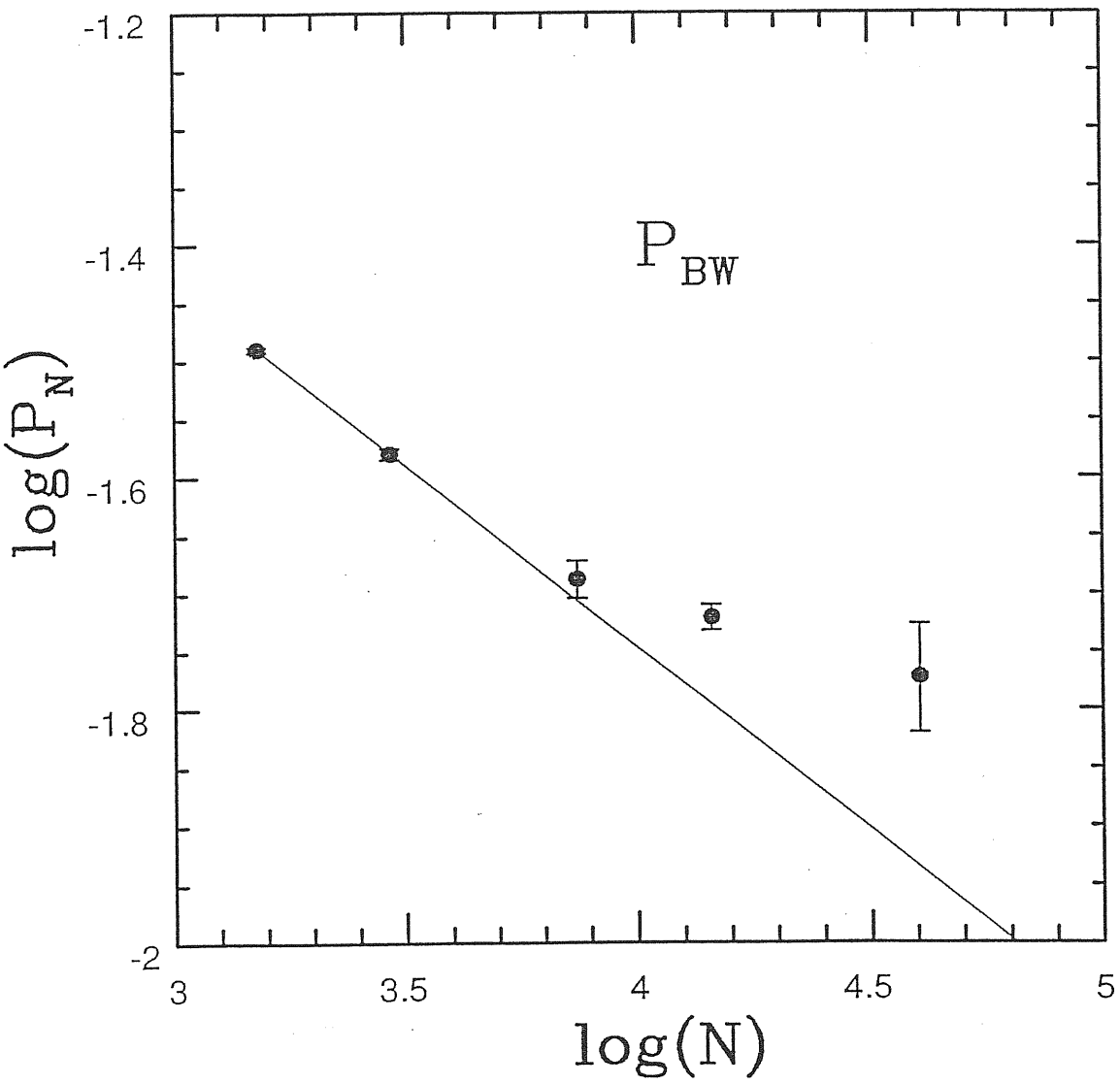


Figure 10: Log-log plot of the finite size behaviour of the P_{BW} order parameter for the K_4–model.

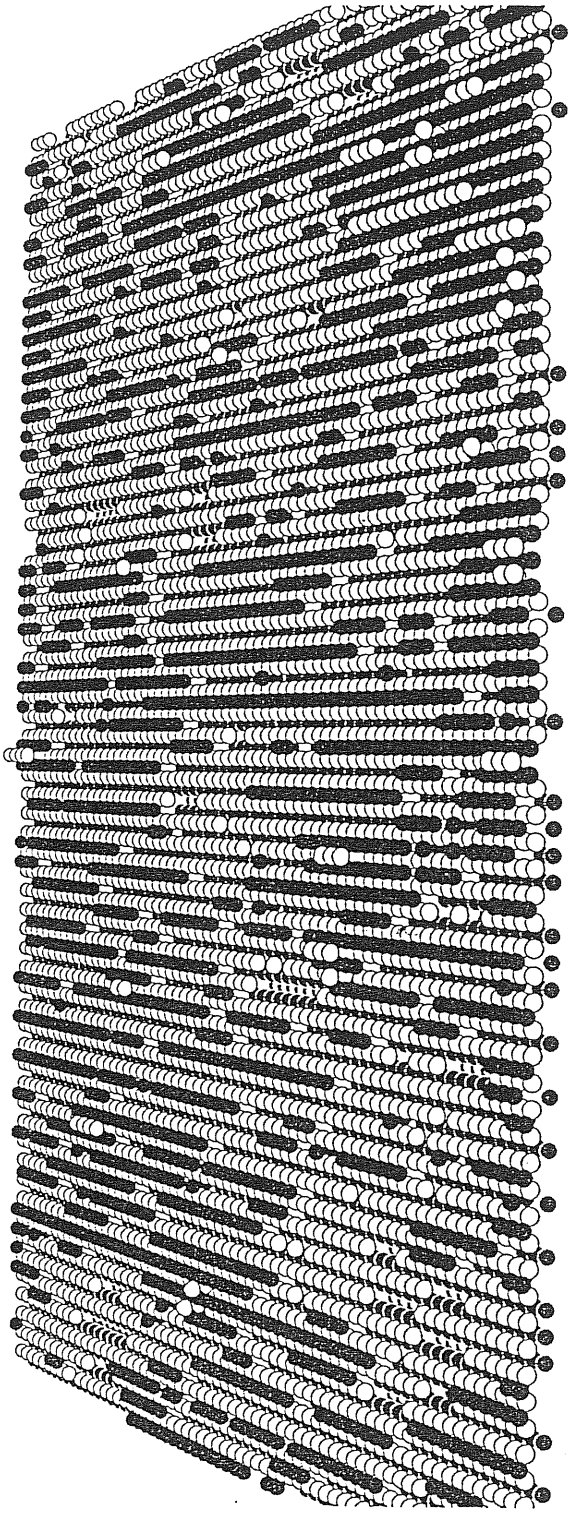


Figure 11: Snapshot of a surface configuration as generated by the Monte Carlo simulation for the K_4–model at a temperature of $2.3K_{2y}$.

5 Conclusions

The original motivation for the present work was a deeper understanding of the nature of the disordered flat phase (or phases) occurring in simple lattice models of fcc (110) surfaces. In particular, in the spirit of the distinction proposed in Ref. [8] between a DEF (Ising wall dominated) phase as opposed to a DOF (step dominated) phase, we wanted to clarify which of the two scenarios, or if perhaps both, was at play in the simple BCSOS-type models studied in Ref. [5] and [10].

It seems at least intuitively obvious that an order parameter P_{BW} counting the difference in the number of local peaks belonging to the white and to the black sublattice should indeed discriminate between the two possibilities. Such an order parameter would have, at least in principle, the nice feature of having some relationship to actual experiments. The coherent part of the specular peak in antiphase for X-ray scattering, in the usual kinematic approximation used by experimentalists, should measure directly P_{BW}. As a note of caution, we observe that a *small* P_{BW} inside a large incoherent background is however not easily accessible.

From the theorist's point of view, the discussion has to consider separately, at this stage, the case of semi–microscopic cell-type models [3] from that of fully microscopic surface models. In the former framework of a coarse-grained description of the system, as the four state clock-step model of den Nijs [3], the stage is clear and the actors are there: walls and steps. Since white atoms stay on top in regions where the reconstruction variable θ is 0 or π, and black atoms do so in regions where θ is $\pi/2$ or $3\pi/2$, the P_{BW} order parameter has to be non-zero in the disordered flat phase found in this model, which may therefore be called DEF. Indeed, the disordering transition resulting in a DEF phase is mostly promoted by walls, which involve a change of π for θ on either side of the defect. On the contrary, P_{BW} is expected to vanish in a hypothetical DOF phase, since in this case the relevant defects are steps, which involve a change of $\pm\pi/2$ for θ. The four values of θ should appear with the same probability in the disordered phase, and there is no way of telling which "color" prevails in the top atoms.

The question of possibly finding a DOF phase in the sense of Ref. [8] in a model of the clock-step type deserves, however, a few comments. Suppose that steps were indeed the most energetically favourable objects in the problem, $E_s \ll E_w$, and imagine wanting to stabilize a DOF phase, i.e., preventing the appearence of steps from making the surface immediately rough. The natural way of doing this is to assign vertex energies to the crossing of steps, in such a way as to *disfavour the crossing of parallel steps* with respect to antiparallel ones.[7] This is indeed the standard mechanism by which a DOF is stabilized in the context of RSOS models for simple cubic (110) surfaces (and, as a matter of fact, the context in which the term itself was first introduced). Such 6-vertex energies have been neglected by den Nijs in deriving the zero-chirality limit phase diagram for the clock-step model.[3] It is therefore an appealing suggestion, deserving further study, that their proper inclusion might open

up the possibility of a genuine DOF phase in the model.[8] What is however also quite clear is that this extra richness is probably lost as soon as one performs a *fermionic* mapping of the model.[18, 19] This is so, not so much due to the strong chirality limit involved (which appears to be only a technical simplification on the final fermionic hamiltonian obtained), but for the very same spirit of a fermionic mapping, which is supposed to catch the correct physics of the high anisotropy limit only. Only T-matrix elements up to *one* kink process are correctly accounted for in a fermionic mapping. However, vertices of the kind required in stabilizing a DOF phase involve a *double* kink for the two fermions involved, a process which is not correctly accounted for. The search of a DOF phase should therefore be pursued within the standard clock-step approach without going over to fermions.

Microscopic SOS models are in many ways more attractive, at first sight, as far as stabilizing a DOF is concerned: they automatically tend to disfavour crossing of parallel steps which involve large height differences. Moreover, tuning the model parameters offers, in principle, the possibility of making steps *or* walls more favourable, at least as far as their $T = 0$ energy is concerned. Things are however not so straightforward in practice. Consider, as a remarkable counterexample, the case of the K_4–model. When $K_{2x}/K_4 > -2$, simple Ising wall defects are energetically more favourable with respect to all kinds of steps (see Table 1). A value of $K_{2x}/K_4 = -0.56$, which is just the one we have simulated, seems therefore a quite promising candidate for making a true, almost ideal, DEF. What we end up with, instead, is a situation quite well represented by the snapshot in Fig. 11. Ising walls in their original form, i.e., that of Fig. 3 with the minimum possible wall width of one lattice spacing a_x, are almost totally absent. What one finds, instead, are extended walls of the Ising type with a width of arbitrary length. These are nothing but large (1×1) unreconstructed regions lying between two opposite (2×1) steps. Such (2×1) steps, which indeed are nothing but the very building blocks of a missing-row structure, are free to move in a fluid-like manner with the only constraint that a step up is necessarily followed by a step down. Occasionally, sequences of up-down (2×1) steps gain positional order by "solidifying" in (2×1) missing-row regions which are, however, always of the same "colour" (more precisely, black, for the phase illustrated in Fig. 11). Overall, the surface seems to have as many black regions as white ones: the $P_{1\times1}$ order parameter, which counts precisely the relative abundance of W and B (1×1) elementary cells, goes to zero in the thermodynamic limit. Correlations between steps, however, or, in more elementary terms, the fact that every (2×1) step always ends into a B top atom, resulting in the above mentioned feature of the absence of white missing-row regions, are such that $P_{B\overline{W}}$ turns out to be different from zero, albeit small. In summary, one has all the ingredients of a DEF (black) phase, including a $P_{B\overline{W}} \neq 0$, but with a DOF-like "look": steps (although *not* (3×1) steps) have fluid-like character and one can find B and W regions roughly in equal abundance. Should we label this phase DEF or DOF? The result of tailoring the $T = 0$ defect energies in such a way as to promote an Ising wall dominated DEF phase, ends up into an amusing illustration of a dimer state at its best (see Ref. [10]).

The fact that the "ideal" defects that one wanted to produce with a certain choice of parameter are not actually seen, is indeed a quite general feature of the simple SOS models we have simulated, and is in sharp contrast to the clear schematic picture coming out of a cell model of the clock-step type. A glance at the snapshot of a typical configuration within the simulation reveals a completely unobvious picture: defects are far from being clearly defined, they mix and modify into one-another, and have a discouraging amount of adatoms around, preventing a simple and direct identification of the expected features of a DEF or DOF phase.

One may even suspect that P_{BW} itself is not a good way of discriminating a DEF from a DOF, in the sense that P_{BW} might for some reason be different from zero in all disordered flat phases of all conceiveable SOS models with the BCSOS-type of height constraint. This doubt is inspired by the well known Lieb-Schultz-Mattis theorem which applies, under quite general circumstances, to spin-1/2 chains, [17] the quantum transfer-matrix limit of generic BCSOS-type models. It states that only two possibilities are allowed: either the system has a unique ground state with gapless excitations above, or it has a gap above a degenerate ground state which breaks some simple spatial symmetry (reflection or translation, typically). P_{BW} is *odd* under translation, and so is most probably any extensive object (made up of local quantities) which distinguishes W and B sublattices. Barring accidental cases, P_{BW} can only vanish, by symmetry, on phases which *do not break translational symmetry* which are however not simple to make-up, in view of the theorem: they have, most probably, a unique ground state with gapless excitations above, a likely candidate to a rough phase.

In conclusion, our study does not allow us to attach names (DEF or DOF) to the disordered flat phase(s) of simple SOS models so far studied. We have shown that the simple criterion of an order parameter like P_{BW} does not do the job as expected. Several possibilities (not mutually exclusive) are open, and some of them might be suitable for further study:

- Only *one* kind of disordered flat phase exist in models of the BCSOS-type, and it has $P_{BW} \neq 0$ (large, or small). A true distinction between DEF and DOF does not exist;
- There is a way of distinguishing a DEF from a DOF, but P_{BW} simply fails to do so on general grounds. One needs to resort to more complicated correlation functions (step-step, or so) to distinguish the two phases.
- We correctly found only a DEF phase, but with non-standard features which do not fit the ideal picture one had in mind. The "features" should be more strictly defined;
- We found only a DOF phase, but with non-standard features which do not fit the ideal picture one had in mind. The "features" should be more strictly defined;

- "Ideal" DEF and/or DOF phases might exist if one complicates the model sufficiently. By which correlation function are they distinguished from the disordered flat phase(s) we have been looking at?

6 Acknowledgments

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