PHYSICAL REVIEW LETTERS

VOLUME 51 | 5 SEPTEMBER 1983 | NUMBER 10

Eight-Vertex Model of Two-Dimensional Domain Walls

Franz S. Rys
Fachbereich Physik, Freie Universitaet Berlin, D-1000 Berlin 33, West Germany
(Received 8 December 1982; revised manuscript received 5 July 1983)

A statistical model of interacting linear domain walls (occurring, e.g., in monolayer adsorbates) is solved on the square lattice with use of exact and numerical results of an equivalent eight-vertex model. For attractive walls a commensurate and an incommensurate phase are separated by a first-order line for stiff walls and by a fluid phase for flexible walls. The phase boundaries with the fluid phase are Ising-like. For repulsive stiff walls an intermediate striped phase with a nonuniversal boundary occurs which vanishes for higher flexibilities. Moreover, disorder lines are located.

PACS numbers: 05.50.+q, 64.60.Cn, 68.40.+e, 82.65.Dp

Two-dimensional phase transitions from a commensurate (C) or a disordered [fluid (FL)] phase to an incommensurate (IC) phase, as well as the melting transition, are presently being extensively studied.[1-3] The statistical properties of these phases are conveniently described in terms of thin linear discommensurations (misfit dislocations or compression walls, also allowing for off-lattice sites) which separate larger nearly homogeneous (or commensurate) domains. This approach is rather general, quite transparent and more appropriate than, for example, a multiparameter lattice-gas model of adsorbed monolayers, evaluated by Monte Carlo techniques (which possibly miss certain topological excitations). However, the difficult problem of the domain-wall (DW) statistics is usually treated in a phenomenological mean-field or Landau-Ginzburg formalism, which is not expected to describe correctly a low-dimensional system of walls.

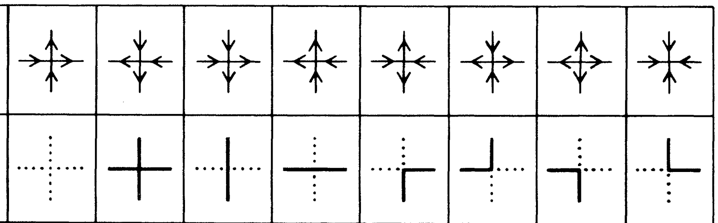
In this Letter, the problem of the line statistics of simple interacting domain walls is formulated rigorously in terms of a lattice model.[4] Only one type of (both horizontal and vertical) mutually interacting DW's with a given stiffness is considered for which no open ends or three-wall junctions occur. This assumption is realized, e.g., for the two-sublattice structures $p(2\times 2)$ or $c(2\times 2)$ on square and $p(2\times 1)$ on rectangular (uniaxial) substrate lattices. "Dilution" walls are neglected for energetic reasons. Any line pattern of DW's, characterized by n_h (n_v) horizontal (vertical) bonds, n_b corners, and n_c crossings, is isomorphic to a bond graph of the eight-vertex (8V) model[5] having weights $\omega_5=\omega_6=\omega_7=\omega_8=1$ [called subsequently the (1234) model]. The energy of a DW configuration is given in terms of four microscopic parameters:

$$E=n_h\epsilon_h+n_v\epsilon_v+n_b\epsilon_b+n_c\epsilon_c. \qquad (1)$$

ϵ_h and ϵ_v are the grand-canonical energies of a horizontal and vertical bond, respectively, ϵ_b is the corner (or bending) energy describing the wall stiffness, and ϵ_c is the crossing energy which is a measure of the wall-wall interaction. A simple example is chosen for which only the wall energies depend on the chemical potential μ of the adsorbate, $\epsilon_h=\epsilon_h{}^0-\mu/2$, $\epsilon_v=\epsilon_v{}^0-\mu/2$, whereas ϵ_b and ϵ_c are μ independent (but a generalization is straightforward).[6] In Fig. 1, the bond representation and the choice of the weights ω_i (for $i=1,\ldots,4$) of the (1234) model are given in terms of the Boltzmann factors $H=\exp(-\beta\epsilon_h/2)$, $V=\exp(-\beta\epsilon_v/2)$, $B=\exp(-\beta\epsilon_b)$, and $C=\exp(-\beta\epsilon_c)$.

Various exact and numerical results on the 8V model are summarized as follows: (i) The symmetric 8V model (solved exactly by Baxter[5])

Arrow Configurations / Bond Configurations



Vertex Weights	$\omega_1 = 1$	$\omega_2 = (HV)^2C$	$\omega_3 = V^2$	$\omega_4 = H^2$	$\omega_5 =$ HVB	$\omega_6 =$ HVB	$\omega_7 =$ HVB	$\omega_8 =$ HVB
Normalised Weights	$\frac{1}{HVB}$	$\frac{HVC}{B}$	$\frac{V}{HB}$	$\frac{H}{VB}$	1	1	1	1

FIG. 1. Arrow and bond configurations of the 8V model. The vertex weights are expressed in terms of the DW Boltzmann factors (see text).

shows a nonuniversal critical behavior (with weight-dependent critical exponents) and corresponds to the isotropic DW model $\epsilon_h = \epsilon_v = \epsilon = -\epsilon_c/2$ and arbitrary ϵ_b. (ii) For the general 8V model various symmetries hold.[5] They imply, for example, the equivalence of the (1234) and the (2143) model. (iii) The free-fermion condition[5] for $\omega_1\omega_2 + \omega_3\omega_4 = 2$ leads to an exact solution of the special case $1 + C = 2B^2$ and describes an Ising-like critical behavior. In particular, the free-fermion condition is fulfilled for the (12) model ($\omega_3 = \ldots = \omega_8 = 1$, i.e., $\epsilon_h = \epsilon_v$, $\epsilon_b = 0$) in the special case of zero crossing energy ($\epsilon_c = 0$) which is identical to the Ising model (as the line graphs are identical with the high-temperature Ising graphs). (iv) Along the disorder line[7] the free energy is analytic, but not necessarily across it. Hence the disorder line does not cross in general any phase boundary. For the (1234) model, it is defined by the equation

$$[1 + (\omega_3\omega_4)^{1/2} - \omega_1][1 + (\omega_3\omega_4)^{1/2} - \omega_2] = 1, \quad \omega_1, \omega_2 \leq 1 + (\omega_3\omega_4)^{1/2} \tag{2}$$

(v) An equivalence[8] relates the general 8V model to the uniaxial Ising model with coupling constants J_0^x, J_0^y, J, and J_4 of the anisotropic nearest-neighbor [nn(x), nn(y)], next-nearest-neighbor, and four-spin interactions around a plaquette, respectively. The J's are uniquely related to the wall energies:

$$\epsilon_h = 2J_0^y + 4J, \quad \epsilon_v = 2J_0^x + 4J, \quad \epsilon_c = -8J, \quad \epsilon_b = -2J + 2J_4. \tag{3}$$

Recent renormalization-group[9-11] and series-expansion[12] calculations on the *isotropic* Ising model yielded the critical surface S in the space of parameters $K_0 = \beta J_0$, $K = \beta J$, $K_4 = \beta J_4$ (cf., e.g., Fig. 1 of Ref. 9). S is symmetric with respect to the "Baxter plane" $K_0 = 0$ and consists of two disconnected parts: the universal blade S_u (with $K_0 + 2K > 0$) containing Ising-like critical points (with the exception of the "Baxter points" with $K_0 = 0$), and the nonuniversal blade S_{nu} (with $K_0 + 2K < 0$). The nonuniversal critical points on the "Baxter line" on S_u and on all of S_{nu} have varying exponents in general. Along the planes $\pm K_0 + 2K = 0$ the two blades approach asymptotically at $T \to 0$. On the low-temperature portion of the Baxter plane, $K_0 = 0$, $K > \{\sinh^{-1}[\exp(-2K_4)]\}/2$, first-order transition points are located (which correspond to a flip of the spontaneous ferroelectric diagonal polarization upon changing the sign of K_0[13]).

With use of Eqs. (3) the phase diagram and the critical behavior of the *isotropic* DW model with $\epsilon_h = \epsilon_v = \epsilon = \epsilon^0 - \mu/2$ is calculated for various values of ϵ_c and ϵ_b yielding the following results:

(1) For *attractive stiff DW's*, $\epsilon_c < 0$, $\epsilon_b > \epsilon_c/2$, the (μ, T) phase diagram [symmetric with respect to $\mu = 0$ because of (ii)] (see Fig. 2) shows a C phase for $\mu < 2\epsilon^0 + 4\epsilon_c$, which is characterized by a nondegenerate "empty" ground state at $T = 0$, a low DW density, and an Ising-like order-disorder phase boundary with the FL phase. For $\mu > 2\epsilon^0 + 4\epsilon_c$, a high-DW-density phase describes a concentrated array of crossing discommensurations with a nondegenerate ground state. It will be termed the IC phase in the following.[14] The IC-FL (order-disorder) boundary is Ising-like (for in both cases the critical points lie on S_u). At $\mu = 2\epsilon^0 + 4\epsilon_c$ a nonuniversal bicritical Baxter point B is located where a vertical first-order line separating the C from the IC phase joins the C-FL

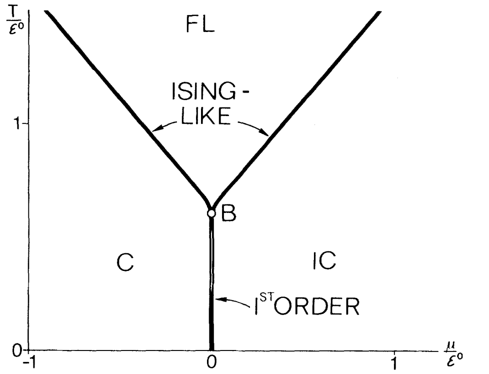


FIG. 2. Schematic phase diagram for $\epsilon_b = \epsilon^0/2$, $\epsilon_c = -2\epsilon^0$. The Ising-like phase boundaries C-FL and IC-FL merge into the first-order C-IC boundary at the bicritical Baxter point B (which decreases with decreasing ϵ_b). For $\epsilon_b < \epsilon_c/2$ a finite FL gap opens for all T (not shown).

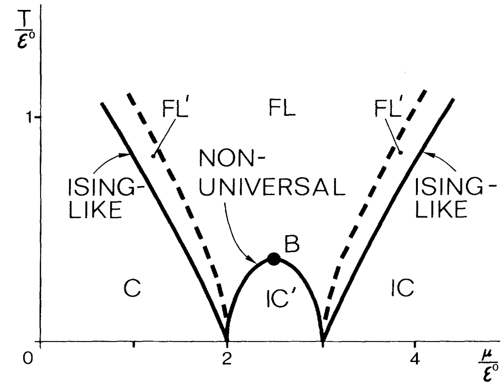


FIG. 3. Schematic phase diagram of the DW model with $\epsilon_b = \epsilon_c = \epsilon^0/2$. The solid lines denote the C-FL and the IC-FL phase boundaries (with Ising-like critical points) and the IC′-FL phase boundary (with nonuniversal critical points, e.g., with $\nu = 0.6$ at B). The broken lines show the disorder lines [Eqs. (2)].

and the IC-FL phase boundaries. The Baxter temperature T_B decreases with ϵ_b (for fixed $\epsilon_c < 0$), and $T_B = 0$ for $\epsilon_b \leq \epsilon_c/2$.

(2) For *attractive flexible DW's*, $\epsilon_c < 0$, $\epsilon_b < \epsilon_c/2$, a finite FL gap opens between the C and the IC phases for $T > 0$ with a highly degenerate ground state. The existence of a first-order transition for attractive DW's which was conjectured for hexagonal patterns[2] is thus proved on square structures for stiff DW's ($\epsilon_b > \epsilon_c/2 > 0$) but disproved for flexible ones ($\epsilon_b < \epsilon_c/2$). Moreover, in the case (1) an order-order C-IC transition (of first order) occurs instead of an intermediate FL phase [as in case (2)]. Interestingly, according to a recent conjecture[3] a FL phase exists always down to $T = 0$ for (2×1) structures on hexagonal substrates.

(3) For *repulsive stiff DW's*, $\epsilon_c > 0$, $\epsilon_b > 0$, a C phase occurs for $\mu < 2\epsilon^0$ and an IC phase for $\mu > 2\epsilon^0 + 2\epsilon_c$ with Ising-like phase boundaries (see Fig. 3). In addition, a qualitatively different intermediate IC′ phase is sandwiched between the C and IC phases. It has a doubly degenerate ground state formed by a parallel array of discommensurations either in the horizontal or the vertical direction.[15] The IC′-FL phase boundary is nonuniversal since its critical points lie on S_{nu}. On the crossing with the symmetry line $\mu = 2\epsilon^0 + \epsilon_c$ a Baxter point B is located. No first-order line occurs in this case. A disorder line [Eq. (2)] appears for $\mu < 2\epsilon^0$ and for $\mu > 2\epsilon^0 + 2\epsilon_c$ and separates in each case two regions of the fluid phase, FL and FL′, in which the correlation functions may have a different behavior.[16]

(4) For *repulsive flexible walls*, $\epsilon_c > 0$, $\epsilon_b < 0$, a qualitatively similar phase diagram as in case (2) shows up.

(5) For the *uniaxial* DW model, no explicit numerical data have yet been calculated. However, it follows from a renormalization-group analysis[10] that all continuous phase boundaries are, in fact, Ising-like.

An alternative DW model for the extreme uniaxial case $\epsilon_h = \infty$ can be formulated in terms of a general six-vertex model, which shows a variety of continuous Ising-like, F-like (or Kosterlitz-Thouless like), and first-order transitions. It will be studied elsewhere.

Other problems are described by this model as well. For example, the (12) model [cf. (i)] is one of the simplest cases of the (anti)ferroelectric 8V model in a diagonal field and is of interest on its own.[17] Also, it is equivalent to the Ising model on the square lattice with local bond disorder defined by the Hamiltonian in Eq. (4) of Ref. 18 with $J = \beta\epsilon$, $F = -\beta\epsilon_c$, locating the bicritical point at $F_{crit} = 2\ln 3 = 2.197\ldots$ (for $q = 2$). The limit of an infinite wall repulsion ($\epsilon_c = \infty$) is the two dimensional, multiplicity-1 case of the loop-gas model.[19] For negative wall energies, $\epsilon < 0$, the (12) model has no phase transitions for $T > 0$.

Furthermore, a special case of the (1234) model is equivalent to a simple lattice gauge model.[20]

In conclusion, the statistical problem of isotropic discommensuration walls on quadratic structures is solved by use of exact and numerical results. For various choices of the bending and crossing energies, the phase diagrams and the critical properties are established. For example, phase transitions in monolayers at oversaturated or submonolayer coverages on square substrate faces [e.g., in H/Pd(100), O/Ni(100)[21]] can be described. In the case of low coverages and strong nearest-neighbor repulsions the phases C, IC′, and IC would correspond, e.g., to the structures $p(2\times 2)$, $p(2\times 1)$, and $c(2\times 2)$, respectively. Unfortunately, at present no experimental critical exponents are available for a quantitative comparison of the model's predictions. A detailed discussion of experimental phase diagrams will be given in an extended paper. Also, a generalized DW model describing several kinds of walls (e.g., on hexagonal structures) will be elaborated.

This work was initiated by an interesting conversation with P. Kleban. Thanks are also due to M. N. Barber, A. N. Berker, W. Helfrich, and V. L. Pokrovskij for stimulating discussions and to S. Reindl and D. Tománek for technical assistance. The project was supported by the Deutsche Forschungsgemeinschaft.

[1]V. L. Pokrovsky and A. L. Talapov, Phys. Rev. Lett. 42, 65 (1979); P. Bak, D. Mukamel, J. Villain, and K. Wentowska, Phys. Rev. B 19, 1610 (1979); F. Haldane and J. Villain, J. Phys. (Paris) 42, 1673 (1981); J. Schulz, Phys. Rev. Lett. 46, 1685 (1981); J. Villain and P. Bak, J. Phys. (Paris) 42, 657 (1981); T. Bohr, Phys. Rev. B 25, 6981 (1982); M. Kardar and A. N. Berker, Phys. Rev. Lett. 48, 1552 (1982); D. Huse and M. E. Fisher, Phys. Rev. Lett. 49, 793 (1982); T. Nattermann, J. Phys. (Paris) 43, 631 (1982); for a review, see, e.g., P. Bak, Rep. Prog. Phys. 45, 587 (1982), and references therein.

[2]See, e.g., P. Bak and T. Bohr, Phys. Rev. B 27, 591 (1983).

[3]S. N. Coppersmith, D. S. Fisher, B. I. Halperin, P. A. Lee, and W. F. Brinkman, Phys. Rev. Lett. 46, 549 (1981).

[4]The lattice approximation to the continuum wall problem is expected to give a good description of the critical properties in analogy to a lattice-gas model of a real gas. In general, the lattice of the DW model is not *a priori* related to any physical lattice (as, e.g., the substrate lattice).

[5]R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, London, 1982).

[6]In a lattice-gas picture, the four parameters ϵ_h, ϵ_v, ϵ_b, and ϵ_c are determined by the effective lateral nearest-neighbor, next-nearest-neighbor, two-body, three-body, four-body, etc., substrate interactions, and μ is determined by the adsorbate coverage θ.

[7]I. Peschel and F. S. Rys, Phys. Lett. 91A, 187 (1982); M. Kardar, Phys. Rev. B 26, 2693 (1982).

[8]L. P. Kadanoff and F. Wegner, Phys. Rev. B 4, 3989 (1971).

[9]M. Nauenberg and B. Nienhuis, Phys. Rev. Lett. 33, 944 (1974).

[10]J. M. J. van Leeuwen, Phys. Rev. Lett. 34, 1056 (1975).

[11]M. P. Nightingale, Phys. Lett. 59A, 486 (1977); R. H. Swendsen and S. Krinsky, Phys. Rev. Lett. 43, 177 (1979); M. N. Barber, J. Phys. A 12, 679 (1979), and 15, 915 (1982).

[12]J. Oitmaa, J. Phys. A 14, 1159 (1981).

[13]Thanks are due to M. N. Barber for an illuminating discussion on this point.

[14]The inclusion of appropriate isotropic interactions between neighboring parallel DW's will presumably lead to a "genuine" floating isotropic IC phase (by "gluing" the DW's). For example, in a corresponding lattice model, isotropic second-neighbor interactions would have to be included.

[15]If appropriate interactions between parallel walls are included, IC′ denotes a doubly degenerate floating incommensurate phase.

[16]W. Selke, K. Binder, and W. Kinzel, Surf. Sci. 125, 74 (1983).

[17]For a positive $\epsilon > 0$, the transitions are Ising-like except for the Baxter point at $\omega_1 = \omega_2 = 3$ (for $\epsilon_c = -2\epsilon$) with nonuniversal exponents $\alpha = \frac{1}{2}$, $\nu = \frac{3}{4}$, etc. The disorder line appears for competing interactions $J < 0, J_4 < 0$ only.

[18]R. H. Swendsen, D. Andelman, and A. N. Berker, Phys. Rev. B 24, 6732 (1981).

[19]The loop-gas model has been formulated recently [F. S. Rys and W. Helfrich, J. Phys. A 15, 599 (1982)] for the excluded-volume interaction of closed ring polymers in two and three dimensions (e.g., for the equilibrium polymerization of sulfur), of the dislocation-mediated smectic-*A* to nematic and melting transitions, and of vortex lines at the superfluid and the superconducting transitions, etc. Moreover, it has applications in recent d-dimensional lattice gauge theories [M. Karowski, H. J. Thun, W. Helfrich, and F. S. Rys, Freie University Report No. FUB/HEP 2/83 (to be published)], in the statistics of membranes and microemulsions, etc. At present, the critical properties of the loop gas are not known.

[20]A. Weinkauf and J. Zittartz, Z. Phys. B 45, 223 (1982).

[21]For H/Pd(100), R. J. Behm, K. Christmann, and G. Ertl, Surf. Sci. 99, 320 (1980). For O/Ni(100), D. E. Taylor and R. L. Park, Surf. Sci. 125, L73 (1982).