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LETTER TO THE EDITOR

Roughening transitions and the zero-temperature triangular Ising antiferromagnet

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Abstract. The zero-temperature triangular Ising antiferromagnet is mapped onto a solid-on-solid (SOS) model. The system undergoes a roughening transition characterised by a critical exponent $\alpha = \frac{1}{2}$, by the absence of excitations in the smooth phase, and by domain wall excitations (stripes) in the rough phase. At infinite SOS temperature the height–height correlation function is explicitly calculated with the aid of known four-point Ising correlations. We point out that a certain six-vertex model with a comparable SOS interpretation has an identical critical temperature, critical exponent and critical amplitude. This is in support of existing ideas on universality in systems with striped phases.

Since the solution of the triangular Ising model by Houtappel (1950), it is known that this model has a phase transition characterised by a specific heat exponent $\alpha = 0$ (there is no phase transition if the strongest interaction is antiferromagnetic and the remaining two are equal). We consider antiferromagnetic couplings K_i (which contain the inverse temperature as a factor), where i equals 1, 2 or 3 and refers to the three nearest-neighbour bond directions on the lattice. We put $K_i = K + \Delta_i$ for $i = 1, 2$ and $K_3 = K$ and let $\Delta_1 \geqslant \Delta_2$ and $\Delta_1 \geqslant 0$. We are interested in the limit $K \to -\infty$. In this limit, the condition for criticality (Houtappel 1950) goes over into a critical line in the Δ_1, Δ_2 plane given by

$$y_1 - y_2 = 1 \qquad \text{where } y_i = e^{2\Delta_i}. \tag{1}$$

Houtappel's expression for the reduced free energy per spin in the thermodynamic limit becomes, after subtraction of the infinite constant $-K$,

$$f(\Delta_1, \Delta_2) = (4\pi)^{-1} \int_0^{2\pi} d\omega \, \ln[\tfrac{1}{2}(y_1 y_2^{-1} + y_1^{-1} y_2 + y_1^{-1} y_2^{-1} + 2y_1^{-1} \cos\omega) + \tfrac{1}{2}|y_1 y_2^{-1} - y_1^{-1} y_2 - y_1^{-1} y_2^{-1} - 2y_1^{-1} \cos\omega|], \tag{2}$$

periodic boundaries being assumed. For $y_1 - y_2 \geqslant 1$ we have an ordered phase. The expression between absolute value signs is non-negative and f reduces to

$$f(\Delta_1, \Delta_2) = \Delta_1 - \Delta_2. \tag{3}$$

For $y_1 - y_2 < 1$ we have a disordered phase. Defining

$$\omega_c(\Delta_1, \Delta_2) = \cos^{-1}[\tfrac{1}{2}(y_1^2 y_2^{-1} - y_2 - y_2^{-1})], \tag{4}$$

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we obtain

$$f(\Delta_1, \Delta_2) = \Delta_1 - \Delta_2 + (2\pi)^{-1} \int_0^{\omega_c(\Delta_1,\Delta_2)} d\omega \ln(y_1^{-2}y_2^2 + y_1^{-2} + 2y_1^{-2}y_2 \cos\omega). \tag{5}$$

To find the energy, we set $\Delta_i = \beta E_i$ and obtain by differentiation

$$\frac{df}{d\beta} = E_1 - E_2 + \frac{\omega_c}{\pi}(-2E_1 + E_2) + \frac{2}{\pi} E_2 \tan^{-1}\left(\frac{y_2^2 - 1}{y_2^2 + 1} \tan\frac{\omega_c}{2}\right). \tag{6}$$

Figure 1 shows $df/d\beta$ versus Δ_1 for the case $\Delta_2 = 0$.

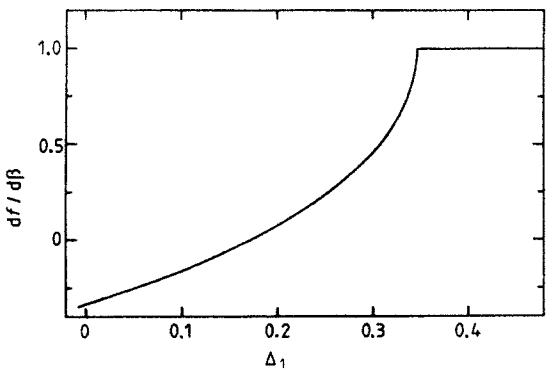

Figure 1. Energy in units $-E_1$ of the Ising model described in the text plotted against Δ_1. At $\Delta_1 > \frac{1}{2}\ln 2$ the system is completely ordered. The quantity plotted along the vertical scale can also be interpreted as the average slope of an SOS model (see text).

In the neighbourhood of the critical point $\beta = \beta_c$, the angle ω_c is of order $(\beta_c - \beta)^{1/2}$ and the leading terms of the energy are given by

$$df/d\beta \approx E_1 - E_2 - (2/\pi) y_1^{-1} y_2^{-1} (y_1 E_1 - y_2 E_2)^{3/2} (\beta_c - \beta)^{1/2}. \tag{7}$$

From (3) we see that the specific heat vanishes in the low temperature phase. From (7) we see that the specific heat C obeys

$$C \sim (\beta_c - \beta)^{-1/2} \qquad \text{as } \beta \uparrow \beta_c. \tag{8}$$

Hence, in contrast to the Houtappel result for finite K, we find a specific heat exponent $\alpha = \frac{1}{2}$.

As already mentioned, the total free energy per particle also contains an infinite constant $-K$: only those configurations which have precisely one pair of parallel spins around each elementary triangle produce non-vanishing terms in Z. This property allows us to interpret the system as a roughening model. To see this, we draw solid lines between all pairs of antiparallel spins. As illustrated in figure 2, there is a one-to-one correspondence (apart from a trivial factor 2) between the allowed spin configurations and the coverings of the lattice by diamonds. The partition function Z is a sum of weighted diamond coverings. The diamond weights can be obtained by sharing the bond weights of nearest-neighbour spin pairs out between adjacent diamonds and are listed in figure 3.

When looking at figure 2 in perspective one can consider it as the irregular surface of a cubic lattice, viewed from the (1, 1, 1) direction. This suggests the assignment of

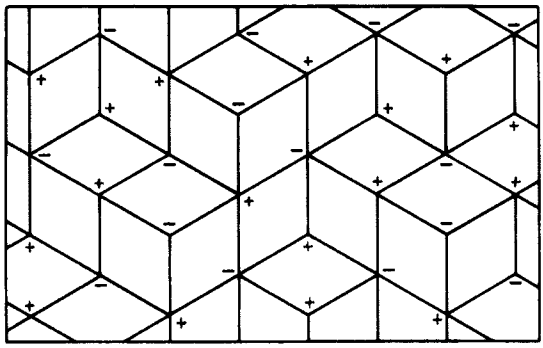

Figure 2. A typical configuration of up spins (+) and down spins (−) on the triangular lattice. Each elementary triangular lattice face contains precisely one pair of parallel nearest-neighbour spins. All antiparallel nearest-neighbour pairs are connected by full lines. This results in a diamond covering of the lattice.

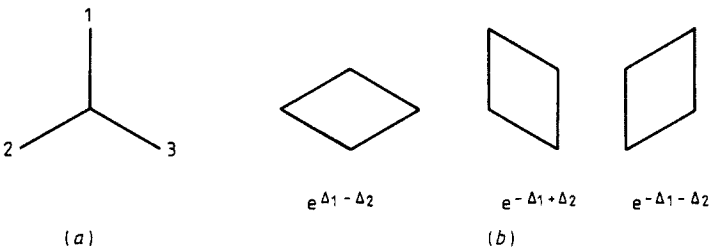

Figure 3. (*a*) Definition of the three main directions of the lattice. The coupling K_i is understood to act along the ith direction. (*b*) The Boltzmann weights of the diamonds.

a height variable h_i to each lattice site i in the following way: (i) let a given site at the origin have height zero; (ii) let there be, between any nearest-neighbour pair of sites connected by a full line, a height difference +1 or −1, depending on their relative position, as indicated in figure 4. Clearly no conflict arises as one travels around a closed loop of full lines. The height differences between nearest-neighbour sites not connected by a full line are easily deduced and have also been listed in figure 4. It

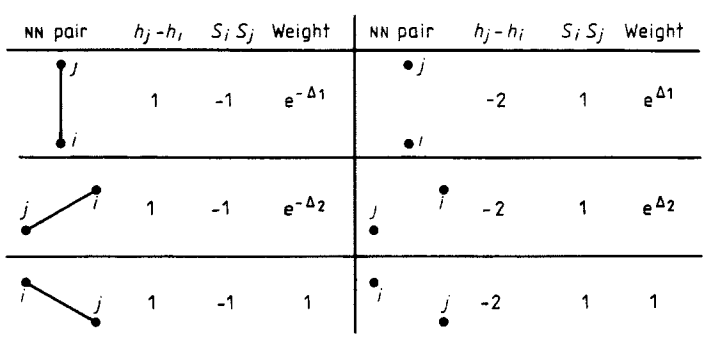

Figure 4. Height differences, spin products and Boltzmann factors for pairs of nearest-neighbour sites i and j. Left-hand side: i and j connected; right-hand side: i and j not connected.

is evident that the energy of a configuration of height variables can be expressed as a sum of interaction energies associated with nearest-neighbour height differences (see the last column of figure 4). Thus we have an SOS model with nearest-neighbour interactions, with height differences subject to the constraints imposed by the diamond covering. We can now analyse the phase transition expressed by equations (2)–(8) in terms of this SOS model.

Because $\Delta_1 \geqslant \Delta_2$, the ground state configuration is the one with a regular covering by diamonds of orientation 1 only (see figure 3(*b*)). The corresponding SOS configuration is a completely flat, but tilted, surface. Excitations from the ground state are obtained by turning diamonds from orientation 1 to orientations 2 or 3. One easily discovers that an elementary excitation must consist of an infinite string of turned diamonds (each having orientation 2 or 3), running from left to right through the system (see figure 5). Such elementary excitations therefore cost an energy proportional to the linear size N. By a simple energy-versus-entropy argument one can find out if any of these excitations are present; this also produces equation (1). Diamond coverings with strings of excitations correspond to a surface with steps in the SOS picture; one step separates two levels as shown in figure 5. The density $\rho(\Delta_1, \Delta_2)$ of string excitations is equal to the density of flipped diamonds, given by

$$\rho(\Delta_1, \Delta_2) = \tfrac{1}{2} - \tfrac{1}{2}\,\partial f/\partial \Delta_1 = \omega_c(\Delta_1, \Delta_2)/\pi. \tag{9}$$

Thus the string density vanishes with a square root singularity at the critical temperature.

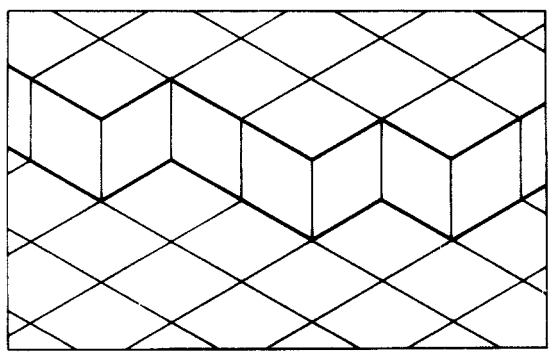

Figure 5. Diamond covering with a string of flipped diamonds. In the SOS picture, the string forms a step on an otherwise flat surface.

A different way to arrive at our present results is via the equivalence of the modified KDP model and the dimer problem on the hexagonal lattice (Wu 1968), which is equal to our diamond problem. It was already found by Kasteleyn (1963) that this dimer problem is characterised by string excitations; the exact solution by Wu (1968) showed that $\alpha = \frac{1}{2}$ for these models. Square root singularities were also reported by Nagle (1975) and by Pokrovsky and Talapov (1979), and later studied in greater detail by others (Villain and Bak 1981, Haldane and Villain 1981); here this singularity has been extracted from the Ising model solution.

Since the distance between successive strings is irregular, SOS configurations in the high-temperature phase have only an average tilt, and their roughness is determined by the fluctuations around this average. It is therefore natural to define $\delta h_i = h_i - \langle h_i \rangle$

(with $\langle \ldots \rangle$ indicating the ensemble average) and to consider the height–height correlation function

$$G(r) = \langle (\delta h_0 - \delta h_r)^2 \rangle, \tag{10}$$

where 0 and r are two lattice sites a distance r apart (measured in units of the nearest-neighbour distance). We suppose now that the lattice vector from 0 to r is along one of the main crystal directions (see figure 3(a)), and that 0 and r are separated by the sites $1, 2, \ldots, r-1$. From figure 4 we see that the height difference between two successive sites ($j = i+1$) can be expressed in terms of Ising spins as

$$\delta h_{i+1} - \delta h_i = -\tfrac{3}{2}(s_i s_{i+1} - \langle s_i s_{i+1} \rangle). \tag{11}$$

Substituting this in (10), we obtain

$$G(r) = \tfrac{9}{4} \sum_{i=1}^{r} \sum_{j=1}^{r} (\langle s_{i-1} s_i s_{j-1} s_j \rangle - \langle s_{i-1} s_i \rangle \langle s_{j-1} s_j \rangle). \tag{12}$$

This shows that the height–height correlation $G(r)$ in the SOS model is directly proportional to the energy fluctuation along a line segment of length r in the Ising model.

There is one special case in which we can calculate $G(r)$ explicitly, namely when $\Delta_1 = \Delta_2 = 0$ (or $\beta = 0$). This case corresponds to the zero-temperature isotropic Ising antiferromagnet, for which Stephenson (1970) has calculated precisely those four-spin correlations which are needed in (12). His result is that

$$\langle s_{i-1} s_i s_{j-1} s_j \rangle - \langle s_{i-1} s_i \rangle \langle s_{j-1} s_j \rangle = \begin{cases} 0 & \text{for } |i-j| = 3, 6, 9, \ldots, \\ -3/\pi^2 (i-j)^2 & \text{otherwise.} \end{cases} \tag{13}$$

Substituting this result in (12), we obtain after some algebra

$$G(r) = (9/\pi^2) \log r + (9/\pi^2)[1 + \gamma + \tfrac{1}{2} \log 3] + O(1/r) \tag{14}$$

where γ is Euler's constant. Thus the critical behaviour of this roughening model is very different from that of the ordinary roughening transition, which is of infinite order (van Beijeren 1977, Knops 1977, José *et al* 1977). The possibility of finite-order roughening transitions has already been mentioned by van Beijeren, and Knops (1979) presented an SOS model with $\alpha = -2$. Whereas in Knops' model the transition is of finite order due to an asymmetry between two sublattices, the obvious cause in our case is the string nature of the excitations.

Haldane and Villain (1981) emphasise that the square root singularity must be general for all systems with excitations of that kind. We investigate this here by confronting our results above with the exact analysis of a second model, namely the six-vertex model with reduced vertex energies $e_1 = -e_2 = h + v$, $e_3 = -e_4 = h - v$, $e_5 = e_6 = 0$, in the usual notation (Lieb and Wu 1972). This system is equivalent to a roughening model by the van Beijeren (1977) mapping (but it is not van Beijeren's SOS model). The solution of this six-vertex model has been sketched by Sutherland *et al* (1967). The model has a transition to the completely polarised state at

$$(e^{2h} - 1)(e^{2v} - 1) = 1 \tag{15}$$

(Lieb and Wu 1972). We now investigate the solution near complete polarisation, i.e. for a relatively small number n of overturned arrows along the transfer direction, along the lines indicated by Lieb and Wu. Using the Bethe ansatz, one finds for a

vertex model of width N and periodic boundaries that the largest eigenvalue λ_n of the transfer matrix in the subspace of n excitations is given by

$$\lambda_n = \exp[N(h+v) - 2nv] / \prod_{j=1}^{n} [\exp(-2h - ik_j) - 1] \tag{16}$$

where the wavenumbers k_j obey, for $n \ll N$, in leading order of $1/N$,

$$k_j \approx (-n - 1 + 2j)\pi / N. \tag{17}$$

Retaining the leading combinations of powers of n and N ($N \gg n \gg 1$) leads to

$$\lambda_n \approx e^{N(h+v)} [e^{-2v}/(1 - e^{-2h})]^n (1 - n^3 \pi^2 / N^2 24 \sinh^2 h). \tag{18}$$

The largest eigenvalue occurs for $\partial \lambda_n / \partial n = 0$ or

$$n/N = (2/\pi) \sinh(h) \{2 \log [e^{-2v}/(1 - e^{-2h})]\}^{1/2} \tag{19}$$

and the reduced free energy per particle $f = \lim_{N \to \infty} (1/N) \log \lambda_n$ is given by

$$f(h, v) = h + v + (4\sqrt{2}/3\pi) \sinh(h) \{\log [e^{-2v}/(1 - e^{-2h})]\}^{3/2}. \tag{20}$$

The transition is, like in our first SOS model, characterised by $\alpha = \frac{1}{2}$ but the similarity goes further. When we suppress vertex 1 ($e_1 = +\infty$) we obtain the modified KDP model; the equivalence of this model with our first SOS model via the mapping of Wu (1968) can also be obtained directly via the one-to-one correspondence between strings of inverted arrows in the KDP model and strings of flipped diamonds such as shown in figure 5. If we use the equivalence $h = \Delta_1$, $v = \Delta_1 - \Delta_2$, our equation (2) agrees, as expected, with the free energy of the $\varepsilon = 0$ modified KDP model (Lieb and Wu 1972, Wu 1968). Further, using this equivalence to express (20) in Δ_1 and Δ_2, and subsequently differentiating with respect to the temperature, reproduces the singular part of (7) exactly. Hence the two models are equivalent at a low excitation density: they have the same critical temperature, critical exponent and critical amplitude. This corroborates and extends the intuitive ideas of Haldane and Villain (1981) on universality in systems with striped phases.

Concluding, we have pointed out the existence of a special limiting case contained in the Houtappel solution of the triangular Ising model, having a specific heat exponent $\alpha = \frac{1}{2}$ and a disordered phase characterised by uniaxial domain walls (stripes), similar to those occuring in the floating phase of ANNNI models (Selke and Fisher 1980). Using a mapping onto an SOS model, we have obtained exact results for a roughening transition. Very similar critical behaviour is found for a second SOS model via the van Beijeren mapping.

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