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LETTER TO THE EDITOR

Exact calculation of the local height probabilities in the body-centred SOS model

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Abstract. The local height probabilities P_a and the mean square height average $\langle h^2 \rangle$ are calculated exactly for the smooth phase of the body-centred solid-on-solid model. Near criticality $P_a \sim K'(-t)^{1/4}$ and $\langle h^2 \rangle \sim K''(-t)^{-1/2}$, where t is the deviation from criticality parameter and K', K'' are constants specified in the text.

In this letter we calculate the local height probabilities P_a and the mean square height average $\langle h^2 \rangle$ for the smooth phase of the body-centred solid-on-solid (BCSOS) model. This is done by first using the van Beijeren (1977) mapping of the BCSOS model to the six-vertex model. We then note that the recently solved eight-vertex SOS model (Andrews *et al* 1984, Forrester and Baxter 1985) contains as a special case the solid-on-solid interpretation of the six-vertex model. From the expressions obtained for the P_a in the eight-vertex SOS model, the P_a for the six-vertex SOS model can then be written down immediately.

We begin with the body-centred cubic(BCC) Ising model. Each site on the BCC lattice $\mathscr{L}$ has a spin + or −. Let there be nearest- and next-nearest-neighbour interactions as shown in figure 1.

Let $\mathscr{L}$ consist of two interlaced simple cubic sublattices $\mathscr{L}_1$ and $\mathscr{L}_2$. Suppose the sites on the outermost layers of $\mathscr{L}$ are on $\mathscr{L}_1$. On the top layer of each sublattice fix the spins to be −; on the bottom layer of each sublattice fix the spins to be +. Now take the limit $J_0 \to \infty$. Then in each column there will be no − spin below a + spin, and the level of the + − interface in each nearest-neighbour columns will differ by +1 or −1. (Here we have taken as unity the height difference between nearest neighbours and the up direction as positive.)

To specify the level of the + − interface in each column, take a plane of spins in the sublattice $\mathscr{L}_1$ approximately halfway between the top and bottom planes and parallel to those planes. On the boundary of this plane fix the spins to be +. Define the + − interface thus specified in the outermost columns to occur at height 0. We measure all other heights of the + − interface as distances above or below this reference level.

To unambiguously specify the ground state of this model let us fix the spins on the boundary of the plane immediately above the reference plane to be +. These spins all lie on $\mathscr{L}_2$. The interface thus specified on the outermost columns of this plane occur at height 1. Note that since the level of the interface in each nearest-neighbour

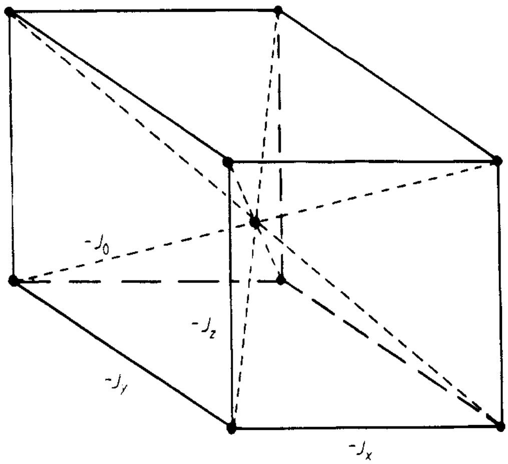

Figure 1. An elementary cube of the body-centred cubic lattice. The spin on the centre site is coupled to the spins on the surrounding cube (nearest neighbours) by the coupling $-J_0$. The spins on the surrounding cube are coupled to each other (next-nearest neighbours) by the couplings $-J_x$, $-J_y$, $-J_z$ in the x, y and z directions respectively.

column must differ by 1, heights on $\mathscr{L}_1$ are even integers, while the heights on $\mathscr{L}_2$ are odd.

The height above the reference plane of the $+-$ interface in each column specifies a configuration of the BCSOS model. Thus the BCSOS model is defined on a square lattice (rotated 45°), at each site there being an integer height with nearest-neighbour heights differing by 1 (see figure 2). Notice that the lattice can be decomposed into even and odd sublattices (corresponding to $\mathscr{L}_1$ and $\mathscr{L}_2$ of the original BCC lattice) which must contain even and odd heights respectively.

There are six allowed face configurations, which we list in figure 3. We associate a (normalised) energy of the interaction between the four nearest-neighbour columns to each allowed face configuration. The face weights are

$$\begin{aligned} a &= W(l, l+1|l-1, l) = W(l, l-1|l+1, l) = \exp(-2J_y/k_B T) \\ b &= W(l+1, l|l, l-1) = W(l-1, l|l, l+1) = \exp(-2J_x/k_B T) \\ c &= W(l+1, l|l, l+1) = W(l-1, l|l, l-1) = 1. \end{aligned} \tag{1}$$

Here the weight $W(l_i, l_j|l_m, l_n)$ corresponds to the face with surrounding sites i, j, n, m ordered anticlockwise starting from the left.

As observed by van Beijeren (1977) each of these configurations can be transformed into a six-vertex configuration by drawing an arrow outward if the height increases as you move clockwise around a face, and inward otherwise (see figure 3). In the symmetrical case $J_x = J_y$, from figure 3 and (1) we see that the allowed energies correspond to the F model (Baxter 1982, p 129).

At low temperatures the F model is in an ordered antiferromagnetic phase. In the BCSOS model this corresponds to a flat phase in which the probability of a site deep within the lattice having height a (a any integer) is non-zero (provided of course a is even (odd) on the even (odd) sublattice). The use of 'a' here to denote height should not be confused with the 'a' in (1) which denotes the weight.

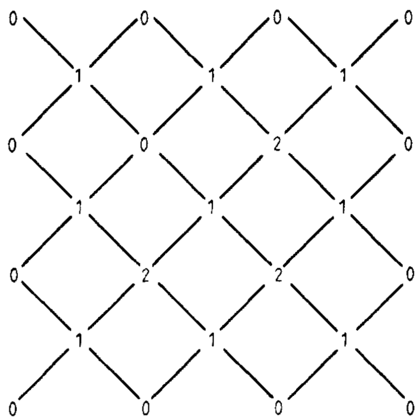

Figure 2. A typical configuration of the BCSOS model with boundary conditions as specified in the text.

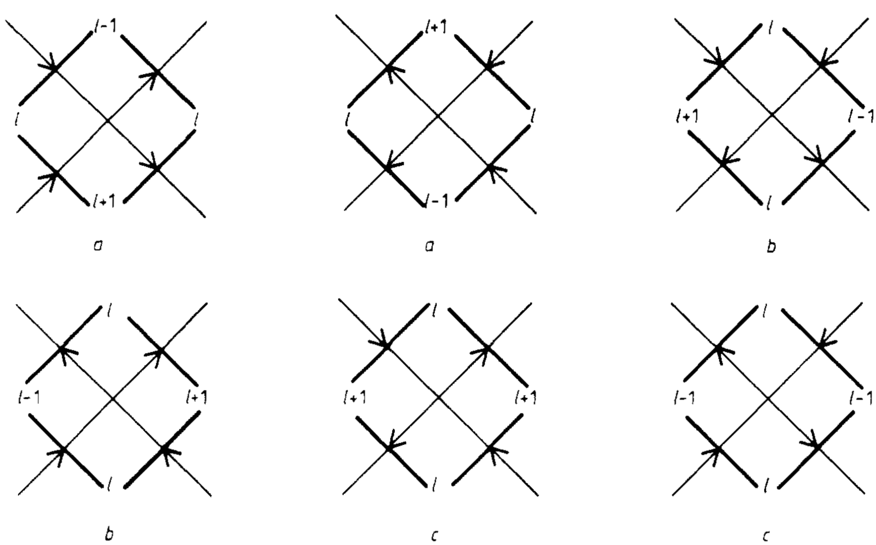

Figure 3. The six allowed configurations of heights round a face of the lattice, and the corresponding vertex configurations.

The local height probability is defined as

$$P_a = \sum \delta(a, l_1) \prod W(l_i, l_j | l_m, l_n) / \sum \prod W(l_i, l_j | l_m, l_n) \tag{2}$$

where the weight function W is given by (1), the product is over all faces (i, j, n, m) of the square lattice, and the sum is over all allowed height configurations. For definiteness, the site with height l is taken to be the centre of the lattice, but any site deep within the lattice will do. With the square lattice rotated 45°, the outer heights are fixed at 0, and the second outer heights at 1 (recall figure 2).

Andrews *et al* (1984) have evaluated the P_a for an infinite sequence of SOS models (the so called eight-vertex SOS model). In that work the weight function W was given by (equation (A37))

$$\begin{aligned}
\alpha_l &= W(l, l+1|l-1, l) = W(l, l-1|l+1, l) = \nu w^{1/2} E(xw^{-1}) \\
\beta_l &= W(l+1, l|l, l-1) = W(l-1, l|l, l+1) = \nu[xE(x^{l-1})E(x^{l+1})/E^2(x^l)w]^{1/2}E(w) \\
\gamma_l &= W(l+1, l|l, l+1) = \nu E(x)E(x^l w)/E(x^l) \\
\delta_l &= W(l-1, l|l, l-1) = \nu E(x)E(x^l/w)/E(x^l)
\end{aligned} \tag{3}$$

where

$$E(x) \equiv E(x, y) = \prod_{n=1}^{\infty} (1-y^{n-1}x)(1-y^n x^{-1})(1-y^n)$$

$$= \sum_{n=-\infty}^{\infty} (-1)^n x^{n(n-1)/2} z^n \tag{4}$$

and

$$y = x^r. \tag{5}$$

Here we have not written some factors in the weights which do not alter the P_a (see Forrester and Baxter 1985, equation (1.4.2)). The heights are restricted to lie in the interval $1 \leqslant l_i \leqslant r-1$, and heights on adjacent sites of the square lattice must differ by unity. Consider regime III of this model so that $w^{1/2} < x < 1$. Now take the limits $r \to \infty$, $l \to \infty$ with x, w and ν fixed in the weights (3). Writing

$$x = \exp(-2\lambda) \qquad w = \exp[-(\lambda + v)] \qquad \nu = \tfrac{1}{2}\rho\, e^{\lambda} \tag{6}$$

we obtain from (3) and (4)

$$\begin{aligned}
&\alpha_l \to \rho \sinh[\tfrac{1}{2}(\lambda - v)] \\
&\beta_l \to \rho \sinh[\tfrac{1}{2}(\lambda + v)] \\
&\gamma_l, \delta_l \to \rho \sinh(\lambda).
\end{aligned} \tag{7}$$

This is precisely the parametrised form of the six-vertex weights a, b, c respectively (Baxter 1982, equation (8.9.7)). By comparing (7) and (1) we see that in the symmetrical case $J_x = J_y$ we must take

$$\begin{aligned}
&\rho = 1/\sinh(\lambda) \\
&v = 0 \\
&\sinh(\lambda/2)/\sinh(\lambda) = \exp(-2J_x/k_B T).
\end{aligned} \tag{8}$$

Thus regime III of the eight-vertex SOS model reduces to the BCSOS model in the limits $r \to \infty$, $l \to \infty$. In this regime the local height probabilities $P_{a'}$ were calculated to be

$$P_{a'} = x^{(1/2)[a'(a'-1)+b(b+1)]} E(x^{a'}, y)\Delta(x)/[E(-x, x^4)E(x^b, y/x)] \tag{9}$$

$$\Delta(x) = x^{-a'b}E[-x^{2(r-2)(r-a')+2rb}, x^{4r(r-2)}] - x^{a'b}E[-x^{2(r-2)(r+a')+2rb}, x^{4r(r-2)}] \tag{10}$$

where the boundary heights were fixed at b, $b+1$.

From (9), by taking the limits r, a', $b \to \infty$, $a' - b = a$ and fixed, we obtain for the BCSOS model

$$P_a = x^{(1/2)(a^2-a)}/E(-x, x^4). \tag{11}$$

If a is on the odd (even) sublattice, a must be odd (even). The mean square height average is

$$\langle h^2\rangle \equiv \tfrac{1}{2}\sum_{a=-\infty}^{\infty} a^2 P_a$$

$$= \sum_{a=1}^{\infty} a^2 x^{(1/2)(a^2-a)}/E(-x, x^4). \tag{12}$$

(The prefactor of $\frac{1}{2}$ accounts for the two sublattices.) Note that these results are identical to the P_a and $\langle h^2\rangle$ of a discrete Gaussian model with single site interactions only, the Boltzmann weight at each site being $x^{(1/2)(a-1/2)^2}$. From (6) and (8), x is given in terms of the original Boltzmann weights (1) by

$$x = \tfrac{1}{2}\{\exp(2J_x/k_B T) + [\exp(4J_x/k_B T) - 4]^{1/2}\}. \tag{13}$$

As $x \to 1^-$ the model becomes critical. From (13) this corresponds to

$$J_x/k_B T \to \tfrac{1}{2}\log 2 \tag{14}$$

which marks the onset of a rough phase in which the P_a are zero for each a and $\langle h^2\rangle$ is infinite. Of particular interest is the singular behaviour of P_a and $\langle h^2\rangle$ as $x \to 1^-$.

Defining the deviation from criticality parameter by

$$t = (T - T_c)/T_c \tag{15}$$

with T_c specified by (14) we have from (13)

$$\log x \sim (2\log 2)^{1/2}|t|^{1/2} \qquad \text{as } t \to 0. \tag{16}$$

As $x \to 1^-$, the theta functions exhibit the familiar behaviour (which can be derived by using the Poisson summation formula (Baxter 1982, p 468))

$$E(-x, x^4) \sim (\pi/4\log x)^{1/2} \tag{17}$$

$$\sum_{a=1}^{\infty} a^2 x^{(1/2)(a^2-a)} \sim (1/4\pi)(\pi/\log x)^{3/2}. \tag{18}$$

Hence from (11), (12), (16)-(18) we have the leading order singular behaviour as $t \to 0^-$

$$P_a \sim K'(-t)^{1/4} \tag{19}$$

$$\langle h^2\rangle \sim K''/(-t)^{1/2} \tag{20}$$

where

$$K' = (2\log 2)^{1/4}(4/\pi)^{1/2} \tag{21}$$

$$K'' = \tfrac{1}{2}(2\log 2)^{-1/2}. \tag{22}$$

It is possible to construct a dynamical theory which well describes the long-wavelength, low-frequency behaviour† of the roughening transition (see e.g. Weeks 1979). In particular, by use of the fluctuation-dissipation theorem, the theory should correctly give the leading order singular behaviour of the height-height correlation $\langle (h_i - h_j)^2\rangle$ for large separations of the sites i and j.

† The following is due essentially to the referee.

Just below T_c the theory predicts

$$\langle (h_i - h_j)^2 \rangle \sim \frac{1}{\pi^2} \log \frac{\xi^2}{1 + \xi^2/(R_{ij})^2} \tag{23}$$

where ξ denotes the correlation length and R_{ij} denotes the distance between sites. (This can be derived from equations (48) and (49) of Weeks (1979).) However in the BCSOS model we must recall that $\langle (h_i - h_j)^2 \rangle$ is zero unless the sublattice of the sites i and j corresponds to the parity of the heights h_i and h_j. This means that for the BCSOS model we must divide the right-hand side of (23) by 2. Remembering this and taking $R_{ij} \to \infty$ in (23) we obtain

$$2\langle h^2 \rangle \sim (1/\pi^2) \log \xi. \tag{24}$$

For the F model it is known that near T_c (Baxter 1982, equation (8.11.24))

$$\xi^{-1} \sim 4 \exp(\pi^2/\log x). \tag{25}$$

Substituting (16) for $\log x$ we obtain from (25) and (24) the behaviour of $\langle h^2 \rangle$ just below T_c as given by the dynamical theory. The result is in precise agreement with the exact result (20) and (22).

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