

The two conditions (15) are of rather different nature physically. Given as masses and cross sections, it is often possible to find a relative density  $n_1/n_2$  such that the first condition is satisfied. On the other hand, the densities do not appear in the second condition. In other words, if the second condition is satisfied, exact solutions can be written down for all values of  $n_1/n_2$ .

\*This work was supported in part by the National Science Foundation under Grant No. NSF-MPS75-15469, in part by the U. S. Energy Research and Development Administration under Grant No. AT(11-1)3227, and by the Division of Engineering and Applied Physics, the Department of Astronomy, and the Center for Earth and Planetary Physics, Harvard University.

<sup>1</sup>M. Krook and T. T. Wu, Phys. Rev. Lett. **36**, 1107 (1976).

## Exactly Solvable Model for the Roughening Transition of a Crystal Surface

Henk van Beijeren

*Institut für Theoretische Physik, Rheinisch Westfälische Technische Hochschule, Aachen, West Germany*

(Received 8 March 1977)

An exactly solvable model of the crystal-vacuum interface is constructed which exhibits a roughening transition. The model is obtained as a special limit of a ferromagnetic Ising model and it is isomorphic to the symmetric six-vertex model. Some of the thermodynamic properties of the system are discussed.

The concept of interface roughening was introduced in the theory of crystal growth by Burton and co-workers<sup>1,2</sup> on the basis of a comparison between a crystal surface and the quadratic Ising model. From a different point of view Gallavotti conjectured<sup>3</sup> that the cubic Ising model might show a roughening transition for an interface between phases of opposite magnetization. His conjecture was supported by Weeks, Gilmer, and Leamy,<sup>4</sup> who used low-temperature expansions to estimate the roughening temperature  $T_R$  of the isotropic cubic Ising model and the solid-on-solid (SOS) model, which is obtained from the cubic Ising model by letting the vertical coupling constant go to infinity while keeping the horizontal coupling constants fixed (an interface is maintained by imposing appropriate boundary conditions). Their estimates of  $T_R$  are well below the bulk critical temperature in either case. Further evidence for the existence of a roughening transition comes from computer simulations of the interface in the SOS model and the discrete Gaussian (DG) model.<sup>5-8</sup> A rigorous proof for the existence of such a transition, however, to our knowledge has not been given before.

Here I discuss an exactly solvable model which does show a roughening transition. We start from a body-centered-cubic Ising model of  $2N \times 2N \times 2N$  sites with ferromagnetic nearest-neighbor coupling  $J_0$  (between particles in the center and on a corner of an elementary cube) and next-nearest-neighbor couplings  $J_x$ ,  $J_y$ , and  $J_z$  in the three main lattice directions. The spins in the two bot-

tom layers are kept positive, those in the two top layers negative, and free boundary conditions are imposed on the side walls (in the crystal interpretation positive spins correspond to occupied lattice sites and negative spins to empty ones). The body-centered solid-on-solid (BCSOS) model is obtained by letting  $J_0$  approach infinity, keeping  $J_x$ ,  $J_y$ , and  $J_z$  constant. In this limit the so-called SOS condition is satisfied (this means that in no column of the lattice is a negative spin to be found below a positive one). In Fig. 1 some spin configurations are sketched on a "ladder" of two neighboring columns of spins on a lattice of height 8. Because of the imposed boundary conditions such a ladder always contains at least one (+-) bond of strength  $+J_0$  [e.g., bond 2 in Fig. 1(a)], but in the limit as  $J_0 \rightarrow \infty$  configurations in which any ladder contains more than one (+-) bond such as in Fig. 1(b) are strictly forbidden. From this the SOS condition follows di-

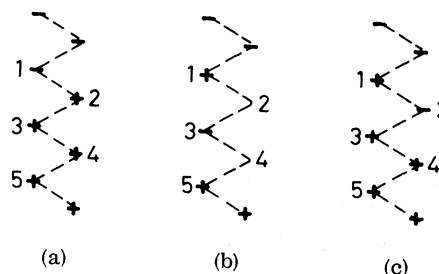


FIG. 1. Some spin configurations on a ladder of two neighboring columns.

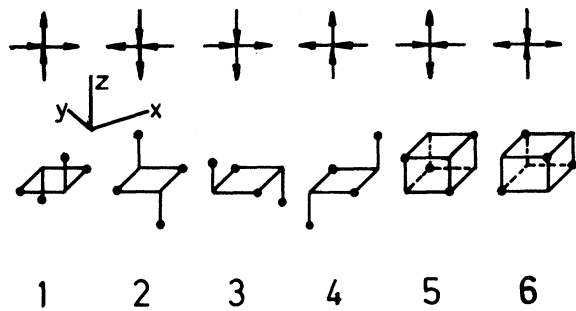


FIG. 2. The allowed six vertices and the corresponding configurations of interface heights.

rectly. As a result, all allowed spin configurations can be specified completely by giving the level of the uppermost positive spin in each column. Between neighboring columns these levels may differ only by  $+\frac{1}{2}$  or  $-\frac{1}{2}$  (our unit of length is the next-nearest-neighbor distance), since otherwise again the ladder containing these columns would possess more than one (+-) bond [see Fig. 1(c)]. Now each allowed spin configuration can be translated into a vertex configuration by drawing arrows of length  $1/\sqrt{2}$  on the dual lattice of the "lattice of vertical columns"; i.e., each arrow bisects a line piece connecting two neighboring columns, and its direction is chosen such that the column with the higher level of positive spins is to the right of the arrow (see Fig. 2). Clearly the vertices generated this way satisfy the ice rule (two arrows in and two arrows out). Conversely each vertex configuration satisfying the ice rule defines an allowed set of positive spin levels, uniquely up to an overall additive integer, resulting from the freedom to shift the interface as a whole upward or downward. As a result the BCSOS model is isomorphic to the six-vertex

model for which the exact solution is known.<sup>9-11</sup>

From the pictures in Fig. 2 we can immediately read off the vertex energies. One finds  $\epsilon_1 = \epsilon_2 = J_y - J_x$ ;  $\epsilon_3 = \epsilon_4 = J_x - J_y$ ;  $\epsilon_5 = \epsilon_6 = J_x - J_y$ . So all different versions of the symmetric six-vertex model are reproduced, dependent on the values of  $J_x$  and  $J_y$ . Notice that the value of  $J_z$  is irrelevant.

Important quantities in the six-vertex model are  $x$  and  $y$ , the polarization per site in the  $x$  and  $y$  directions, respectively. In the BCSOS model these quantities translate into  $\sqrt{2}$  times the height increase of the interface per unit length in the  $(-1, -1)$  and  $(1, -1)$  directions, respectively. All values of  $x$  and  $y$  between  $+1$  and  $-1$  can be forced on the system by prescribing appropriate boundary conditions on the side walls.

The most interesting case is the isotropic ferromagnet with  $J_x = J_y = \frac{1}{2}\epsilon > 0$ . This corresponds to the  $F$  model, for which the thermodynamic properties are discussed extensively in Ref. 11. The system has a phase transition at  $T_R = \epsilon/(k_B \times \ln 2)$ , where  $k_B$  is Boltzmann's constant. This transition is of infinite order, the singular part of the free energy behaves as  $\exp(-\alpha|T - T_R|^{-1/2})$  where  $\alpha$  is some constant, all derivatives of the free energy with respect to temperature are continuous, and a plot of, for example, specific heat versus temperature does not show any visible sign of a phase transition at  $T_R$ . All critical exponents are infinite.<sup>12-15</sup> Hence the critical behavior of the BCSOS model is entirely different from that of the quadratic Ising model, which has been used widely to describe the crystal-solution interface.

A quantity which is not discussed in much detail in Ref. 11 is the energy per unit length,  $E$ , of a single step on the interface.<sup>16</sup> For diagonal and horizontal steps one obtains fairly straightforwardly from Refs. 11 and 10, respectively,

$$E_{\text{diag}}^{\text{BCSOS}}/\epsilon = 2\sqrt{2}[1 - 4 \exp(-2\beta\epsilon)]^{-1/2} \left\{ \frac{1}{2} + \sum_{n=1}^{\infty} (-1)^n [1 + (n-1)\tanh((n-1)\lambda) - n \tanh(n\lambda)] \right\}, \quad (1a)$$

$$E_{\text{hor}}^{\text{BCSOS}}/\epsilon = 2[1 - 4 \exp(-2\beta\epsilon)]^{-1/2} \left\{ \frac{1}{4} + \sum_{n=1}^{\infty} (-1)^n \left[ \frac{1}{2} + (n - \frac{3}{4})\tanh((n - \frac{3}{4})\lambda) - (n - \frac{1}{4})\tanh((n - \frac{1}{4})\lambda) \right] \right\}, \quad (1b)$$

where  $\beta = (k_B T)^{-1}$  and

$$\lambda = 2 \left\{ \beta\epsilon + \ln \left( \frac{1 + [1 - 4 \exp(-2\beta\epsilon)]^{1/2}}{2} \right) \right\}.$$

In Fig. 3 these quantities are plotted as a function of the reduced temperature  $\tilde{T} = k_B T/\epsilon$ , together with the step energies in the quadratic Ising model as given by Onsager<sup>17</sup> and by Fisher and Ferdinand.<sup>18</sup> At low temperatures the step energies for the two models are equal as one

might expect. The behavior near the critical point is, again, entirely different for the two models. In the Ising model the step energies approach their nonzero critical value linearly, whereas in the BCSOS model the step energies approach zero (as predicted by Leamy and Gilmer<sup>6</sup>), again as  $\exp(-\alpha|T - T_R|^{-1/2})$ . As in the Ising model,<sup>18</sup> the step energy becomes isotropic

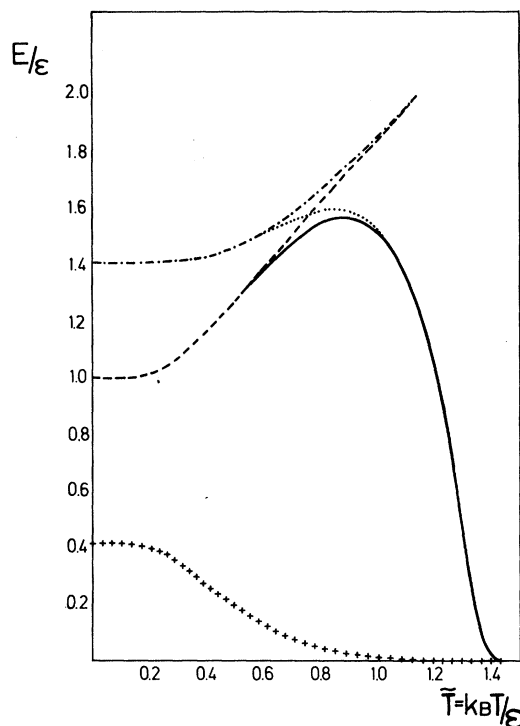


FIG. 3. Step energies vs temperature for a single horizontal and diagonal step in BCSOS and quadratic Ising model. Solid line,  $E_{\text{hor}}^{\text{BCSOS}}/\epsilon$ ; dashed line,  $E_{\text{hor}}^{\text{Ising}}/\epsilon$ ; dotted line,  $E_{\text{diag}}^{\text{BCSOS}}/\epsilon$ ; and dash-dotted line,  $E_{\text{diag}}^{\text{Ising}}/\epsilon$ . The quantity  $(E_{\text{diag}} - E_{\text{hor}})/\epsilon$  is plotted as crosses. Within the precision of this graph it is the same for the two models.

as  $T_R$  is approached. Remarkable is that the difference  $(E_{\text{diag}} - E_{\text{hor}})/\epsilon$  (see Fig. 3) is almost the same for the two models (within 0.002 at all temperatures). The step free energy, like the step energy, vanishes at  $T_R$ . Hence one may conclude that the phase transition at  $T_R$  is indeed a roughening transition: At this temperature the interface loses its resistance against the formation of arbitrarily long ridges. Finally we want to quote the fact<sup>11</sup> that a phase transition occurs only for  $x = y = 0$ ; for nonzero values of  $x$  and  $y$  the interface is already rough at  $T = 0$ .

It is interesting that the symmetric eight-vertex model<sup>12</sup> can also be interpreted as an interface model, if one identifies the vertices 7 and 8 with end points of screw dislocations, to which then have to be attributed certain well-defined energies. It is well known that the inclusion of such impurities reduces the critical exponents to finite values.<sup>12-15</sup>

Although the existence of a roughening transition in the BCSOS model does not prove anything

about the ordinary SOS model or the isotropic simple-cubic Ising model, it certainly makes the existence of a roughening transition in the latter two models more plausible. On the basis of universality of critical behavior for systems with the same symmetry properties<sup>19</sup> one might furthermore expect that the roughening transition for these models will be of the same infinite-order type as for the BCSOS model. Chui and Weeks<sup>20</sup> recently showed that the DG model can be mapped on the two-dimensional Coulomb gas and should have the same critical behavior as the latter. Indeed the same type of infinite-order transition as exhibited by the  $F$  model has been found by Kosterlitz for the two-dimensional Coulomb gas<sup>21</sup>; from Sutherland's calculation of the vertical-arrow correlation function in the  $F$  model for  $T = 2T_R$  (presumably a typical above-critical temperature)<sup>22,11</sup> it follows that the square of the height difference in the BCSOS model  $\langle (h_i - h_j)^2 \rangle_{\text{av}}$  is proportional to  $\ln R_{ij}$  (where  $R_{ij}$  is the distance between the sites  $i$  and  $j$ ), just as in the DG model,<sup>20</sup> and Swendsen's computer data for the DG model<sup>7</sup> also look consistent with equivalent critical behavior of the two models.

Computer results obtained for the SOS model<sup>6,7</sup> on *finite size* lattices appear very similar to my results for the BCSOS model as well, but Swendsen's investigations of the size dependence of specific heat and step specific heat in this model suggest that these quantities may become divergent at  $T_R$  in the infinite-size limit. In my opinion his data are not decisive and the possibility of a large but finite maximum in the specific heat (or a minimum in the step specific heat) close to  $T_R$  cannot be excluded. A definite determination of the critical behavior of the SOS model seems to require either the computer simulation of still larger systems or a better theoretical understanding of the type of interface models discussed here and the relations between them. If the various models indeed have different critical behavior it is an interesting question where and why universality breaks down.

For the BCSOS model itself various quantities of interest are still to be calculated. In principle the free energy is known for arbitrary  $x$  and  $y$ <sup>10</sup> (although no practically useful form has appeared in the literature so far), which would offer the opportunity to calculate the direction dependence of step free energies as well as free energies for systems with interacting steps.

I wish to thank Dr. B. U. Felderhof for his careful reading of the manuscript.

- <sup>1</sup>W. K. Burton and N. Cabrera, *Disc. Faraday Soc.* **5**, 33 (1949).
- <sup>2</sup>W. K. Burton, N. Cabrera, and F. C. Frank, *Philos. Trans. Roy. Soc.* **243**, 299 (1951).
- <sup>3</sup>H. van Beijeren and G. Gallavotti, *Lett. Nuovo Cimento* **4**, 699 (1972).
- <sup>4</sup>J. D. Weeks, G. H. Gilmer, and H. J. Leamy, *Phys. Rev. Lett.* **31**, 549 (1973).
- <sup>5</sup>G. H. Gilmer and P. Bennema, *J. Appl. Phys.* **43**, 1347 (1972).
- <sup>6</sup>H. J. Leamy and G. H. Gilmer, *J. Crys. Growth* **24/25**, 499 (1974).
- <sup>7</sup>R. H. Swendsen, *Phys. Rev. Lett.* **38**, 615 (1977).
- <sup>8</sup>H. J. Leamy, G. H. Gilmer, and K. A. Jackson, in *Surface Physics of Crystalline Materials* (Academic, New York, 1975).
- <sup>9</sup>E. H. Lieb, *Phys. Rev.* **162**, 162 (1967), and *Phys. Rev. Lett.* **18**, 692, 1046 (1967), and **19**, 108 (1967); B. Sutherland, *Phys. Rev. Lett.* **19**, 103 (1967); M. L. Glasser, *Phys. Rev.* **184**, 839 (1969).
- <sup>10</sup>C. P. Yang, *Phys. Rev. Lett.* **19**, 586 (1967); B. Sutherland, C. N. Yang, and C. P. Yang, *Phys. Rev. Lett.* **19**, 588 (1967).
- <sup>11</sup>E. H. Lieb and F. Y. Wu, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 1.
- <sup>12</sup>R. J. Baxter, *Ann. Phys. (N.Y.)* **70**, 193 (1972).
- <sup>13</sup>J. D. Johnson, S. Krinsky, and B. M. McCoy, *Phys. Rev. Lett.* **29**, 492 (1972).
- <sup>14</sup>R. J. Baxter, *J. Statist. Phys.* **8**, 25 (1973).
- <sup>15</sup>R. J. Baxter and S. B. Kelland, *J. Phys. C* **7**, L403 (1974).
- <sup>16</sup>The presence of a step means that there is a height difference of one-half unit between two sides of the crystal;  $E$  is related to the free energy  $\sigma$  per unit length of a step by  $E = \partial(\beta\sigma)/\partial\beta$ .
- <sup>17</sup>L. Onsager, *Phys. Rev.* **65**, 117 (1944).
- <sup>18</sup>M. E. Fisher and A. E. Ferdinand, *Phys. Rev. Lett.* **19**, 169 (1967).
- <sup>19</sup>See, e.g., L. P. Kadanoff, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1976), Vol. 5A.
- <sup>20</sup>S. T. Chui and J. D. Weeks, *Phys. Rev. B* **14**, 4978 (1976).
- <sup>21</sup>J. M. Kosterlitz, *J. Phys. C* **7**, 1046 (1974).
- <sup>22</sup>B. Sutherland, *Phys. Lett.* **26A**, 532 (1968).

## Properties of Inclusive $\pi^\pm$ Production in 100-GeV/c Antiproton-Proton Interactions

J. Whitmore, B. Y. Oh, M. Pratap, G. Sionakides, and G. A. Smith

*Department of Physics, Michigan State University, East Lansing, Michigan 48824\**

and

R. E. Ansorge, C. P. Bust, J. R. Carter, W. W. Neale, J. G. Rushbrooke and D. R. Ward

*Cavendish Laboratory, Cambridge, England†*

and

C. T. Murphy, R. Raja, and L. Voyvodic

*Fermi National Accelerator Laboratory, Batavia, Illinois 60510‡*

(Received 31 January 1977)

Inclusive spectra are presented for  $\pi^\pm$  production in 100-GeV/c  $\bar{p}p$  interactions. The rapidity distribution for the difference ( $\bar{p}p - pp$ ) approximately scales as the difference in total cross sections in the fragmentation region between 12 and 100 GeV/c and exhibits an approximate  $s^{-1/2}$  dependence in the central region.

Extensive data from the CERN intersecting storage rings (ISR) and from Fermilab now exist on inclusive particle production in baryon-baryon and meson-baryon scattering at high energies. Multipion production in antinucleon-nucleon interactions, however, has not been published above a laboratory momentum of 15 GeV/c.<sup>1</sup> Consequently, nothing is known about the high-energy behavior of multiparticle production in  $\bar{p}p$  interactions and, in particular, about the baryon annihilation process above  $\sim 12$  GeV/c.<sup>2</sup> In this Letter we present the first results on inclusive  $\pi^\pm$  produc-

tion in  $\bar{p}p$  interactions at 100 GeV/c. These data permit a study of the center-of-mass- (c.m.) energy dependence of inclusive  $\pi^\pm$  production in both the fragmentation and central regions. Although individual annihilation events cannot be identified in this experiment, by making comparisons with similar data from  $pp$  interactions we infer some features of inclusive pion production which may describe high-energy baryon annihilation.

The data result from a 98 000-picture exposure of the Fermilab 30-in. hydrogen bubble chamber, wide-gap spark chamber hybrid system to a 100-