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Antiferromagnetic restricted solid-on-solid model: Ising models on rough surfaces

Marcel den Nijs
Department of Physics, University of Washington, Seattle, Washington 98195
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The antiferromagnetic, restricted, solid-on-solid model describes a surface which above its roughening temperature undergoes a transition due to the melting of looplike internal degrees of freedom. This model belongs to the same universality class as an Ising model on a two-dimensional lattice with transverse vibrations, and describes commensurate melting of monolayers adsorbed on rough substrates with annealed steps. Finite-size-scaling calculations confirm this. q-state antiferromagnetic clock models describe antiferromagnetic Ising models on lattices with dislocations of Burgers vector q.

The phase diagram of the antiferromagnetic restricted solid-on-solid (RSOS) model is discussed. Ferromagnetic SOS models are well known and describe roughening.[1] The surface is characterized by integer-valued column-height variables h_r at the sites of a square lattice:

$$Z_{\mathrm{RSOS}}=\sum_{\{h_r\}}\exp\left(\sum_{\langle r,r'\rangle} J[1-(h_r-h_{r'})^2]\right) . \tag{1}$$

The RSOS model is the special version where only steps of height one are allowed, $dh(r,r')=0, \pm 1$. In the ferromagnetic region this does not change the nature of the roughening transition while it facilitates numerical studies.[2] The RSOS model is also equivalent to a spin-one quantum chain.[3]

The purpose of this paper is to point out that the antiferromagnetic RSOS model also undergoes a phase transition, to determine its scaling properties (using analytical arguments and a numerical finite-size-scaling calculation), and to mention some possible experimental realizations of phase transitions in the same universality class.

The antiferromagnetic RSOS model describes a surface which is rough at all temperatures, but with looplike internal degrees of freedom. It undergoes a phase transition when meander entropy causes these loops to melt. Moreover, because these loops behave as Bloch walls in an Ising model, this model belongs to the same universality class as an Ising model on a lattice with transverse vibrations and can serve as a prototype to describe melting of monolayers with two competing commensurate ground states adsorbed on substrates with annealed steps.[4] It will be argued that, for weak coupling between these two types of degrees of freedom, the lattice vibrations do not alter the scaling properties of the Ising transition, except that the renormalized Gaussian coupling constant K_G, which characterizes the roughness of the surface

$$\langle (h_{r+r_0}-h_{r_0})^2\rangle \simeq (\pi K_G)^{-1}\ln(r), \quad \text{when } r>>1 , \tag{2}$$

has a logarithmic singularity.[5] Finally, this is confirmed numerically within the context of the RSOS model using finite-size scaling.

Further, antiferromagnetic clock models (antiferromagnetic RSOS models with screw dislocations) belong to the same universality class as Ising models on vibrating lattices with screw dislocations and serve as prototypes to study some intriguing aspects of the melting of incommensurate adsorbed monolayers with orientational degrees of freedom. The orientational degrees of freedom can preempt the Kosterlitz-Thouless nature of the positional melting.[6] This new identification of antiferromagnetic SOS and clock models with the melting of two coupled degrees of freedom (Ising spins and vibrations or orientational and positional order) is especially useful in determining the scaling properties of these complicated transitions. It facilitates numerical studies because the essential features of the RSOS model and the clock models are described using a minimum of degrees of freedom.

The body-centered solid-on-solid (BCSOS) model is the simplest model that describes surface roughening.[7] It requires steps $dh(r,r')=\pm 1$ between all nearest-neighbor columns (the flat surface is represented by an alternating step-up step-down order), is equivalent to the six-vertex model, and is exactly soluble.[8] The RSOS model will be interpreted as a BCSOS model coupled to an Ising model. For $J<0$ steps, $dh(r,r')=\pm 1$ are more likely than $dh(r,r')=0$. At zero temperature, where the $dh(r,r')=0$ states are frozen out, the model reduces to the BCSOS model. The surface remains rough; the BCSOS model is at its so-called ice point where all Boltzmann weights are equal and where $K_G=\pi/6$.[6,8] The $dh(r,r')=0$ states behave like strings of impurities. They line up to form closed loops, because they must follow contours of the surface. They obey the same topological rules as Bloch walls in the Ising model. Therefore, the RSOS model can be rewritten as an Ising model coupled to a BCSOS model by introducing an Ising spin $S=\pm 1$ at the top of each column r,

$$Z_{\rm RSOS}=\sum_{\{S_r\}}\left[\exp\left(\sum_{\langle r,r'\rangle}\frac{J}{2}(1-S_rS_{r'})\right)Z_{\rm BCSOS}(\{S_r\})\right] , \quad (3)$$

with $Z_{\rm BCSOS}(\{S_r\})$ the partition function of a modified BCSOS model still at its ice point, but now on a lattice where all bonds (r,r') containing a Bloch wall $S_rS_{r'}=-1$ have been removed and h_r is set equal to $h_{r'}$. The Bloch walls impose contours on the surface and suppress the local surface roughness.

As usual, the rough interface can be described by the Gaussian model with coupling constant K_G [see Eq. (1)]; at large length scales (under renormalization) the discreteness of the h_r variables is irrelevant and is replaced by a continuous variable $-\infty<\phi_r<\infty$ (Ref. 1). The RSOS model becomes a Gaussian model coupled to an Ising model

$$Z=\sum_{\{S_r,\phi_r\}}\exp\left(\sum_{\langle r,r'\rangle}\frac{K_E}{2}(\phi_r-\phi_{r'})^2-\frac{C}{2}(\phi_r-\phi_{r'})^2(1-S_rS_{r'})+\frac{K_I}{2}(1-S_rS_{r'})\right) . \quad (4)$$

The Bloch walls decrease the Gaussian coupling constant locally, by an amount C. They suppress the Gaussian fluctuations and prefer certain contours. This is also an Ising model on a lattice with transverse vibrations; C is the change in the Ising coupling constant due to fluctuations in the spin distances. The vibrating lattice can be a substrate surface above its roughening temperature, and the Ising spins can represent a commensurate adsorbed monolayer (in a lattice-gas or cell-spin description). The spin distances fluctuate because of step excitations. Bloch walls are accompanied by steps because the energy of antiparallel spins can be lowered by increasing the spin distance. The RSOS model retains the essential aspects which describe this: Two states $dh=\pm 1$ is the minimum needed to describe interface roughness and only one state $dh=0$ is used to describe the Ising spins and their coupling to the steps. This extreme economy in degrees of freedom makes the RSOS model well suited for numerical studies. Each Bloch wall removes one step instead of adding steps, but the sign of C should not be important, and in some systems the spin distance may indeed decrease. Since the Bloch walls flatten the surface, its roughness will decrease with temperature.

The lattice vibrations should not change the universality class of the Ising model. The coupling between the Gaussian and Ising degrees of freedom is irrelevant at the Ising critical point in the decoupled (fixed-point) model $C=0$. The crossover exponent is equal to $y_C=y_G+y_T-2=-1$, because the Gaussian operator $(\phi_r-\phi_{r'})^2$ is marginal $(y_G=0)$, while the Ising energy operator $S_rS_{r'}$ scales with the thermal critical exponent $y_T=1$.[9] The renormalized elastic constant K_G is allowed to become singular at the Ising transition because y_C is marginal when the Ising degrees of freedom are not critical $(y_C=y_G)$. The RSOS model is simple enough that this may be checked numerically. The finite-size-scaling behavior of surface tensions in semi-infinite strips of width $N\leq 10$ is obtained, as usual, from the largest eigenvalues of the transfer matrix by changing the boundary conditions at the strip edge.[10]

The model of Eq. (4) has two types of surface tensions. The free energy of the Bloch walls per unit length η_I is equal to the difference in free energy between the energies for the cases of antiperiodic and periodic boundary conditions for the Ising spins. It is customary to multiply surface tensions with the strip width $S_I=N\eta_I$. In the ordered phase S_I diverges (η_I is finite), at high temperatures S_I goes to zero (η_I is zero), and at the Ising transition S_I converges to a constant value B (η_I goes to zero as the inverse of the strip width N). The critical temperature can be determined from the crossing points $S_I(N')=S_I(N)$.[10] Recently, it has been recognized that the amplitude B is a universal property of the phase transition,[11] proportional to the magnetic critical exponent $B=(2-y_H)2\pi$; $y_H=\frac{15}{8}$ in the Ising model. The thermal critical exponent y_T can be obtained from the first derivative of the surface tension $dS_I/dJ\sim N^{-y_T}$; $y_T=1$ in the Ising model.

A second type of interface is obtained by imposing a step in the Gaussian variables at the edge of the strip, $\phi_{N,y}=\phi_{0,y}+\epsilon$. In the decoupled Gaussian model this surface tension is equal to $S_G(\epsilon)=K_G\epsilon^2/2$. This follows trivially by restoring the periodic boundary conditions via the transformation $\tilde{\phi}_{x,y}=\phi_{x,y}-\epsilon x/N$.[10] When applied to the coupled Gaussian-Ising model this transformation gives, trivially,

$$S_G(\epsilon)=\epsilon^2\frac{K_G}{2}=\epsilon^2\left[\frac{K_E}{2}-C\left(\frac{\partial f}{\partial K_I}\right)_{K_E,C}\right] . \quad (5)$$

The elastic constant K_E is renormalized by an amount proportional to the first derivative of the total free energy with respect to the Ising coupling constant. K_G has a $(J-J_S)\ln(J-J_S)$ singularity if the Ising transition is unchanged.[5]

In the RSOS model, surface tensions are obtained by imposing steps $h_{N,y}=h_{0,y}+\epsilon$, with ϵ an integer. The two-step surface tension S_2 behaves like $S_G(2)$. The one-step surface tension S_1 is a combination $S_1=S_G(1)\pm S_I$ [with the + (−) sign for even (odd) strip widths], because a Bloch wall automatically removes a step. This is easy to understand at low temperatures. For $J<<0$ the Bloch walls are absent if both N and ϵ are even. One Bloch wall parallel to the edge must be included if ϵ is odd. For odd strip widths this is reversed; a Bloch wall appears when ϵ is even. A Bloch wall effectively decreases the strip width by one:

$$S_1=\tfrac{1}{2}K_G\frac{N}{N-1}\pm N(J-f_{\rm ice}) , \quad (6a)$$

$$S_2=\tfrac{1}{2}4K_G , \quad (6b)$$

for $J<<0$, with $K_G=\pi/6$ and $f_{\rm ice}=(\frac{3}{2})\ln(\frac{4}{3})$ the free energy per site at the ice point of the 6-vertex model.[6,8,12]

Figures 1 and 2 show the finite-size scaling behavior of S_1 and S_2. The string melting takes place at $J_S=-0.4815\pm 0.0005$ (see Table I). This is close to the critical temperature $J_I=\ln(\sqrt{2}-1)+f_{\rm ice}=-0.44985$ of an Ising model on a rigid lattice with a Bloch-wall energy $J-f_{\rm ice}$. Below the string-melting temperature $J<J_S$ the surface is rough (criti-

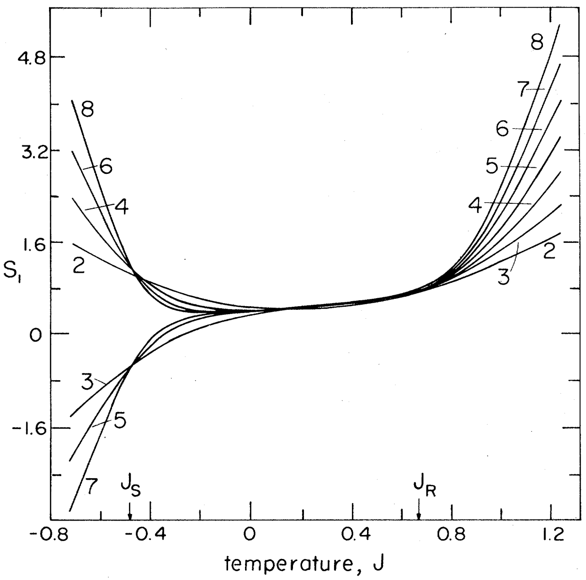

FIG. 1. The one-step surface tension times the strip width N of the RSOS model for $N=2$–8.

cal), while the Ising spins are ordered; $\eta_2=S_2/N$ scales as $1/N$ while $\eta_1=S_1/N$ is finite. Above the string-melting transition $J>J_S$ the surface is rough while the Ising spins are disordered; both surface tensions scale as $1/N$, while the free energy of the Bloch wall $S_I=S_1-S_2/4$ vanishes. As expected, the surface roughness decreases with temperature; S_1 and S_2 increase. $J>0$ is the familiar ferromagnetic side of the phase diagram. $J_R=0.632\pm0.005$ (Ref. 13) is the roughening temperature, where the Bloch walls suppress the surface roughness sufficiently to induce a (reversed) roughening transition. For $J>J_R$ the surface is flat; both surface tensions are finite.

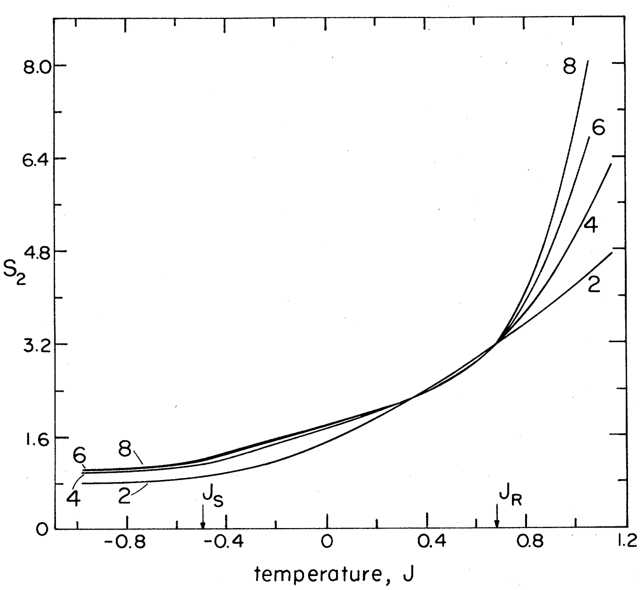

FIG. 2. The two-step surface tension times the strip width N of the RSOS model for $N=2, 4, 6, 8$.

TABLE I. String-melting temperature approximants from crossing points.

Widths N'	N	J where $S(N')=S(N)$ in S_1	in $S_I=S_1-S_2/4$
4	2	−0.4572	−0.4854
6	4	−0.4783	−0.4849
8	6	−0.4805	−0.4830
10	8	−0.4812	−0.4825
5	3	−0.4904	
7	5	−0.4837	
9	7	−0.4822	

The thermal critical exponent at J_S follows from the scaling behavior of $dS_I/dJ \sim N^{-y_T}$, and converges rapidly towards the exact Ising value, $y_T=1.000\pm0.003$ (see Table II). The error is dominated by the uncertainty in J_S. The magnetic critical exponent follows from the universal amplitude, and is much more sensitive to the uncertainty in J_S, $x_H=2-y_H=0.1265\pm0.002$ (see Table III).

At J_S the loops have reduced the surface roughness by 20%, $K_G=S_2/2=0.638\pm0.0006$ (see Table III). K_G has the expected logarithmic singularity [see Eqs. (5) and (6)]. dS_2/dJ diverges (see Fig. 3), and $dS_2/dJ=p+q\ln(N)$ gives a good fit for all N (see Table II).

Following the same line of reasoning as presented above, it can be shown that antiferromagnetic q-state clock models describe antiferromagnetic Ising models on rough surfaces with annealed dislocations of Burgers vector $\pm q$. Odd values of q are most interesting, because then the odd vorticity frustrates the antiferromagnetic Ising order. Unfortunately, the dislocations in surfaces are quenched, but there are other, more realistic, applications, like melting of incommensurate monolayers with internal degrees of freedom as for N_2 adsorbed on graphite.[14] Here the orientational degrees of freedom are more complicated, but similar to the Ising spins, and (in the incommensurate solid phase) the positional degrees of freedom (described by two coupled Gaussian models) are similar to the height variables describing the rough surface.

As discussed earlier,[6] there are three typical melting sequences for such a system. In one of them, which is realized in N_2 on graphite, the orientational order vanishes first. As in the RSOS model the dislocations will not change the universality class of the orientational transition, except that again the renormalized elastic constants are singular.[5]

In one of the other two melting sequences, the melting of

TABLE II. Approximants at $J=-0.4815$ for the energy exponent $y_T=\ln[S_I(N')/S_I(N)]/\ln(N'/N)$ and $dS_2/dJ=p+q\ln(N)$.

N'	N	y_T	p	q
4	2	1.0456	0.3113	0.4166
6	4	1.0115	0.3045	0.4216
8	6	1.0028	0.3049	0.4213
10	8	1.0002	0.3080	0.4198

TABLE III. Approximants for the surface roughness and magnetic exponent at $J=-0.4815$.

N	$K_G=S_2(N)/2$	$x_H=2-y_H=S_I(N)/2$
2	0.4638	0.1309
4	0.5748	0.1296
6	0.6026	0.1284
8	0.6134	0.1280
10	0.6186	0.1276

the orientational degrees of freedom can induce the positional degrees to melt simultaneously. This happens at the earlier discussed string-melting transitions in antiferromagnetic clock models.[6] The third possibility is that the positional order vanishes first. Also, this is realized in specific corners of the phase diagrams of antiferromagnetic clock models. After the positional order has vanished, the clock model describes an antiferromagnetic Ising model on an annealed disordered lattice (a fluid). Such a system undergoes a phase transition or at least has a so-called disorder point[6] at the temperature where the surface tension of the Ising Bloch walls (the loops) vanishes; the Ising spins "disorder" (the staggered magnetization is zero in the entire low-temperature phase and also in the fluid phase due to gauge invariance[15]). Numerical studies (using finite-size scaling) of these two types of transitions are in progress.

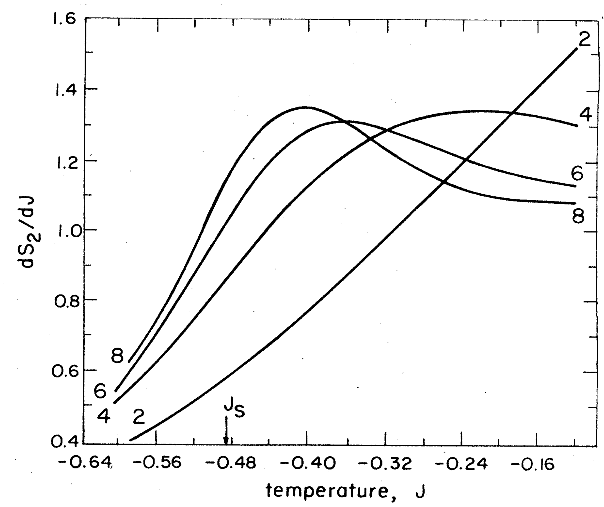

FIG. 3. The first derivative with respect to temperature of the two-step surface tension times the strip width N of the RSOS model for $N=2, 4, 6, 8$.

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[12]$K_G=S_2/2=0.523\,57\pm0.000\,02$ and $f_{\rm ice}=0.431\,525\pm0.000\,002$; using a N^{-2} extrapolation in accordance with the known corrections to scaling.

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