

Field-dependent crystal forms and shape transitions in two-dimensions

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1985 J. Phys. A: Math. Gen. 18 1533

(<http://iopscience.iop.org/0305-4470/18/9/032>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 31/05/2010 at 09:55

Please note that [terms and conditions apply](#).

Field-dependent crystal forms and shape transitions in two dimensions

P A Slotte and P C Hemmer

Institutt for teoretisk fysikk, Universitetet i Trondheim, N-7034 Trondheim-NTH, Norway

Received 27 September 1984, in final form 17 December 1984

Abstract. We determine equilibrium crystal shapes for a triangular Ising model with isotropic nearest-neighbour interactions. At zero temperature the shape is an equilateral hexagon for ferromagnetic interactions, and an equilateral triangle for antiferromagnetic interactions in the presence of a weak field, $H \leq 2J$. When the magnetic field is increased beyond $2J$ the shape varies continuously with the field, in the form of a hexagon with three-fold symmetry. For still higher fields, $H \geq 4J$, the shape is again an equilateral triangle, now oriented $\pi/3$ relative to low-field crystals. Finite-temperature shapes are determined by means of a solid-on-solid calculation of the orientation-dependent interfacial free energy.

1. Introduction

Under thermodynamic conditions that allow two phases to coexist the question of the average equilibrium shape of a large inclusion of one phase (e.g. a crystal or a droplet) in the background of another is an old problem which goes back to the turn of the century (Wulff 1901). The difficult part of the problem is to calculate the interfacial free energy per unit length (the surface tension) as a function of the orientation of the interface. From this the shape of the inclusion can be determined directly by the Wulff construction (see Rottman and Wortis 1984a for a review). The problem has received considerable attention recently (Rottman and Wortis 1981, 1984a, b, Zia and Avron 1982, Avron *et al* 1982), partly because exact results for all temperatures are available for the two-dimensional square lattice Ising model.

In this paper we report on an investigation of equilibrium shapes for a triangular Ising model. This model can be used to describe shapes of magnetic domains in a two-dimensional magnet and equilibrium shapes for adsorption of particles on a surface. For attractive (ferromagnetic) nearest-neighbour interactions equilibrium shapes have sixfold symmetry due to the sixfold symmetry of the underlying lattice. We are, however, interested in the *repulsive* (antiferromagnetic) case. In a non-zero magnetic field this model has a triply degenerate ground state. We study the shape of a large inclusion of one of these phases in the background of another.

The results are interesting and unexpected. At zero temperature there exist three regions for the magnetic field strength H , a low-field region $0 < H \leq H_1$, an intermediate region $H_1 < H < H_2$ and a high-field region $H_2 \leq H < 6J$. In the low-field region the shape of the inclusion is an equilateral triangle with sides oriented orthogonal to the lattice directions, in the intermediate region the contour is a hexagon with threefold symmetry and field-dependent shape, and in the high-field region a triangular shape

again appears, now rotated by $\pi/3$ with respect to the low-field triangles. The same effects are visible at non-zero temperatures, now in domains with smoothly curved contours.

The outline of this paper is as follows. In § 2 we present the exact analysis at $T = 0$. The low-temperature expansion of the interfacial free energy is discussed. To obtain the orientation dependent finite-temperature free energy we take in § 3 recourse to a solid-on-solid approximation. At low temperatures the resulting free energy should constitute an excellent approximation to the exact results. The equilibrium shapes are obtained via the Wulff construction.

2. Zero-temperature results

2.1. The Wulff construction

The equilibrium shape of an inclusion of one phase in an environment of another is obtained by applying the Wulff construction. Specifically, assume that the surface tension, $\sigma(\hat{n})$, for an interface orthogonal to \hat{n} , is known. Draw a polar plot of $\sigma(\hat{n})$ and at each point on the curve draw a straight line perpendicular to the radius. The inner envelope of these lines defines the equilibrium shape of the inclusion. (Adjustment to the actual area is obtained by a multiplicative factor.)

A kink in the polar plot produces a facet (straight boundary) on the inclusion. Since the interface here is a one-dimensional object this happens only at zero temperature.

2.2. The model

The Hamiltonian has the form

$$\mathcal{H} = J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i \quad (1)$$

with $J > 0$ and $s_i = \pm 1$. The sums run over nearest-neighbour pairs, and all spins, respectively. By symmetry it suffices to consider positive external magnetic fields, $H > 0$.

In the ground state the minus spins populate any one of the three sublattices, the plus spins the two other sublattices. The degeneracy is therefore three. Figure 1 shows an inclusion of one of these phases in the background of another. The region of the temperature-field plane where the phases are stable is also indicated.

The triangular lattice by itself has six symmetry axes, parallel and orthogonal to the lattice directions. The selection of two out of three phases reduces the number of symmetry axes to three, namely those orthogonal to the lattice directions (see figure 1). Hence the surface tension will have this reduced symmetry.

2.3. $T = 0$ behaviour

At zero temperature the surface tension, $\sigma(\hat{n}, T)$, is simply the minimum energy per unit length required to make a macroscopic interface perpendicular to \hat{n} .

Let us start by giving the values of the surface tensions for interfaces along the symmetry directions, i.e. perpendicular to the lattice directions. The two different interfaces are shown in figures 2 and 3, and for each direction the interface comes in two different versions, depending upon the value of the magnetic field. Simple counting

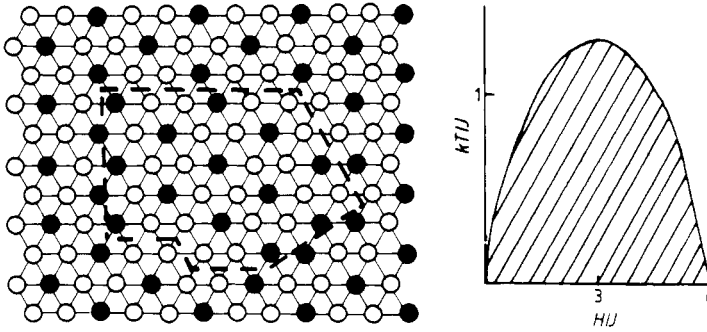


Figure 1. A small inclusion. Note that the plus spins (open circles) on one sublattice can be considered as belonging to either phase. The part of the H - T plane where the three phases are stable is indicated by the hatched area in the diagram on the right-hand side (Kinzel and Schick 1981).

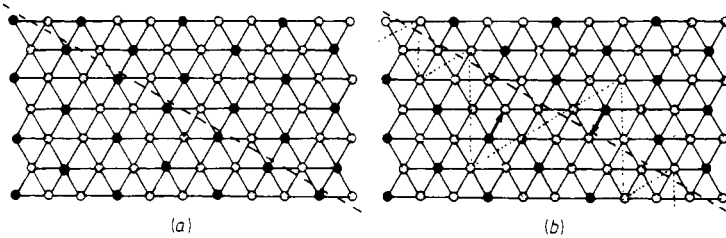


Figure 2. The interface α . When $0 < H < 4J$ the energy minimum is obtained as shown in (a). This is a 'heavy' domain wall (Kardar and Berker 1982. Huse and Fisher, 1982, 1984, use a slightly different nomenclature.) When $4J < H < 6J$ it pays to flip one minus spin in every pair of neighbouring minus spins, as shown in (b), forming a 'superlight' domain wall. Notice the entropy connected with the latter interface since some $+/-$ pairs, indicated by the arrows, can flip without energy cost. The degenerate interface may be conceived of as consisting of segments in the β direction alternating with segments running in the vertical direction ('light' walls). For the case when the two arrow-marked spin-pairs are flipped this interface representation is shown as the dotted line.

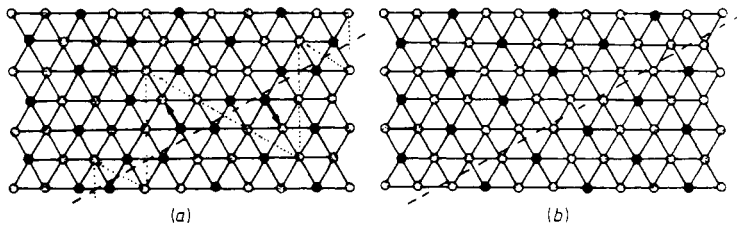


Figure 3. The interface β . The version (a) is for low fields. As in figure 2(b) an extensive entropy is again involved. The 'superheavy' domain wall (broken) may break up into 'heavy' segments as indicated by the arrows and the dotted line. For $H > 2J$ it pays to turn every other minus spin along the interface. The latter interface, a 'light' domain wall, is non-degenerate.

gives

$$\sqrt{3}\sigma_\alpha = 4J - \frac{1}{3}H - |H - 4J| \tag{2}$$

and

$$\sqrt{3}\sigma_\beta = 2J + \frac{1}{3}H - |H - 2J|. \tag{3}$$

Notice the symmetry around $H = 3J$

$$\sigma_\beta(6J - H) = \sigma_\alpha(H). \tag{4}$$

We let θ denote the angle between the direction of the interface and the horizontal lattice direction in figures 2 and 3. Symmetry allows us to consider values of θ limited to the angular interval $(-\pi/6, \pi/6)$.

In the present case with merely nearest-neighbour interactions there are several microscopic minimum-energy interfaces for a given macroscopic interface between two points A and B a distance L apart (figure 4), corresponding to a finite zero-temperature entropy (see § 2.4). In figures 2(b) and 3(a) we have indicated examples of how by flipping spin pairs one may shift the microscopic interface without changing the interface energy. Moreover, figure 4(a) shows the nature of the collection of step-like microscopic interfaces which all yield the same minimum energy. In this section we find these minimum-energy interfaces by inspection, but the results for the minimum energy itself and the degeneracy (the entropy) can be verified by taking the low-temperature limit of the interface free energy calculated in § 3 from the partition function.

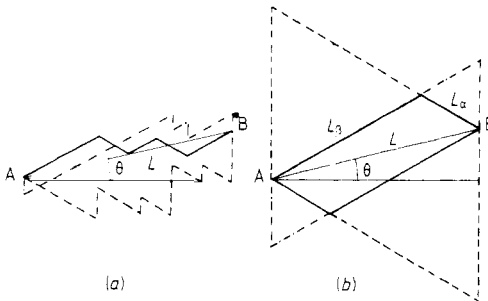


Figure 4. Examples of microscopic minimum-energy interfaces from A to B, with macroscopic length and orientation L and θ respectively, (a). The fully drawn interface refers to the intermediate field region, the broken interface to the low-field region, and the chain interface to the high-field region. The microscopic interface from A and B is confined to the parallelograms shown for the three field regions in (b). The horizontal lines runs in one of the lattice directions.

It is convenient to calculate the free energy of the interface between A and B by using one special microscopic interface, namely one that first progresses a distance L_β in the direction β and then a distance L_α in the direction α (figure 4(b)). With the results (2), (3) for the surface tensions in these directions we have

$$\sigma = (\sigma_\alpha L_\alpha + \sigma_\beta L_\beta) / L. \tag{5}$$

Simple geometric considerations give

$$L_\alpha = \frac{2}{3}\sqrt{3}[\sin(\frac{1}{6}\pi - \theta)]L, \quad L_\beta = \frac{2}{3}\sqrt{3}[\sin(\frac{1}{6}\pi + \theta)]L. \tag{6}$$

Hence the angle-dependent interfacial energy, $\sigma(\theta, 0)$ is given by

$$\sqrt{3}\sigma(\theta, 0) = 2\sigma_\alpha \sin(\frac{1}{6}\pi - \theta) + 2\sigma_\beta \sin(\frac{1}{6}\pi + \theta) \tag{7}$$

for $|\theta| \leq \frac{1}{6}\pi$.

Wulff constructions are shown in figure 5. (Note that the direction \hat{n} of the surface tension $\sigma(\hat{n}, T)$, the input in the Wulff construction, is by definition *orthogonal* to the interface.) For all temperatures the change of roles of the including and the included phase (i.e. letting the lower phase in figures 2 and 3 be the included phase) amounts to a change of signs of the angles, or equivalently, a rotation of the inclusion by $\pi/3$ (see figures 2 and 3). At zero temperature a similar rotation is also induced by replacing the magnetic field H by $6J - H$.

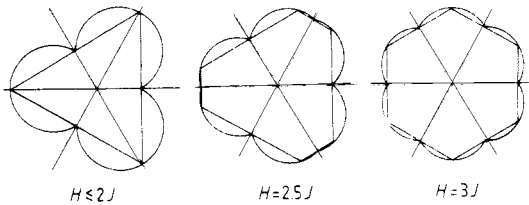


Figure 5. Wulff constructions for $T=0$. The outer curves are the interfacial free energy $\sigma(\hat{n}, 0)$. The inner lines are the corresponding equilibrium shapes obtained by the Wulff construction. The lattice directions are defined by the three intersecting lines.

For low fields, $H < 2J$, $\sigma_\beta = 2\sigma_\alpha$ and consequently the shape is field independent. The resulting form is a triangle which only uses the minimum energy directions α . The energy difference, $\sigma_\beta - \sigma_\alpha$, is so large that it does not pay, for a given area, to make the total interface shorter. In the interval $2J < H < 4J$ the ratio $\sigma_\beta/\sigma_\alpha$ is smaller, and field dependent. The inclusion has now, as shown in figure 5, a hexagonal form. Only at $H = 3J$ is the hexagon equilateral. The ratio between the lengths of the facets is

$$\rho = (4J - H)/(H - 2J). \tag{8}$$

For $H > 4J$ the directions α and β exchange roles compared with the low-field region, as is evident from the symmetry relation (4). The equilibrium shape is again triangular, but the triangle is rotated by $\pi/3$ with respect to the low-field triangles.

2.4. Low-temperature expansion

If $g_0(L, \theta)$ is the number of ways an interface, of macroscopic length and orientation L and θ , respectively (see figure 4), can be constructed with a minimum energy E_0 , then the low-temperature surface tension is

$$\begin{aligned} \sigma(\theta, T) &= -(kT/L) \ln[g_0 \exp(-E_0/kT)] \\ &= (E_0 - kT \ln g_0)/L, \end{aligned} \tag{9}$$

up to exponentially small terms. Here k is the Boltzmann constant.

Since the microscopic interface consists of alternating segments running in one out of two directions (see figure 4(a)) the degeneracy g_0 is simply the number of ways one can select $N_a = L_a/\sqrt{3}$ steps in one direction and $N_b = L_b/\sqrt{3}$ steps in the other

direction. Hence the degeneracy is given by the combinatorial factor

$$g_0 = \binom{N_a + N_b}{N_a}. \tag{10}$$

One sees from figure 4(b) that $L_a = L_\alpha$ and $L_b = L_\beta$ in the intermediate field region, while $L_a = L_\alpha + L_\beta$ and $L_b = L_\beta$ in the low-field region, and $L_a = L_\alpha$ and $L_b = L_\alpha + L_\beta$ in the high-field region. This gives, up to exponentially small terms, the low-temperature expansions:

$$\sigma(\theta, T) = \sigma(\theta, 0) + \frac{3}{2}kT \{ \sin(\pi/6 + \theta) \ln[\sin(\pi/6 + \theta)] + \cos \theta \ln(\cos \theta) - \sqrt{3} \sin(\pi/3 + \theta) \ln[\sqrt{3} \sin(\pi/3 + \theta)] \} \tag{11}$$

for $H < 2J$,

$$\sigma(\theta, T) = \sigma(\theta, 0) + \frac{3}{2}kT \{ \sin(\pi/6 + \theta) \ln[\sin(\pi/6 + \theta)] + \sin(\pi/6 - \theta) \ln[\sin(\pi/6 - \theta)] - \cos \theta \ln(\cos \theta) \} \tag{12}$$

for $2J \leq H \leq 4J$, and

$$\sigma(\theta, T) = \sigma(\theta, 0) + \frac{3}{2}kT \{ \sin(\pi/6 - \theta) \ln[\sin(\pi/6 - \theta)] + \cos \theta \ln(\cos \theta) - \sqrt{3} \sin(\pi/3 - \theta) \ln[\sqrt{3} \sin(\pi/3 - \theta)] \} \tag{13}$$

for $H > 4J$.

The relevance of the first-order terms in (11)-(13) for the finite-temperature shapes will be discussed below.

3. Finite temperatures

To investigate finite-temperature effects we have applied a solid-on-solid approximation to the interfacial free energy. Thus we only consider interface configurations without overhangs and without islands of different states within the opposing phases. We also discard the possibility of the third phase intervening at the interface. (For a discussion of the solid-on-solid approximation for the square lattice, and for references, see Zia and Avron 1982.)

The configurations used are illustrated in figure 6, and can be characterised by a set of integers, $\{k_i, l_i, m_i, n_i\}$, representing the number of overturned spins in each column, relative to a reference interface. Since the magnetisation of one of the sublattices is equal in the two phases under consideration, *only nearest-neighbour-column height differences* enter the energy expression:

$$E(\{k_i, l_i, m_i, n_i\}) = \sum_{i=1}^{N/3} [E_1(l_i - k_i) + E_2(m_i - l_i) + E_3(n_i - m_i) + E_1(k_{i+1} - n_i)] \tag{14}$$

where N is the length of the projection of the interface onto the $\theta = 0$ axis, in units of the lattice spacing, and

$$E_1(\delta) = \begin{cases} (8J - \frac{4}{3}H)\delta + \frac{2}{3}H - 4J & \delta > 0 \\ -\frac{4}{3}H\delta + \frac{2}{3}H & \delta \leq 0, \end{cases} \tag{15}$$

$$E_2(\delta) = \begin{cases} \frac{2}{3}H\delta & \delta > 0 \\ -(4J - \frac{2}{3}H)\delta & \delta \leq 0, \end{cases} \tag{16}$$

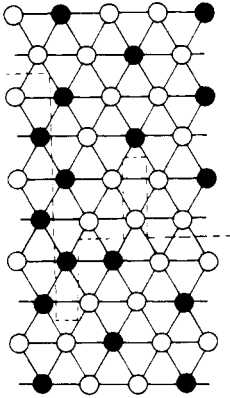


Figure 6. A typical interface configuration. The interface shown can be characterised by the set of integers $\{k_1, l_1, m_1, n_1, k_2, l_2\} = \{2, -1, 0, 1, 0, 0\}$.

and

$$E_3(\delta) = E_1(\delta + 1). \tag{17}$$

The field energy contributions have been judiciously distributed to secure convergence over the whole field range $0 < H < 6J$ in the evaluation of the partition function.

The partition function is

$$Z = \sum_{\{\delta_i\}} \exp\left(-\beta E(\{\delta_i\}) - \mu \sum_i \delta_i\right) \tag{18}$$

where $\{\delta_i\}$ is a set of height differences, and $\beta = 1/kT$. The 'chemical potential' μ regulates the macroscopic direction with the mean value of the interface angle given by

$$\tan \theta = -\sqrt{3} N^{-1} (\partial/\partial \mu) \ln Z. \tag{19}$$

The free energy per unit length of the interface is given by

$$\begin{aligned} N\sigma(\theta, T) &= -kT \cos \theta (1 + \mu \partial/\partial \mu) \ln Z \\ &= -kT (\cos \theta \ln Z + \frac{1}{3}\sqrt{3} \mu \sin \theta). \end{aligned} \tag{20}$$

The evaluation of the partition function amounts to summing geometric series, with the result

$$\ln Z = \frac{2}{3} N \ln(t_1 t_2) \tag{21}$$

with

$$\begin{aligned} t_1 &= \frac{\sinh(\frac{2}{3}h - \frac{1}{2}\mu) + \sinh(4K - \frac{2}{3}h + \frac{1}{2}\mu)}{\cosh 4K - \cosh(4K - \frac{4}{3}h + \mu)} \\ t_2 &= \frac{\sinh 2K}{\cosh 2K - \cosh(2K - \frac{2}{3}h - \mu)} \end{aligned} \tag{22}$$

where $K = \beta J$ and $h = \beta H$.

Hence, if one defines

$$d_i = (\partial/\partial \mu) \ln t_i, \tag{23}$$

the angular dependence of the free energy is determined by elimination of μ between

the two equations

$$\begin{aligned}\tan \theta &= -\frac{2}{3}\sqrt{3}(d_1 + d_2) \\ \sigma/J &= -(2 \cos \theta \ln(t_1 t_2) + \sqrt{3}\mu \sin \theta)/3K.\end{aligned}\quad (24)$$

Notice that (24) is symmetric under the transformation

$$H \rightarrow 6J - H, \quad \mu \rightarrow -\mu, \quad \theta \rightarrow -\theta \quad (25)$$

which implies that the shape of an inclusion at a field $6J - H$ is identical with the shape at a field value H , the only difference being a rotation by $\pi/3$. This symmetry is exact at zero temperature (see (4) and (7)), but the exact free energy is *not* expected to have this symmetry since this would lead to the phase diagram being symmetric around $H = 3J$ which it apparently is not (Kinzel and Schick 1981). We expect that a solid-on-solid type approximation that takes into account configurations with the third phase intervening at the interface would do away with the symmetry (25).

In contrast to the exact free energy (24) is not symmetric around the $|\theta| = \pi/6$ axes. We have cured this by using (24) in the angular interval $(-\pi/6, \pi/6)$ around the horizontal direction where the solid-on-solid approximation is expected to be best, and enforcing the symmetry. The differences between the two versions are small near the symmetry axes, $|\theta| = \pi/6$, as long as one is not close to the critical region. In an approximate theory, like the present one, the temperature at which the interfacial free energy vanishes, will in general depend on the direction. Severe critical shape distortions will inevitably result. The exact free energy, on the other hand, approaches the *isotropic* scaling form.

From the examples of equilibrium shapes shown in figures 7-9 we notice that the shapes become very nearly circular already when the temperature is raised to the value $T = 0.75J/k$, about half of the maximum critical temperature. We expect the solid-on-solid approximation to be very good up to this temperature range. In this connection let us mention that by taking the low-temperature limit of the solid-on-solid result (24) one can show that the low-temperature expansions (11)-(13) are exactly reproduced. Notice also from the figures that the free energy in the directions where it is minimal changes very slowly with temperature as long as the anisotropies are not small. This is also borne out by the low-temperature expansions (11)-(13) since the derivative, with respect to the temperature, of the free energy is zero in these directions.

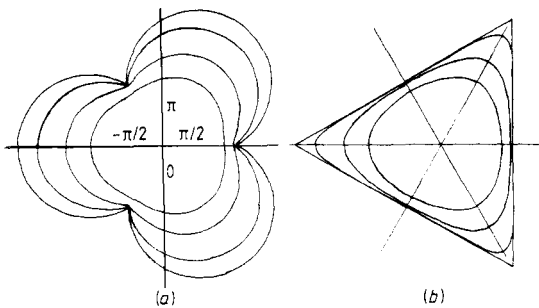


Figure 7. Interfacial free energy (a) and equilibrium shapes (b) at different temperatures in the magnetic field $H = 2J$. The temperatures are 0 (outermost curves), 0.2, 0.5 and 0.75 (innermost curve), in units of J/k . The values of the angle θ are indicated in (a). The three intersecting lines in (b) define the lattice directions.

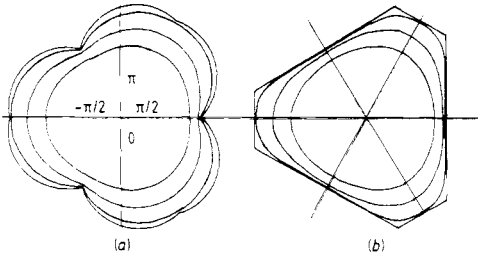


Figure 8. As figure 7, but in the magnetic field $H = 2.5J$.

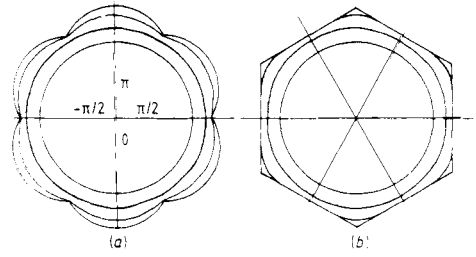


Figure 9. As figure 7, but in the magnetic field $H = 3J$.

4. Concluding remarks

We have shown, for a two-dimensional model, the existence of characteristic magnetic fields H_1 , H_2 , at which qualitative shape changes take place at low temperatures. At zero temperature these changes are genuine 'shape transitions', with discontinuities in the number of facets.

There is every reason to believe that similar subcritical shape transitions occur under more general circumstances. In three dimensions these transitions are expected to extend to finite temperatures.

References

- Avron J E, van Beijeren H, Schulman L S and Zia R K P 1982 *J. Phys. A: Math. Gen.* **15** L81
 Huse D A and Fisher M E 1982 *Phys. Rev. Lett.* **49** 793
 — 1984 *Phys. Rev. B* **29** 239
 Kardar M and Berker A N 1982 *Phys. Rev. Lett.* **48** 1552
 Kinzel W and Schick M 1981 *Phys. Rev. B* **23** 3435
 Rottman C and Wortis M 1981 *Phys. Rev. B* **24** 6274
 — 1984a *Phys. Rep.* **103** 59
 — 1984b *Phys. Rev. B* **29** 328
 Wulff G 1901 *Z. Kristallogr.* **34** 449
 Zia R K P and Avron J E 1982 *Phys. Rev. B* **25** 2042