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The semi-infinite Domb model

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Abstract. The semi-infinite Domb model with volume-dependent bulk exchange interactions $J(v)$ and modified exchange interactions on the free surface $J_S(v) = (1 + \Delta)J(v)$ is studied through a variational method based on the Bogoliubov inequality for the free energy. The phase diagram of global temperature against Δ is obtained and it is shown that the orders of some transition lines depend on the value of the pressure. It is also shown that the phase diagram is qualitatively rather different from that obtained for systems having constant exchange interactions and first-order bulk behaviour.

1. Introduction

The semi-infinite Ising model on a rigid simple cubic lattice with modified exchange interaction on the free surface constitutes a simple model for the study of surface effects in magnetic materials (see [1] and references therein). The global phase diagram when the bulk undergoes a second-order transition is well understood. For a sufficiently high surface coupling enhancement the system orders on the surface before it orders in the bulk, whereas for low surface couplings the surface orders when the bulk does. In addition, all the critical lines are also of second order. However, the phase diagram may change for systems that undergo a first-order transition within the bulk. A general treatment within the framework of Landau theory has shown that the model can exhibit a surface-induced disordering transition where surface quantities present a critical behaviour although the bulk quantities are discontinuous [2, 3].

On the other hand, compressible magnetic systems have also been the subject of many theoretical studies (see, e.g., [4, 5]). It has been shown that the critical behaviour in the bulk is strongly dependent on the space boundary conditions as well as on the specific type of fluctuations (for a recent discussion of such effects, see, e.g., [6]). However, the mathematical complications in the calculations for these systems with realistic position fluctuations are rather involved. Nevertheless, some very simple models have been proposed in order to treat compressible Ising Hamiltonians such as the Domb model [7] and the Baker–Essam model [8]. When the effect of pure ion position fluctuations is considered to an extreme degree in the shearless Baker–Essam model at constant volume the bulk presents a renormalized second-order behaviour. In contrast, when the effect of volume fluctuations are taken into account as in the case of the Domb model, which includes a volume-dependent exchange parameter, the bulk presents second- and first-order types of behaviour depending on the value of the pressure (see, e.g., [9]). In a realistic system, both types of fluctuations should be present and therefore the character of the transition will depend on which one of these predominates.

In the present work we study the semi-infinite compressible Ising model. Of course, as the elastic effects have a long range, the physical properties of an elastic medium with a surface will also be quite sensitive to the space boundary conditions. Such effects, however, are not taken into account in this paper. We treat the semi-infinite Domb model by assuming that the average lattice spacing on the free surface is the same as that deep in the bulk. As this simple model displays both first- and second-order behaviour, the presence of a surface should affect the global phase diagram in different ways, depending on the order of the bulk transition. Moreover, the first-order bulk behaviour is accomplished by a volume discontinuity (also involving a discontinuity in the exchange interactions) implying that the effective mean-field boundary conditions at the surface also change in a discontinuous way. Such an effect has not been treated in the previous framework of Landau theory [2, 3].

In order to obtain the thermodynamic properties and the magnetization profiles of the semi-infinite Domb model we employ the mean-field approximation by means of a variational method based on the Bogoliubov inequality for the free energy. The Hamiltonian model, the formalism and the bulk phase diagram in the temperature–pressure plane are given in section 2. In section 3 global phase diagrams that take into account the presence of the free surface are discussed and compared with the diagram obtained for models having constant bulk exchange interactions [2, 3]. A brief conclusion is given in section 4.

2. Model, formalism and bulk phase diagram

2.1. The Hamiltonian model

A general compressible Ising model can be defined by the following Hamiltonian:

$$H = -\sum_{(i,j)} J(|\boldsymbol{r}_{ij}|)\sigma_i\sigma_j + \sum_{i,j} \varphi_{\mathrm{el}}(|\boldsymbol{r}_{ij}|) \tag{1}$$

where the first sum includes a magnetic term with nearest–neighbour interactions of ions with spin $\frac{1}{2}(\sigma_i = \pm 1)$ and the elastic energy is given by the second sum (the corresponding kinetic energy term has been suppressed). The elastic energy and the exchange integral depend on the relative positions of the ions $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$. The Domb model is obtained by expanding the above Hamiltonian about the equilibrium energy and by neglecting the local position fluctuations. The model (1) may then be written as (for further details see [6])

$$H = H_{\mathrm{L}} + H_{\mathrm{I}} \tag{2}$$

with the purely elastic term H_{L} given by

$$H_{\mathrm{L}} = \tfrac{1}{2}N^3 c(v - v_0)^2 \tag{3}$$

where N^3 is the total number of sites in the semi-infinite simple cubic structure, v is the volume of a unit cell, v_0 is a positive parameter and c is a positive constant related to the inverse of the compressibility of the lattice. The effective spin Hamiltonian is

$$H_I = -\sum_{(i,j)} J_{ij}(v)\sigma_i\sigma_j \tag{4}$$

where, in the infinite Domb model, we have

$$J(v) = J_0 - J_1(v - v_0) = J_{ij}(v) \tag{5}$$

with J_0 and J_1 being positive constants. In order to treat the Domb model with a free surface we have simply to assume that the exchange interactions $J_{ij}(v)$ for nearest-neighbour spins in the bulk are given by equation (5) while for nearest-neighbour spins on the free surface the exchange interactions take the value

$$J_S(v) = (1 + \Delta)J(v). \tag{6}$$

Here Δ is the surface coupling enhancement.

2.2. *Formalism*

In order to obtain the free energy related to H_I we use a variational method based on the Bogoliubov inequality [10]

$$F_I(T, v) \leqslant F_0(T) + \langle H - H_0\rangle_0 = \Phi(\gamma_i), \tag{7}$$

where $F_0(T)$ is the free energy corresponding to the trial Hamiltonian H_0, the brackets indicate an average over an ensemble defined by H_0, and γ_i are variational parameters. An approximate value of the free energy is obtained by minimizing Φ with respect to γ_i.

The mean-field approximation is obtained by considering

$$H_0 = -\sum_{i=1}^{N^3} \gamma_i\sigma_i. \tag{8}$$

Thus, we have

$$\begin{aligned} F_0(T) &= -k_BT\sum_{i=1}^{N^3} \ln(2\cosh\beta\gamma_i) \\ \langle H - H_0\rangle_0 &= -\sum_{(i,j)} J_{ij}(v)m_im_j + \sum_{i=1}^{N^3} \gamma_i m_i \end{aligned} \tag{9}$$

where $\beta = 1/k_BT$ and $m_i = \tanh\beta\gamma_i$. Assuming that the magnetizations in the planes parallel to the free surface are homogeneous (i.e. in the ferromagnetic phase where $J(v) > 0$) we get

$$\begin{aligned} \Phi(\gamma_i) = &-N^2k_BT\sum_{i=1}^{N} \ln(2\cosh\beta\gamma_i) + N^2\sum_{i=1}^{N}\gamma_i m_i \\ &- 2N^2J_S(v)m_1^2 - 2N^2J(v)\sum_{i=2}^{N} m_i^2 - N^2J(v)\sum_{i=1}^{N} m_im_{i+1} \end{aligned} \tag{10}$$

where i now labels layers parallel to the surface. Minimization of equation (10) leads to

$$\gamma_1 = 4J_S(v)m_1 + J(v)m_2 \tag{11}$$

$$m_1 = \tanh\beta\gamma_1 \tag{12}$$

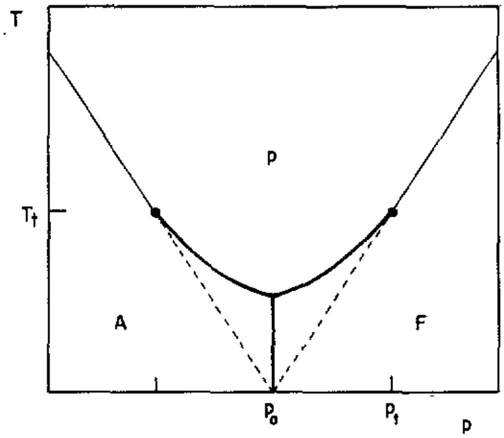

Figure 1. Sketch of the bulk (T, p) phase diagram. The tricritical point (T_t, p_t) separates regions of first- and second-order transitions: bold full curves, first-order transitions; full lines, second-order transitions.

for, respectively, the variational parameter and the magnetization of the free surface, and

$$\gamma_i = 4J(v)m_i + J(v)(m_{i-1} + m_{i+1}) \tag{13}$$

$$m_i = \tanh \beta\gamma_i \tag{14}$$

where the last two equations hold for $i \geq 2$. The Ising free energy F_I is then given by equations (10)–(14) and we have for the total free energy

$$F(T, v) = F_L(T, v) + F_I(T, v) \tag{15}$$

where F_L is also given by the right-hand side of equation (3).

As the bulk transition always occurs at definite values of temperature and pressure, it is more convenient to work with the Gibbs potential, which can be easily obtained by performing the Legendre transformation,

$$G(T, p) = F(T, v) + N^3pv \tag{16}$$

where the pressure p is defined as

$$p = -N^{-3}\, \partial F(T, v)/\partial v. \tag{17}$$

The bulk free energy per spin g_B is obtained from (16) via

$$g_B(T, p) = \lim_{N\to\infty} G(T, p)/N^3 \tag{18}$$

and the corresponding surface free energy is given by

$$g_S(T, p) = \lim_{N\to\infty} [G(T, p) - N^3 g_B(T, p)]/N^2. \tag{19}$$

Finally, the antiferromagnetic case (i.e. for pressure values so that $J(v) < 0$) is obtained in a quite analogous way. We have to consider two sublattices and two different variational parameters inside each plane parallel to the surface. If m_i is assumed to be the sublattice magnetization we obtain the same formulae above with $|J(v)|$ substituted for $J(v)$.

2.3. *Bulk phase diagram*

The bulk phase diagram in the temperature–pressure plane of the present model (which, for completeness, is shown in figure 1) has already been studied according to this approximation [9]. It is entirely symmetric with respect to $p_0 = -J_0c/J_1$. There are first-order transition lines where the magnetization and the volume undergo discontinuous changes: a vertical ferromagnetic–antiferromagnetic transition line and two symmetric curves of ferromagnetic–paramagnetic (on the right) and antiferromagnetic–paramagnetic (on the left) transitions. Although these lines are computed numerically, the second-order lines and the tricritical points can be obtained analytically through a Landau expansion of the Gibbs free energy giving, respectively,

$$T_{cB} = \pm 6J_0/k_B \pm 6J_1p/k_Bc \tag{20}$$

$$T_t = 54J_1^2/k_Bc. \tag{21}$$

In equation (20) the upper (lower) sign holds for the ferromagnetic (antiferromagnetic) phase. It should be mentioned that the minor differences between the equations above and those of [9] result from the fact that here we are writing the elastic energy and the exchange interactions in terms of the volume v while there they are given in terms of the average lattice spacing a (however, if the volume is expanded about v_0, $v - v_0$ is, up to first order, just proportional to the corresponding lattice spacing $a - a_0$).

3. Global phase diagram

As the results for the ferromagnetic and antiferromagnetic phases are analogous, we shall discuss below only the case $J(v) > 0$, where the bulk is ferromagnetic. The main qualitative features are the same when $J(v) < 0$.

3.1. *The case $p \geqslant p_t$*

In this case, the bulk undergoes a second-order phase transition (see figure 1) at T_{cB} given by equation (20). For $T > T_{cB}$ and close to the surface transition the magnetization m_1 can be calculated by inverting equations (12) and (14) and then expanding for $m_i \ll 1$. We get

$$m_2 = am_1 + bm_1^3 \tag{22}$$

$$m_i = X_i m_2 - X_{i-1} m_1 \qquad i \geqslant 3 \tag{23}$$

where

$$a = 1/\beta J(v) - 4J_S(v) \tag{24a}$$

$$b = 1/3\beta J(v) \tag{24b}$$

and we define

$$z = (1/\beta)J(v) - 4. \tag{24c}$$

Here $X_i = X_i(z)$ are polynomials of degree $i - 2$ in z (with z defined above) obeying the following recursion relation:

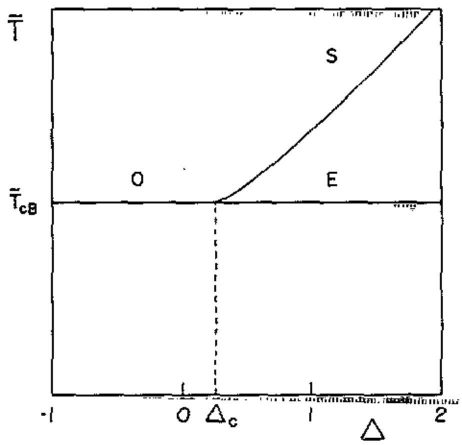

Figure 2. Global $(\tilde{T}, \Delta)$ phase diagram for $p \geqslant p_t$. All transition lines are second order and they are denoted by O, E and S. $\tilde{T}_{cB}$ and the surface transition line S are given by equations (20) and (29), respectively.

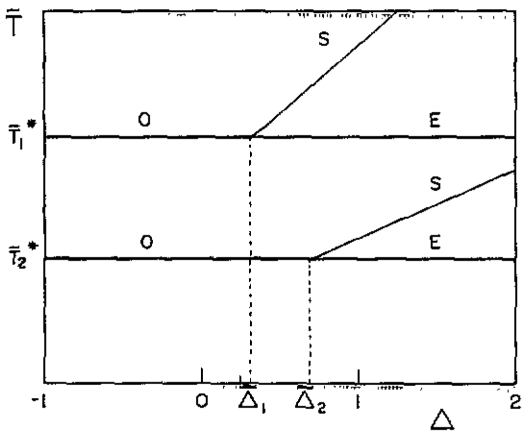

Figure 3. Global $(\tilde{T}, \Delta)$ phase diagram for two different values of pressure: $p_t > p_1 > p_2$. The transitions O and E are first order while S is second order. The results were taken for $J_1^2/J_0c = 0.1$, $k_BT_1^*/J_0 = 4.0$, $p_1J_1/J_0c = -0.34$, $\bar{\Delta}_1 = 0.32$; $k_BT_2^*/J_0 = 2.0$, $p_2J_1/J_0c = -0.17$, $\bar{\Delta}_2 = 0.66$.

$$X_i = zX_{i-1} - X_{i-2} \qquad i \geqslant 4 \tag{25}$$

$$X_2 = 1 \qquad X_3 = z. \tag{26}$$

Taking the limit $i \to \infty$ we have

$$m_{i\to\infty} = m_B = 0; (X_i/X_{i-1})_{i\to\infty} = y$$

and for temperatures such that $z \geqslant 2$ equation (25) leads to

$$y = \tfrac{1}{2}[z + (z^2 - 4)^{1/2}]. \tag{27}$$

Finally, from equations (22) and (23) we obtain

$$m_1^2 = (1 - ay)/by. \tag{28}$$

The surface critical temperature T_{cS} is then given by

$$1 - ay = 0 \tag{29}$$

with the surface critical exponent $\beta_1 = \frac{1}{2}$. The global $(\tilde{T}, \Delta)$ phase diagram for a given value of the pressure p is shown in figure 2 where the reduced temperature $\tilde{T}$ is defined

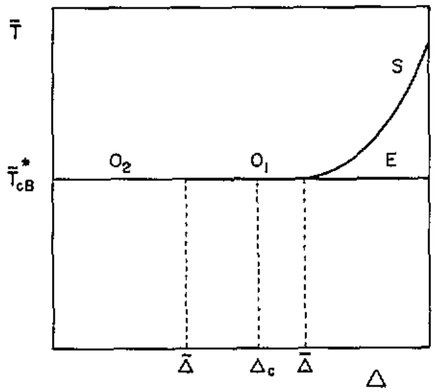

Figure 4. Sketch of the global ($\bar{T}$, Δ) phase diagram for models having first-order bulk behaviour at T^*_{cB} with constant bulk exchange interactions according to [3]. The surface transition line S is also first order. The surface magnetization m_1 is continuous at E ($\Delta > \bar{\Delta}$), discontinuous at O_1 ($\tilde{\Delta} < \Delta < \bar{\Delta}$) and goes continuously to zero at O_2 ($\Delta \leqslant \tilde{\Delta}$). At $\Delta = \Delta_c$, $m_1 = m_B$.

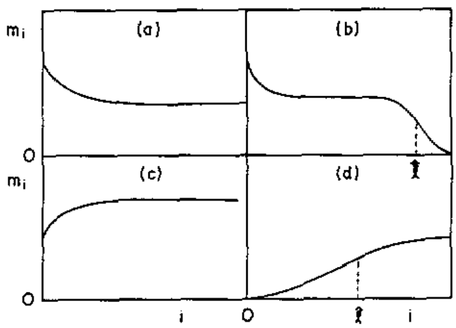

Figure 5. Generic shapes of the magnetization profile related to the phase diagram depicted in figure 4: (a), in the ordered state at the transition E and O_1 for $\Delta_c < \Delta < \bar{\Delta}$; (b), in the disordered state at the transition E; (c), in the ordered state at the transition O_1 for $\tilde{\Delta} < \Delta < \Delta_c$; (d), in the ordered state at the transition O_2. In figures (b) and (d) there is an interface at $i = \bar{l}$ and $i = \tilde{l}$, respectively.

by $\bar{T} = k_B T/J_0$. At $\bar{T}_{cS} = \bar{T}_{cB}$ we get the mean-field value $\Delta_c = 0.25$, which is independent of the pressure and, from equation (24*c*), we have $z = 2$ meaning that the lines O, E and S meet in a critical endpoint at the surface. So, as expected, all the known features concerning the criticality at surfaces with the bulk undergoing a second-order transition are obtained in this case. Moreover, at $p = p_t$, $T_{cB} = T_t$ and we have critical behaviour at the surface at a tricritical transition in the bulk [11].

3.2. *The case* $p_0 < p < p_t$

In this range the bulk shows a first-order behaviour at a temperature T^* where the magnetization and the volume undergo discontinuous changes. This implies that the exchange interaction and the relative position of the sites on the free surface are also discontinuous. In this case, however, T^* has to be computed numerically for some given values of the theoretical parameters. The magnetization profile may also be obtained by investigating the set of equations (12) and (14) on a computer. The global ($\bar{T}$, Δ) phase diagram thus obtained is shown in figure 3 for two different values of pressure. For completeness we also show in figure 4 a sketch of the global phase diagram and, in figure 5, the generic shapes of the magnetization profile obtained according to an equivalent mean-field-like approximation for models having a first-order bulk behaviour with constant bulk exchange interactions (for further details see [3]). In order to compare the present results with those of [3] we discuss below each line of the phase diagram in figure 3 separately.

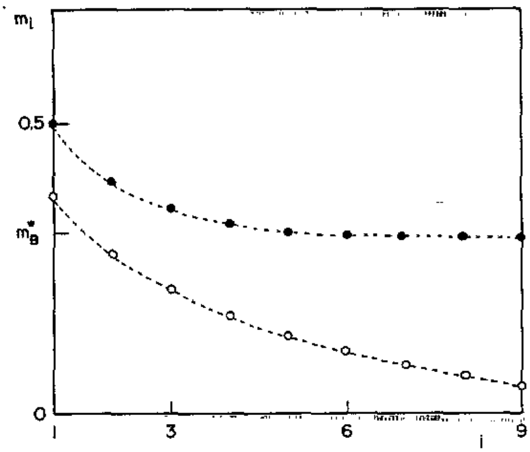

Figure 6. Magnetization profile at the transition E where the ordered bulk state (●) and the disordered bulk state (○) coexist: $J_1^2/J_0c = 0.1$, $k_BT^*/J_0 = 5.0$, $pJ_1/J_0c = -0.17$, $\Delta = 0.4$ ($\bar{\Delta} = 0.27$).

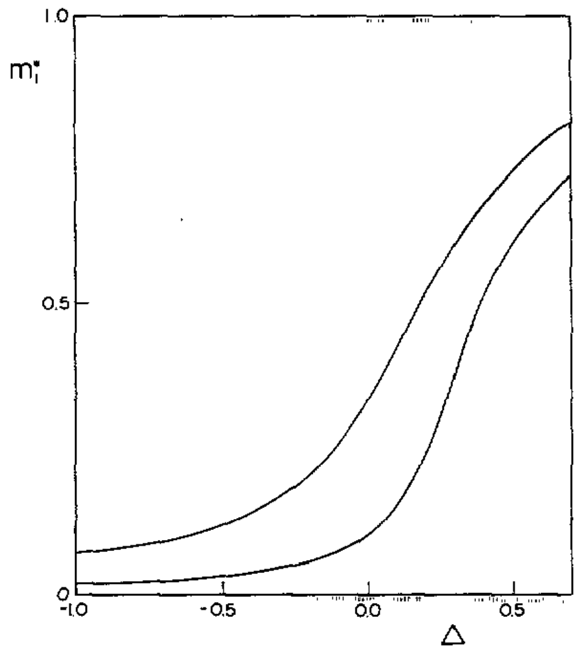

Figure 7. The ordered surface magnetization m_1^* as a function of Δ in the ordered phase at the transition O ($T = T^*$), $J_1^2/J_0c = 0.1$. Upper curve: $k_BT^*/J_0 = 4.0$, $pJ_1/J_0c = -0.34$. Lower curve: $k_BT^*/J_0 = 5.0$, $pJ_1/J_0c = -0.17$.

Let us first consider the transition line E, which is now first-order. Because of the discontinuity of $J(v)$, the magnetization m_1, as well as the whole profile, is also discontinuous at E. However, except for the ordered bulk magnetization m_B^*, the profile jumps from a finite value to another finite value as shown in figure 6. The generic shape of the profile in the ordered state is the same as that in figure 5(a) while in the disordered state it goes smoothly to zero as a function of i without a characteristic length scale separating the ordered surface layer from the disordered bulk as in figure 5(b).

At the transition line O, which is also first order, the surface magnetization (as well as the bulk one) jumps from $m_1^* \neq 0$ in the ordered state to zero in the disordered one. The shape of the order parameter profile in the ordered state is the same as those of figures 5(*a*) and 5(*c*) and we obtain, in this case, the same qualitative features of the transition designated by O_1 in figure 4. However, this model does not exhibit a surface disordering transition where the surface quantities undergo a critical behaviour while the bulk quantities are discontinuous. In figure 7 we show the ordered surface magnetization m_1^* at $T = T^*$ as a function of Δ for two transition temperatures. We note that although m_1^* is small as $J_S \to 0$ it never goes to zero. It can be shown that $m_1 = 0$ is not a solution of equations (12) and (14) as long as $m_B \neq 0$. Thus, the magnetization profiles, such as that shown in figure 5(*d*), cannot be predicted by this model.

Finally, the phase boundary S is determined by magnetization profiles such that $g_S = 0$. For $T > T^*$, we have $m_B = 0$ and through an expansion of the surface free energy (19) we find indeed that $g_S = 0$ only if $m_1 = 0$. Thus, unlike the model treated in [3], the surface transition in this case remains second order with T_{cS} given by the same equation, (29). At $\Delta = \bar{\Delta}$, $T_{cS} = T^*$, where $\bar{\Delta} > \Delta_c$ is now dependent on pressure (see figure 3). In this case, however, the lines O, E and S do not meet in a kind of surface critical endpoint once some unphysical solutions for $T_{cS} < T^*$ and $\Delta < \bar{\Delta}$ are obtained from equation (29). At $\Delta = \Delta_c$, $m_1 = m_B$ and the extrapolation length goes to infinity.

Most of the differences concerning the phase diagram and magnetization profiles for both the models discussed above, such as the behaviour at the transition lines O and E, can be ascribed to the fact that in the present model the first-order transition is induced by the pressure with a discontinuity in the exchange interaction $J(v)$. The parameters in the Landau free-energy expansion of [3] do not take into account, in principle, such a dependence. For example, by expanding the total free energy (16) close to the tricritical point ($p \leqslant p_t$) and taking the continuum limit we obtain a free-energy function whose parameters depend on T and p. Following the usual procedure of minimizing G we obtain, at the transition O, a cubic equation for $(m_1^*)^2$ that has always an ordered solution $m_1^* \neq 0$, as long as $m_B \neq 0$, for any value of $\Delta \geqslant -1$, and the surface is indeed not critical along this line. Thus, the Landau theory procedure in the continuum limit can also be extended in order to treat more general models such as the present one. On the other hand, the second-order transition line S can be understood once for $T > T^*$, $m_B = 0$ and from equations (5) and (17) it can be shown that the bulk exchange interaction is independent of Δ for a given value of the pressure p. Thus, we have in this case just a simple semi-infinite Ising model, which should exhibit a surface ordering that is critical. On the contrary, for systems having a bulk first-order behaviour, such as the one treated in [3], it implies that the surface is also described by the same model on a lattice of dimension $d - 1$. Therefore, the mean-field solutions will give a similar behaviour to the bulk for the criticality at the surface.

4. Concluding remarks

The semi-infinite Domb model with bulk exchange interactions $J(v)$ and modified exchange interactions on the free surface $J_S(v) = (1 + \Delta)J(v)$ has been studied within a variational approach based on the Bogoliubov inequality for the free energy. Although this model is rather too simple to give a true picture of a realistic semi-infinite compressible Ising model it can be considered as a starting point for the study of surface effects in models with a first-order transition in the bulk caused by discontinuities in the volume interactions and in the exchange interactions. In other respects, as the mean-field approach can account for the main features of the critical behaviour at the surfaces of rigid lattices we expect that this approximation should also satisfactorily describe the present more general model.

It has been shown that when the bulk undergoes a second-order phase transition, the global $(\tilde{T}, \Delta)$ phase diagram is completely analogous to that of the rigid model, which exhibits only second-order transition lines. However, at the first-order bulk transition, the lines O and E in figure 3 are now first order. The surface magnetization m_1 is continuous at S and behaves like the bulk magnetization m_B at O and is discontinuous, but finite, at E. The phase diagram in this case is qualitatively different from that obtained for systems with a first-order bulk behaviour but having constant bulk exchange interactions. It is also expected that the global phase diagram of the semi-infinite Baker–Essam model should be similar to that shown in figure 2 once this model presents only second-order bulk behaviour.

Because of the simple form assumed for $J_S(v)$, that is, $J_S(v)$ is simply proportional to $J(v)$, the results for the global phase diagram are qualitatively the same for ferromagnetic or antiferromagnetic bulk ordering. Nevertheless, more general models can also be studied theoretically within the present context by changing the surface interaction J_S. One can consider, for instance, $J_S = (1 + \Delta)J_0$ (which is volume independent), which allows for a ferromagnetic surface coupling with an antiferromagnetic bulk ordering.

Finally, an infinite pseudospin compressible Ising model Hamiltonian, similar to the one considered here, has been proposed previously to study the pressure–temperature phase diagram of the hydrogen-bonded ferroelectric crystal CsD_2PO_4 [12]. In these crystals, an antiferromagnetic phase appears to be induced by the pressure [13, 14]. Thus, experimental results for the critical surface behaviour in such crystals or similar magnetic materials would be highly valuable.

Acknowledgments

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