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Roughening transition in the Blume–Emery–Griffiths model

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Abstract. Studying the ground-state properties of the three-dimensional Blume–Emery–Griffiths model, it is shown that a continuous phase transition is always preceded by the roughening transition. In contrast, with a discontinuous phase transition there is always associated a non-rough interface. A possible behaviour of the roughening transition in this model at non-zero temperatures is suggested.

1. Introduction

A knowledge of interfacial behaviour is essential to understand bulk critical behaviour [1]. Using some scaling arguments, one can show that the correlation length, which is the fundamental quantity for the bulk critical behaviour, and the interface thickness diverge almost in the same way while approaching the critical point. In contrast, at discontinuous phase transitions both these quantities usually remain finite.

Apart from the thickness, another characteristic of the interface is its roughness. For the two- or higher-than-three-dimensional models, the change of roughness during approach of the critical point is only quantitative. In the first case the interface is always rough, while in the second case it is always bounded [2]. The roughness is of particular importance, however, for studying three-dimensional models where the interface can undergo the roughening transition [3]. Is the roughness of the interface somehow connected with the kind of phase transition? In this paper we address this problem, which up to now has seemingly evaded more thorough consideration.

Our results are based mostly on ground-state analysis of the Blume–Emery–Griffiths (BEG) model, which is performed in section 2. A discussion extended to non-zero temperatures is presented in section 3. Section 4 contains our conclusions.

2. BEG model—ground-state properties

Consider the three-dimensional $S = 1$ Ising model with the biquadratic interaction K and the one-ion anisotropy D, described by the following Hamiltonian

$$\mathcal{H} = J \sum_{\langle i,j \rangle} S_i S_j - K \sum_{\langle i,j \rangle} S_i^2 S_j^2 - D \sum_{i=1}^{N} S_i^2 \tag{2.1}$$

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where $S_i = 0, \pm 1$ and $\langle i, j \rangle$ stands for the summation over the nearest-neighbouring pairs. The model is arranged on the simple cubic lattice of side $L (N = L^3)$. Hereafter, the bilinear coupling constant J is set to unity.

The model (2.1) is the so-called BEG model, which was originally introduced to describe phase separation and superfluidity in ^{3}He–^{4}He mixtures [4]. This model has been the subject of many theoretical studies and its thermodynamical properties, especially in the two- and three-dimensional cases, are already well known. Recent results obtained by extensive Monte Carlo simulations, as well as some references to previous works, can be found in Wang *et al* [5, 6]. At the ground state, the thermodynamical properties can be summarized as follows.

(i) $D < 0$. For $K > -\frac{1}{3}D - 1$, there is a ferromagnetic ordering ($-$) with all $S_i = -1$ or (+) with all $S_i = 1$, while for $K < -\frac{1}{3}D - 1$ there is a paramagnetic ordering (0) with all $S_i = 0$. The phase transition between these two phases is discontinuous (thick, dashed line in figure 1). In actual fact, this is a triple line where all three phases (+), ($-$) and (0) coexist.

(ii) $D > 0$. For $K > -\frac{1}{6}D - 1$, there is a ferromagnetic ordering, while for $K < -\frac{1}{6}D - 1$ there is a staggered ordering (in the first sublattice all $S_i = 0$ and in the second one $S_i = \pm 1$ at random). The nature of the phase transition between these two phases (tilted, thick, solid line in figure 1) is not absolutely certain but there are strong arguments that this is a continuous phase transition [6]. The phase transition between the staggered and paramagnetic phases (vertical, thick, solid line in figure 1) is also continuous.

Assuming that the parameters K and D have such values that the model is ferromagnetically ordered, let us impose on the surface of the cube the boundary conditions which induce the (+) phase in the upper part of the cube and the ($-$) phase in the lower part (figure 2).

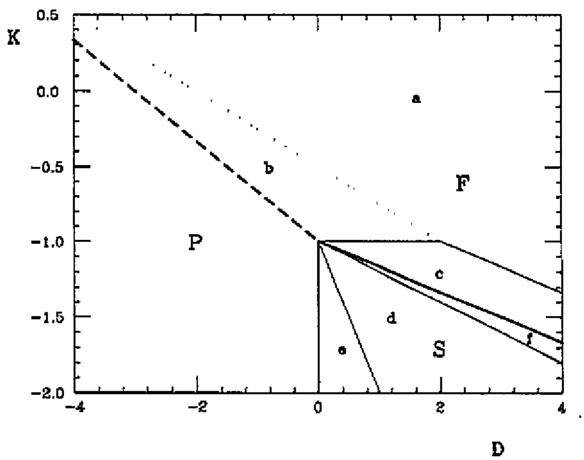

Figure 1. The ground-state phase diagram of the model (2.1). The thick, solid, and dashed lines denote the bulk continuous and discontinuous phase transitions, respectively, which separate the paramagnetic (P), ferromagnetic (F), and the staggered (S) phases. The region of different interface structures (a)–(f) are described in the text.

Rigorous determination of the structure of the created ground-state interface is a non-trivial problem. Our approach to this problem is certainly non-rigorous but in our opinion

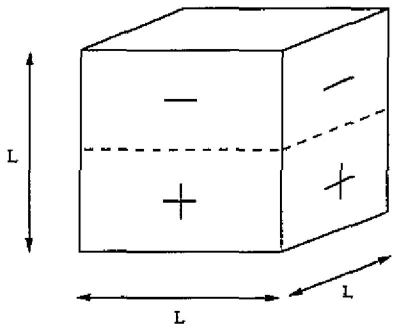

Figure 2. The boundary conditions on the surface of the $L \times L \times L$ cube which induce the interface between the two ferromagnetic phases (+) and (−).

it leads to the exact result. First let us assume that the ground-state interface has the SOS structure (it is possible to show that some simple bulbs or 'backwards bends' increase the energy but we are not sure whether we can eliminate all such non-SOS configurations). Moreover, it is obvious that for some values of parameters (K, D) the interface has the same simple structure as the ground-state interface in the $S = \frac{1}{2}$ ferromagnetic Ising model (it must be so at least for $K = 0$ and $D \to \infty$). For some other values of parameters, we expect that the interface is covered by 0 states. The next assumption is that the thickness of this covering layer is one (this assumption might not be satisfied for the boundary conditions which induce a step in the interface; here, we believe, it is correct). We are thus led to find the minimum energy configurations among such configurations as the one shown in figure 3 (this is actually its section but it is easy to imagine the three-dimensional extension). The excess energy of such configurations is given by

$$E = DL^2 + N_b(1 + K) \tag{2.2}$$

where N_b is the number of broken bonds. Notice that due to the last assumption the first term is constant for all such configurations. Thus we arrive at the following conclusion. For $1 + K > 0$, the excess energy E is minimal for minimal N_b, i.e. the intruding 0 states constitute a flat single layer, while for $1 + K < 0$, N_b must be maximal, i.e. the intruding 0 states constitute a fluctuating surface (such configurations are described below and an example is shown in figure 4(*c*)). It seems to us that the nearest-neighbours interaction and the homogeneous nature of (+) and (−) phases should not lead to more complicated configurations of the ground-state interface. A rigorous approach to this problem is left for a further study.

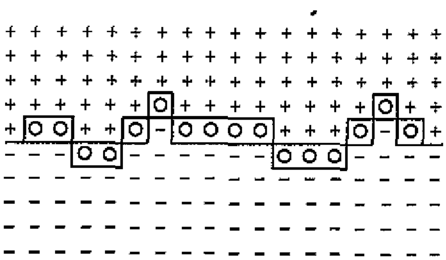

Figure 3. Atypical configuration of the interface with an intruding layer of the 0 states.

Once the candidates for the minimal energy configurations have been 'guessed', we can easily calculate their energy and determine the region of their existence. In the limit $L \to \infty$, the results are as follows.

(a) $4 + 6K + D > 0$ and $2 + 4K + D > 0$. The interface is composed of two layers of opposite spins. It resembles the ground-state interface in the $S = \frac{1}{2}$ ferromagnetic Ising model.

(b) $2 + 4K + D < 0$ and $K > -1$. The interface is also flat but the (+) and (−) phases are separated by an additional single layer of 0 states. Of course, there is a twofold degeneracy.

(c) $4+6K+D < 0$ and $K < -1$. The interface is strongly degenerate. The phases (+) and (−) are also separated by 0 states. However, the intruding layer is not flat, it always changes its height at neighbouring sites by one. Except for the intruding layer, the interface resembles the ground-state interface in the three-dimensional antiferromagnetic Ising model for a sufficiently strong magnetic field [7].

The regions described in cases (a)–(c) are shown in figure 1. For $K = 0$, the interfacial behaviour of the model (2.1) has already been studied [8] but, of course, the fluctuating ground state (c) does not appear in this case.

The same considerations can be given to the two-dimensional BEG model as well. Then the configurations of the two-dimensional interface described in cases (a)–(c) have their one-dimensional analogues, which are depicted in figure 4. Of course, the regions of the existence of the ground states shown in figure 4 for the two-dimensional BEG model are modified, but the topology of the ground-state phase diagram is the same as that in figure 1. This topology is preserved also for higher-dimensional ($d > 3$) cases.

Now let us assume that the parameters K and D are chosen in such a way that the model exhibits staggered ordering. We can again impose on the surface of the cube the appropriate boundary conditions which induce an interface. The structure of this interface is now as follows:

(d) $-(D/5) - 1 > K > -D - 1$. The interface is composed of two flat layers with staggered ordering which is arranged in an unfavourable way: a 0 state from one layer has as its nearest neighbour in the second layer also a 0 state. Analogously, randomly distributed ± states have as neighbours in the other layer also ± states. Notice that the pairs of neighbouring non-zero states are either both in the + state (++) or both in the − state (−−). The interface is also strongly degenerate ($\sim 2^{L^2/2}$) but this degeneracy does not allow the interface to wander. The corresponding situation for the two-dimensional model is shown in figure 5(*d*).

(e) $K < -D - 1$. The non-zero states now become even more unfavourable and as a result one spin of (++) or (−−) pairs is switched into a 0 state. Hence, the interface can be regarded as consisting of two layers of 0 states. There are again a lot of configurations of the interface with the same energy and the situation is basically similar to that described in case (c). The analogous situation for the two-dimensional model is depicted in figure 5(*e*).

(f) $K > -(D/5) - 1$. This time the 0 states become unfavourable and one spin of each (00) pair is switched into a non-zero state. The interface can now be seen as a random surface (of thickness two) of non-zero states (all spins in the (+) are all in the (−) states). There is again a strong degeneracy of the interface and the ensemble of interfaces resemble the ones already described in (c) and (e). Notice that all spins of the interface, in contrast to the spins in the bulk, have to be in the same state. This is the onset of the ferromagnetic ordering which will be created after the order–order phase transition. For the two-dimensional model the analogous situation is presented in figure 5(*f*).

As we have already mentioned, the ground-state transition between the staggered and

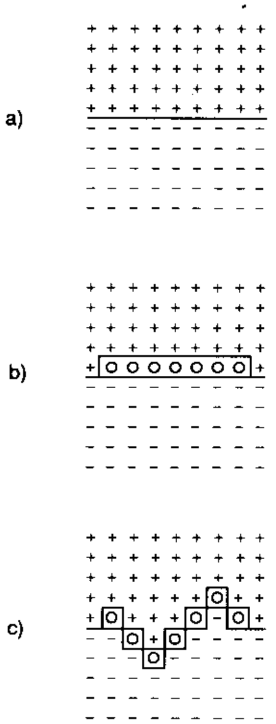

Figure 4. The interface structure for the two-dimensional BEG model in cases analogous to the cases (a), (b), and (c) described in the text.

ferromagnetic phases and the staggered and paramagnetic phases is regarded as a continuous one, but arguments for this are non-rigorous and mostly based on the numerical results [5, 6]. In agreement with the general notion that the surface tension vanishes at the continuous phase transition, our results provide further support for the continuity of these transitions. Namely, it is elementary to show that the excess energy for the interface in the cases (c), (e) and (f) vanishes along the solid thick lines. In contrast, along the dashed thick line the excess energy of the configuration (b) does not vanish. This confirms that this is a discontinuous phase transition. The order of phase transitions as suggested by numerical results is confirmed in the same way also for the two-dimensional model.

3. Thermodynamics and roughening transition for non-zero temperatures

As is well known, the characteristic feature of the interfacial behaviour in the three-dimensional models is the presence of the roughening transitions [3]. In spite of considerable efforts to find more, there is still only one exactly solvable model which exhibits the roughening transition, namely the so-called BCSOS model [9]. The existence of this transition, however, is proven also for other models [10] and it seems that, unless there are some special reasons, the roughening transition should be present in models such as (2.1) as well. In the previous section we have shown, however, that for some values of the parameters K and D the ground-state interface is strongly degenerate and resembles a wandering, fluctuating surface. It is easy to show that the ensemble of these fluctuating

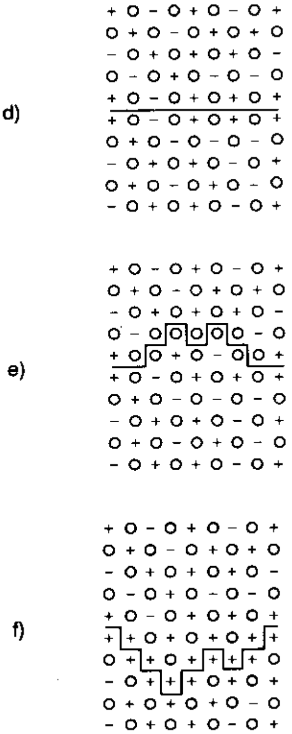

Figure 5. The interface structure for the two-dimensional BEG model in cases analogous to the cases (d), (e), and (f) described in the text.

interfaces is equivalent to the high-temperature limit of the already mentioned BCSOS model. As an immediate consequence we obtain that the ground-state interface is rough, which for the antiferromagnetic Ising model was also confirmed in Monte Carlo simulations [7]. The thin solid lines in figure 1 can thus be regarded as the lines of the ground-state roughening transitions. Another consequence of the equivalency with the BCSOS model is that in the limit $L \to \infty$ the degeneracy of the ground-state interface behaves like q^{L^2} where $q = (\frac{4}{3})^{3/2} \approx 1.539$. This follows from the equivalency of the BCSOS with the six-vertex model [11]. For two-dimensional models, the degeneracy of such a rough ground-state interface is equal to the number of random walks which return to the origin after L steps, and hence asymptotically it behaves like 2^L.

There is one striking feature of the phase diagram in figure 1. The continuous phase transition from the staggered to the paramagnetic phase is always preceded by the ground-state roughening transition. The roughening transition also precedes the continuous phase transition between the staggered and ferromagnetic phases. On the other hand, the discontinuous phase transition between the ferromagnetic and paramagnetic phases is not preceded by such roughening transition. As a consequence we obtain that at the ground-state the line of the roughening transitions join the bulk phase boundary exactly at the junction of the lines of continuous and discontinuous phase transitions.

A qualitative analysis of the bulk phase diagram in the (K, T) plane (where T is the temperature, and the Boltzmann constant k_B is set to unity) in connection with the interfacial behaviour, and for some representative values of D, is given below. Although we have put a scale on the temperature axis, the values of the critical temperature and the roughening temperature are very approximate.

(i) $D = 1$. The bulk phase diagram (thick, solid lines denote continuous phase transitions) and the conjectured behaviour of the roughening transition (thin, solid line) are presented in figure 6. As regards the ground-state structure of the interface, this case is the richest. Lowering the value of K, according to figure 1, we encounter four changes of ground state. Since there is no physical reason why the rough ground-state interface should become localized for higher temperatures, we expect vanishing of the roughening transition for $K = -1, -\frac{6}{5}$, and -2. In the same way as for the antiferromagnetic Ising model, this vanishing can be understood as being caused by the vanishing of the elasticity of the interface as K approaches the above listed values [12].

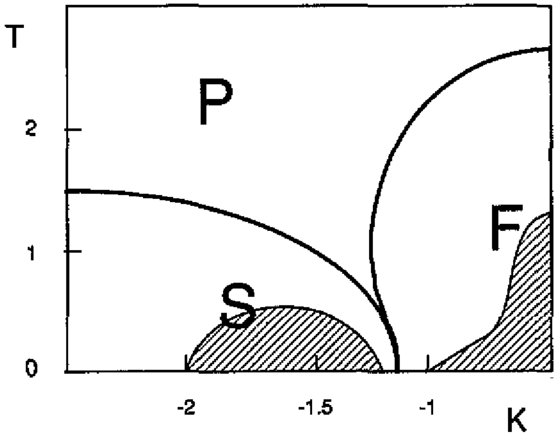

Figure 6. The bulk phase diagram in the (K, T) plane for $D = 1$. Thick, solid lines denote the continuous phase transitions while the conjectured behaviour of the roughening transition is denoted by the thin solid line. A non-rough interface exists in the dashed region.

Vanishing of the roughening temperature T_R can be also explained using a simple energy–entropy argument. Consider the roughening transition in the ferromagnetic phase for $-1 < K < -\frac{3}{4}$ (and $D = 1$). According to figure 6, the ground state is a non-rough interface (b). Due to the very strong degeneracy of the rough configurations (c), we expect that for a sufficiently high temperature the interface will be rough. Simple comparison of free energies leads to the following estimation of the roughening temperature:

$$T_R = \frac{2(1+K)}{\ln q} \sim 4.64(1+K) \qquad q = 1.539\ldots \tag{3.1}$$

As K approaches -1 from above, T_R vanishes linearly. For $K > -\frac{3}{4}$ the ground-state interface does not have the intruding layer of 0 states and the same considerations give the following expression for the roughening temperature:

$$T_R = \frac{4+D+6K}{\ln q} \sim 2.32(4+D+6K). \tag{3.2}$$

This change of the ground state is responsible for the change of a slope at $K = -\frac{3}{4}$ in figure 6. For low temperatures these simple considerations should be accurate. Similar results can be obtained for the interface in the staggered phase.

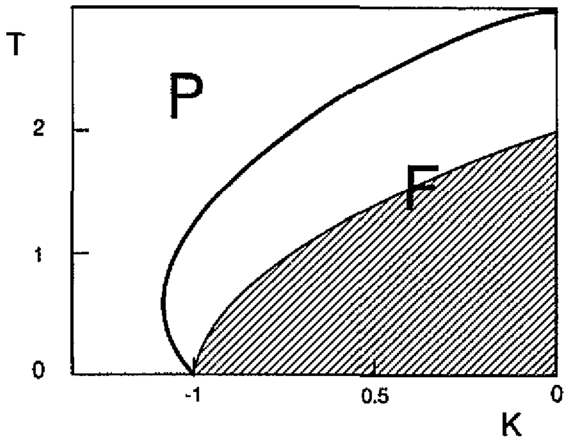

Figure 7. The bulk phase diagram in the (K, T) plane for $D = 0$.

The interesting phenomenon is the ground-state roughening at $K = -2$. It follows from figure 1 that for $D = 1$ and $K < -2$ the system enters the rough region (e), which precedes the continuous phase transition along the vertical line. However, in the reduced parameter space (K, T), this is difficult to observe.

(ii) $D = 0$. With decrease of the value of D the critical temperature between the staggered and paramagnetic phases (figure 6) also decreases. At the marginal value $D = 0$, the staggered ordering becomes absent, even at the ground state, and the resulting phase diagram is shown in figure 7. The ground-state roughening takes place at $K = -1$. The line of roughening transition joins the bulk phase diagram at the ground state.

(iii) $D = -1$. There is no staggered phase in this case either. The lines of continuous and discontinuous (thick, dashed line) phase transitions meet at the tricritical point (black circle in figure 8).

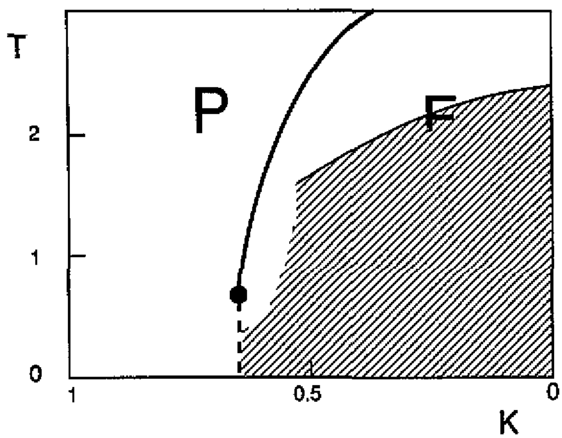

Figure 8. The bulk phase diagram in the (K, T) plane for $D = -1$. Thick dashed lines denote the discontinuous phase transitions. The tricritical point is denoted by a black circle. The behaviour of the roughening transition in the vicinity of the bulk phase boundary is unknown.

How should we draw the line of the roughening transition? In the ordered phase, the ground-state interface is non-rough. Hence the roughening transition should not vanish at least up to the phase boundary. Recalling the ground-state diagram (figure 1), one can be tempted to draw the line of the roughening transition in such a way that it meets the phase boundary exactly at the tricritical point. In the same way as previously we can obtain some estimations of T_R using energy–entropy considerations. Comparing these estimations with the scarce numerical data [6], we can see that they locate the roughening transition considerably higher than the tricritical point. The situation is schematically depicted in figure 8.

Some indications that the interface is non-rough along the triple line (at least at low temperatures) come also from studies of the so-called interfacial adsorption [13]. As we have already mentioned in the previous section, in the regions (b), (c) and (e) the phases (+) and (−) are separated by the intruding layer of 0 states. This intruding layer will persist even at non-zero temperatures. The interesting phenomenon appears while approaching the bulk phase boundary. The width of the intruding layer remains finite at the critical point for the continuous phase transition and it diverges for the discontinuous one [13]. Some scaling arguments show [14] that for the two-dimensional model the divergence of the width of the intruding layer is well described by the model of unbinding of a one-dimensional interface from a rigid wall. The phenomenon can be regarded as unbinding from a rigid wall also in the three-dimensional model [8]. In this case, the interface undergoes a series of discontinuous layering transitions, which suggests that the interface is non-rough [15]. Such discontinuous layering transitions were detected, however, only at low temperatures and it would be desirable to check if such behaviour extends up to the tricritical point.

The above arguments certainly do not resolve the question as to whether the roughening transition join the bulk phase diagram at the tricritical point or not. Nevertheless, such possibility is, in our opinion, not excluded. It seems quite possible that upon approaching the bulk phase boundary the large critical fluctuations will bend the roughening transition curve downward.

Even if the roughening transition crosses the bulk phase boundary at the tricritical point in the BEG model, this coincidence does not appear in some other models. In particular, we have found that in the $S = 1$ antiferromagnetic Ising model the interface can be rough even at the ground-state discontinuous phase transition (results will be published in the near future). One can argue, however, that in the latter model the Hamiltonian of the interface includes the next-nearest-neighbours interaction which might be responsible for non-vanishing of the excess interface energy at the phase boundary.

4. Conclusions

In the present paper we have shown that for the BEG model the ground-state phase transitions are essentially connected with the interfacial properties. In particular, the continuous phase transitions are accompanied by strongly degenerate and fluctuating interfaces. On the other hand, discontinuous phase transitions are accompanied by non-fluctuating interfaces. As a result, for the three-dimensional model the line of roughening transitions meets the bulk ground-state phase boundary exactly at the junction of the continuous and discontinuous phase transitions.

Using a simple energy–entropy argument, our results enable us to draw some conclusions concerning the behaviour of the roughening transition in the BEG model even for finite temperatures. The most interesting and unresolved problem is the case $D < 0$, where the model exhibits a tricritical behaviour. At low temperatures, where the model exhibits discontinuous phase transition, our estimations, as well as some other results [8], suggest that the interface might be non-rough even up to the triple line. Does this non-rough character extend up to the tricritical point as it does at the ground-state? Such a behaviour would reveal an intriguing connection between bulk and interfacial behaviour. Even if it is so, it is probably a property of only a particular class of models. In general, the next-nearest-neighbours interaction, which is common in experimentally accessible systems, will change the energy of interfaces and modify this behaviour.

Acknowledgments

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References

[1] Widom B 1972 *Phase Transitions and Critical Phenomena* vol 2, ed C Domb and M S Green (New York: Academic)
[2] Bricmont J, El Mellouki A and Fröhlich J 1986 *J. Stat. Phys.* **42** 743
[3] van Beijeren H and Nolden I 1987 *Structures and Dynamics of Surfaces II Phenomena, Models and Methods, Topics in Current Physics* vol 43, ed W Schommers and P van Blanckenhagen (Berlin: Springer)
[4] Blume M, Emery V J and Griffiths R B 1971 *Phys. Rev.* B **4** 1071
[5] Wang Y L, Lee F and Kimel J D 1987 *Phys. Rev.* B **36** 8945
[6] Wang Y L and Wentworth C 1987 *J. Appl. Phys.* **61** 4411
[7] Lipowski A and Suzuki M 1993 *Phys. Lett.* **177A** 447
[8] Upton P and Yeomans J M 1987 *J. Phys. A: Math. Gen.* **20** 2989
[9] van Beijeren H 1977 *Phys. Rev. Lett.* **38** 993
[10] Fröhlich J and Spencer T 1981 *Commun. Math. Phys.* **81** 527
[11] Lieb E H and Wu F Y 1972 *Phase Transitions and Critical Phenomena* vol 1, ed C Domb and M S Green (New York: Academic)
[12] Lipowski A and Suzuki M 1993 *J. Phys. A: Math. Gen.* **26** 5687
[13] Selke W and Yeomans J M 1983 *J. Phys. A: Math. Gen.* **16** 2789
[14] Selke W, Huse D A and Kroll D M 1984 *J. Phys. A: Math. Gen.* **17** 3019
[15] Pandit R, Schick M and Wortis M 1982 *Phys. Rev.* B **26** 5112