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Model with roughening transition at low temperatures

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We note that for the Ising model on a body-centered-cubic lattice the temperature $T_R(J)$ of the roughening transition approaches zero when the second-neighbor coupling J vanishes; the interface (100) between regions of opposite magnetization is, at low temperatures, rigid for J positive and becomes rough for J negative. A reinterpretation of van Beijeren's body-centered solid-on-solid model yields a rigorous description of the asymptotic behavior around the limit point $T=0$, $J=0$. In particular, the roughening transition of the solid-on-solid model corresponds to a roughening transition of the isotropic Ising model when crossing a line with critical slope at $T=0$, $J=0$.

The equilibrium shape of a crystal and the phenomenon of the roughening transition of its faces has been recently studied both theoretically and experimentally.[1] Ising models may serve for a simplified description of this phenomenon by considering the equilibrium shape of a "droplet" surrounded by the opposite phase or the roughening transition of an interface between phases of opposite magnetization.[2] If a surface is stabilized in a macroscopic sense by submitting a large volume of a lattice to a boundary condition specified by the configuration with all spins above the surface fixed to be, say, $+1$ while below they are -1, the roughening transition of the corresponding interface may be viewed as a substantial change in the "microscopic resistivity of the system against propagation of this particular boundary condition inside the bulk." Let us describe it more explicitly in terms of the Gibbs ensemble in the considered volume (or better, its thermodynamic limit for infinite volume) under the mentioned boundary conditions. If typical, i.e., most probable, microscopic configurations inside the volume are essentially prolongations of the boundary configuration, with only small deviations from it, we say that the interface is rigid.[3] If, on the contrary, typical configurations differ significantly from the boundary configuration, the surface cannot be reconstructed inside the volume and we say that the interface is rough. The roughening transition is the transition between these two types of behavior.

In this note, we shall consider the Ising model on a body-centered-cubic (bcc) lattice. We shall argue that the roughening transition temperature for the (100) interface depends on the next-nearest-neighbor coupling in the way drawn schematically in Fig. 1.[4]

A bcc lattice consists of two simple cubic lattices in $\mathbb{Z}^3$, to be called the sublattices A and B, which are mutually shifted by the vector $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$. A lattice site i in, say, sublattice A has eight nearest neighbors (NN), all of them belonging to the sublattice B, and six next-nearest neighbors (NNN) belonging again to A. The energy of the corresponding Ising model is given by

$$H=-J_0\sum_{\mathrm{NN}}\sigma_i\sigma_j-J\sum_{\mathrm{NNN}}\sigma_i\sigma_j ,$$

where the first sum runs over all pairs of NN's while the second over all pairs of NNN's. We shall restrict ourselves to ferromagnetic NN coupling ($J_0>0$) bearing in mind that all the results may be transformed into the corresponding ones for $J_0<0$ by a transformation consisting in the change of the sign of all configurations (as well as boundary conditions) on, say, the sublattice A.[5]

Our aim is to study the roughening transition for a horizontal interface [perpendicular to the vector (100)]. We consider thus the boundary configuration $\bar{\sigma}$ defined for a lattice site $i=(i_1,i_2,i_3)$ to be $\bar{\sigma}_i=+1$ whenever $i_1\geq 0$, and $\bar{\sigma}_i=-1$ whenever $i_1<0$.

Let us evaluate the behavior of the model in a neighborhood of the point $T=0$, $J=0$. To this end we shall inspect the ground state compatible with the above boundary condition. Considering the system in a volume V, for concreteness, say, in a large cube with the center at the point $(000)\in A$, and denoting by $H_V(\sigma_V\,|\,\bar{\sigma})$ the energy of a configuration $\sigma_V=\{\sigma_i\,|\,i\in V\}$ in V under the boundary condition $\bar{\sigma}$ outside V, we look for configurations σ_V which minimize this energy. It turns out that a lot of such ground configurations may be found, their number tending to infinity in the thermodynamic limit. Thus, already at $T=0$ the system is governed by a nontrivial Gibbs ensemble, the ground state, to which every ground configuration contributes with the same probability.[6] To get some information about this ground state we shall notice that it is equivalent to the exactly solvable body-centered solid-on-solid (BCSOS) model introduced by van Biejeren[7] and

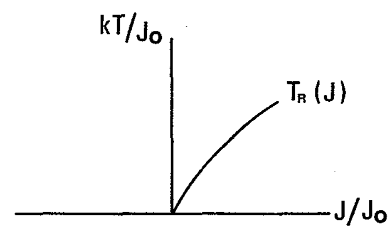

FIG. 1. The roughening temperature T_R for the facet (100) as a function of the NNN interaction J. A rigid interface exists for positive J and $T<T_R(J)$. The function $T_R(J)$ ends at the point $J=0$, $T=0$.

that there is a one-to-one correspondence between the ground configurations and the configurations of the BCSOS model.

Let us denote by S the orthogonal projection of the bcc lattice onto the horizontal plane $i_1=0$ [$S=S_A \cup S_B$, where S_A and S_B, the projections of sublattices A and B, are square lattices mutually shifted by the vector $(\frac{1}{2}\frac{1}{2})$]. The BCSOS model is defined on this lattice S with the configurations given by the height variables $h(s)$ associated with sites $s=(i_2,i_3)\in S$ in such a way that $h(s)\in \mathbb{Z}$ [$h(s)\in \mathbb{Z}+\frac{1}{2}$] for $s\in S_A$ ($s\in S_B$) and $|h(s)-h(r)|=\frac{1}{2}$ whenever r and s are NN's in S (i.e., their distance is $1/\sqrt{2}$).

Suppressing for awhile the condition $|h(s)-h(r)|=\frac{1}{2}$, let us assign to every collection of heights the configuration $\sigma_V=\{\sigma_i \mid i\in V\}$ of the bcc Ising model by $\sigma_i=+1$ if $i_1\geq h(i_2,i_3)$, and $\sigma_i=-1$ if $i_1<h(i_2,i_3)$. Then the energy $H_V(\sigma_V\mid\bar{\sigma})$ in terms of the heights is

$$H_V(\sigma_V\mid\bar{\sigma})-H_V(\bar{\sigma}_V\mid\bar{\sigma})=4J_0\sum_{\text{NN}}[\,|h(r)-h(s)|-\tfrac{1}{2}] +2J\sum_{\text{NNN}}|h(r)-h(s)|\ ,$$

where the first sum is taken over NN's in S and the second one over NNN's in S (i.e., pairs of sites the mutual distance of which is 1). In both sums the heights $h(s)=0$ if $s\in S_A$ and $h(s)=\frac{1}{2}$ if $s\in S_B$, corresponding to the boundary configuration $\bar{\sigma}$, are taken outside V and only those pairs of sites for which at least one of them lies inside V are considered. It is easy to see that for $J=0$ the configurations of the BCSOS model correspond exactly to the ground configurations of the bcc Ising model.

Since we are interested in describing the asymptotic behavior around the point $T=0$, $J=0$, let us observe that the ground state actually depends on a direction of approaching this point in the (T,J) plane. Namely, one may consider the limit of the Gibbs ensemble along the line $J=\alpha kT$ for $T\to 0$ $(-\infty<\alpha<\infty)$. One easily sees that again only ground configurations contribute to the limiting ensemble; but this time, taking into account the above formula for the energy in terms of height variables, with weights proportional to $\exp[-2\alpha\sum|h(s)-h(r)|]$. Now we may use the equivalence of the BCSOS model with the six-vertex model discovered by van Beijeren[7] to conclude that the limiting ensemble is equivalent to the six-vertex model with the weights[8] $\omega_1=\omega_2=\omega_3=\omega_4=e^{-2\alpha}$, $\omega_5=\omega_6=1$. Thus we may reinterpret all results about the BCSOS model[7,9] as statements about the limiting ensemble for different α and hence as statements about the Ising model on a bcc lattice in a neighborhood of the point $T=0$, $J=0$. In particular, from what is known about the BCSOS model, we may conclude (Fig. 2) that the inverse slope of the tangent to the function $T_R(J)$ at this point is $\alpha_c=(\frac{1}{2})\ln 2=0.35$, the value corresponding to the transition of the six-vertex model into a ferroelectric phase, that the (100) interface is rigid for $\alpha>\alpha_c$ and rough for $\alpha<\alpha_c$, and that the transition is of infinite order.[10,11]

The expectation that the interface is rigid to the right of the line $T_R(J)$ and it is rough to the left of it may be further supported by inspection of ground states for $J>0$ and $J<0$. It turns out that for $J>0$ there is only one ground

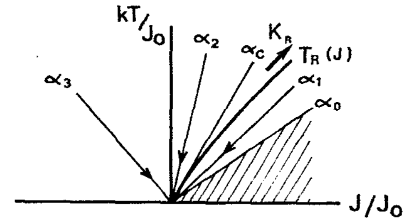

FIG. 2. Representation of results. For J and T in the shadowed region the rigidity of the interface is proved. The limiting behavior when $T\to 0$ along the lines $J=\alpha kT$ has been studied. For inverse slopes $\alpha>\alpha_c$ (e.g., α_1) the limiting system has a rigid interface, while for $\alpha<\alpha_c$ (e.g., α_2,α_3) the interface is rough. The function $T_R(J)$ has for $J\to\infty$ an asymptote in the direction K_R.

configuration consistent with the boundary condition, namely, the configuration $\bar{\sigma}$ itself. It may be actually proved, e.g., by the method of Dobrushin[3] that this ground configuration, at low temperatures, is stable with respect to thermal fluctuations. Using another method due to van Beijeren,[12] we proved[13] the rigidity of the interface for all J and T in the region shadowed in Fig. 2. Namely, the region where $J\geq\alpha_0 kT$, with $\alpha_0=(\frac{1}{2})\ln(\sqrt{2}+1)=0.44$ denoting the critical value of the coupling constant for the Ising model on a two-dimensional square lattice. If $J<0$, the configuration $\bar{\sigma}$ is not a ground configuration any more and the existing ground configurations are not stable at low temperatures. There are excitations of bounded energy for which the interface is elevated above regions of unlimited area. This situation reminds one of the case of the interface for the Ising model on a square lattice where the roughness for all positive temperatures was indeed proved.[14]

Let us notice that the limit $J_0\to 0$ for which the model decouples into two independent Ising models on the simple cubic lattices A and B with a reduced coupling constant K corresponds to the limiting point of the family of parallel lines $J/J_0=K(kT/J_0)+C$ (the point at infinity in the direction $J/kT=K$). Thus we expect that the function $T_R(J)$ approaches asymptotically such a line with the value $K=K_R$ corresponding to the roughening transition of the Ising model on a simple cubic lattice. Notice that it is known[12] that $K_R<\alpha_0$ and that the estimated value[15] is $K_R=0.40=0.9\alpha_0$.

In conclusion, we are arguing that the behavior of the Ising model on a bcc lattice around the point $T=0$, $J=0$ is governed by the ground Gibbs state characterized by the slope α along which one approaches this point. This consideration is actually true also for other boundary conditions $\bar{\sigma}(\mathbf{k})$ corresponding to inclined interfaces with normal $\mathbf{k}$. It turns out that whenever the condition $-k_1\leq k_2+k_3\leq k_1$ is fulfilled, the ground state is equivalent to the BCSOS model in terms of heights over the plane $i_1=0$ and with the corresponding boundary condition [similarly for $-k_2\leq k_3+k_1\leq k_2$ $(-k_3\leq k_1+k_2\leq k_3)$ we get a BCSOS model over the $i_2=0$ $(i_3=0)$ plane]. Such a BCSOS model is, in its turn, equivalent to a six-vertex model with the boundary condition corresponding to the fixed polarizations $x=(k_2+k_3)/k_1$, $y=(k_2-k_3)/k_1$.[16] The same ground Gibbs state, when considered under the boundary conditions $\bar{\sigma}(\mathbf{k})$ with normals $\mathbf{k}$ not covered above, leads in an analogous way to TISOS models[17] (SOS models on a triangular lattice) over the planes $i_1 \pm i_2 \pm i_3 = 0$. These equivalences imply, in particular, that for every α, the (110) interface is rigid while the (111) interface is rough.

Finally, let us remark that the above equivalences may be used to study the facet formation on the equilibrium shape of a crystal, respectively, a droplet in the Ising model. The assumption that the roughening transition may be detected as faceted transition suggests a change of the equilibrium crystal shape as illustrated in Fig. 3. In fact, one may express the surface tension with respect to an interface labeled by $\mathbf{k}$ in the lowest order at low temperature as a sum of the energy of the corresponding ground state plus the free energy of the associated SOS model with fixed boundary conditions. Combining then the results of Jayaprakash, Saam, and Teitel[9,18] and Nienhuis, Hilhorst, and Blöte[17] concerning BCSOS and TISOS models one gets a quantitative description of the faceted transition for α crossing α_c. The details of the above considerations will be given in a forthcoming publication.

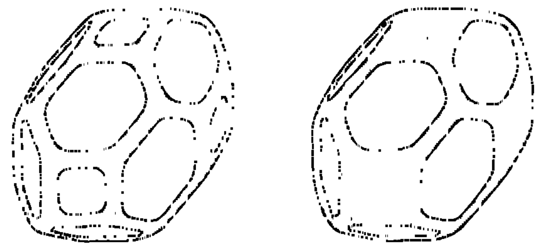

FIG. 3. Equilibrium crystal shapes for small positive NNN interaction J. When the temperature increases the six facets orthogonal to the lattice axis [type (100)] disappear at $T_R(J)$ leaving only the 12 facets of type (110) for temperatures larger than $T_R(J)$ but small enough.

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[1]For a recent review, see, e.g., C. Rottman and M. Wortis, Phys. Rev. **103**, 59 (1984).

[2]Ising models were recently used for a study of crystal shapes in, e.g., J. E. Avron, H. van Beijeren, L. S. Schulman, and R. K. Zia, J. Phys. A **15**, L81 (1982); C. Rottman and M. Wortis, Phys. Rev. B **29**, 328 (1984). For critical remarks concerning the relevance of short-range lattice models for the description of real crystals, see D. S. Fisher and J. D. Weeks, Phys. Rev. Lett. **50**, 1077 (1983).

[3]This is, e.g., the case of a (100) interface for the nearest-neighbor Ising ferromagnet on a simple cubic lattice at low temperatures as was first proven by R. L. Dobrushin, Teor. Veroyatn. Primen. **17**, 619 (1972) [Theory Prob. Appl. **17**, 582 (1972)].

[4]A model for which the roughening temperature may approach zero was investigated by R. L. Dobrushin and S. B. Shlosman [Sov. Sci. Rev. C **5**, 54 (1985)], who considered the Ising antiferromagnet in an external magnetic field. Our argument, developed in the present paper, may be used also for this model and presumably for isotropic Ising models on other lattices, e.g., fcc lattice, in the neighborhood of particular values of the coupling constants.

[5]For the conjectured phase diagram, see J. R. Banavar, D. Jasnow, and D. P. Landau, Phys. Rev. B **20**, 3820 (1979). We shall consider the region $J > -(\frac{2}{3})J_0$ at small temperatures, where two ferromagnetically ordered phases coexist.

[6]Such ground states and their description in terms of SOS models were studied for Ising (anti)ferromagnet and some other models by Dobrushin and Shlosman (cf. Ref. 4).

[7]H. van Beijeren, Phys. Rev. Lett. **38**, 993 (1977).

[8]For the details of the correspondence of BCSOS and vertex models consult the original van Beijeren paper (Ref. 7) or, more recently, Ref. 9.

[9]C. Jayaprakash, W. F. Saam, and S. Teitel, Phys. Rev. Lett. **50**, 2017 (1983).

[10]Let us remark that what is called temperature in BCSOS model corresponds to our parameter α. Reinterpreting the BCSOS model for a description of the asymptotic behavior of the isotropic Ising model around the point $T = 0$, $J = 0$, we are thus suggesting a more physical solution to the puzzle of the significance of the BCSOS model illustrated, e.g., by the remark 21 in the recent paper of Jayaprakash and Saam (Ref. 18): "Technically, the SOS condition can be imposed by introducing anisotropic nearest-neighbor bonds, and letting those bonds with components normal to the surface in question go to infinity. This device is a bit unphysical, and we shall merely assume that voids and overhangs are not crucial to the qualitative physics at all T. . . ."

[11]In connection with the preceding remark, let us also notice that since, after letting the vertical bonds go to infinity, the energy of the SOS interfaces depends on both (horizontal) NN and NNN couplings. One may in some cases calculate the dependence of the roughening temperature of the SOS model on the coupling constants [cf. Eq. (A4b), Ref. 18]. But, as explained above, "the SOS roughening temperature" is not the same as our Ising model $T_R(J)$.

[12]H. van Beijeren, Commun. Math. Phys. **40**, 1 (1975).

[13]The details of the proofs will be given in a forthcoming publication.

[14]G. Gallavotti, Commun. Math. Phys. **27**, 103 (1972).

[15]J. D. Weeks, G. H. Gilmer, and H. J. Leamy, Phys. Rev. Lett. **31**, 549 (1973).

[16]For a study of six-vertex models with polarizations, see, for instance, E. H. Lieb and F. Y. Wu, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1972), Vol. 1.

[17]This beautiful description was introduced for the (111) ground state of an Ising antiferromganet on a simple cubic lattice in Ref. 4. The same SOS model was independently introduced and exactly solved by E. Nienhuis, H. S. Hilhorst, and H. W. J. Blöte, J. Phys. A **17**, 3559 (1984).

[18]C. Jayaprakash and W. F. Saam, Phys. Rev. B **30**, 3916 (1984).