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Roughening Transition for the Ising Model on a BCC Lattice. A Case in the Theory of Ground States

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For the Ising model on a bcc lattice we analyze the ground states associated with different interfaces and discuss some consequences on the roughening transition.

KEY WORDS: Roughening transition; equilibrium crystal shape; ground states; Ising model; bcc lattice.

1. INTRODUCTION

Recently a great deal of effort has been devoted to the study of the equilibrium crystal shapes and the related roughening transitions of their facets (see Refs. 1–4 for recent reviews of both experimental and theoretical results). In the present work we discuss some of these problems for the case of the Ising model on a bcc (body-centered cubic) lattice. We study the ground states corresponding to different interfaces between phases of opposite magnetizations and use the information gained for a description of the equilibrium shape of a "droplet" surrounded by the opposite phase. The point is that the set of these ground states has a rather rich structure. Under a fixed boundary condition a large amount of ground configurations may contribute to the ground state and the corresponding interface may turn out to be either smooth (rigid) or rough.

For the (100) interface, we rely on the pioneering work of van Beijeren,[5] who introduced the so-called body-centred solid-on-solid

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(BCSOS) model as a limit of the Ising model on a bcc lattice with nearest neighbor coupling tending to infinity, and submitted a rigorous description of a roughening transition for the BCSOS model. Reinterpreting slightly his approach and considering the low-temperature behavior at fixed nearest neighbor coupling and with the next nearest neighbor coupling vanishing along lines $J=\alpha T$, we show how the BCSOS model may be used to describe the ground states obtained in the limit, and how the resulting behavior depends on the value of the slope α of these lines. The existence of a critical value α_R at which a smooth (100) interface becomes rough suggests that there is a curve of roughening temperatures $T_R(J)$ approaching the point $J=0$, $T=0$ with the slope α_R.

There is actually a whole class of interfaces with general orientations for which we again get an equivalence of ground states with the states of the BCSOS model under the corresponding boundary conditions. A representative of another class of interfaces is the (111) interface. It turns out that in this case the ground state is equivalent to a state of the so-called triangular Ising solid-on-solid (TISOS) model introduced by Blöte and Hilhorst[6] and further studied in Ref. 7. An important fact is that all interfaces fall into one of the above classes and thus one has a rigorous description of all related ground states and corresponding surface tensions (interface free energies). This information may be further used for a description of the low-temperature asymptotic behavior of the equilibrium crystal shape. Here we rely on the standard Wulf construction,[1-3] even though its rigorous and direct statistical mechanical verification has only begun to emerge.[8]

Our paper is organized as follows. First we clarify what we mean by ground states. We introduce them in Section 2 together with some related notions following the presentation of Dobrushin and Shlosman.[9] Section 3 is devoted to a study of interfaces for the Ising model on a bcc lattice. In addition to the discussion of ground states as described above, the rigidity of the (100) and the (110) interfaces is proved for couplings J and temperatures T inside certain regions of the (J, T) plane. Equilibrium crystal shapes in the low-temperature region are then discussed in Section 4. The main results of the present paper were announced in Ref. 10 and presented in Ref. 11.

2. GROUND STATES

Our aim in this section is to introduce some general notation and different notions concerning ground states. We follow, with minor modifications, the terminology of Dobrushin and Shlosman.[9]

We consider a model on a lattice $\mathbb{L}$, with configuration space $\Omega = S^{\mathbb{L}}$, where S is a finite set of values of the spin attached to each lattice site, and with a finite-range interaction $\{\varphi_A\}$, $A \subset \mathbb{L}$. The functions φ_A: $S^A \to \mathbb{R}$ may also be understood as A-cylindrical functions on Ω. Denoting by σ_V the restriction of a configuration $\sigma \in \Omega$ to a subset $V \subset \mathbb{L}$, $\sigma_V = \{\sigma_x\}_{x \in V}$, and by $\sigma_V \cup \sigma_{V^c}$ the configuration (in Ω) whose restrictions to V and its complement $V^c = \mathbb{L} \backslash V$ are σ_V and σ_{V^c}, respectively, we introduce the Hamiltonian in V under a boundary condition $\bar{\sigma} \in \Omega$ by

$$H_V(\sigma_V \mid \bar{\sigma}) = \sum_{A : A \cap V \neq \varnothing} \varphi_A(\sigma_V \cup \bar{\sigma}_{V^c})$$

The finite-volume Gibbs states on $\Omega_V = S^V$ (a specification)

$$\mu_V^{\beta H}(\sigma_V \mid \bar{\sigma}) = Z_V(\bar{\sigma})^{-1} \exp[-\beta H_V(\sigma_V \mid \bar{\sigma})]$$

where

$$Z_V(\bar{\sigma}) = \sum_{\sigma_V \in \Omega_V} \exp[-\beta H_V(\sigma_V \mid \bar{\sigma})]$$

determine (by the DLR equations) the set $\mathscr{G}(\beta H)$ of Gibbs states (on $\mathbb{L}$) corresponding to a Hamiltonian H at an inverse temperature β (see, e.g., Ref. 12 for an exposition of the theory of Gibbs states suitable for our purposes). If a Gibbs state $\mu \in \mathscr{G}(\beta H)$ happens to equal the limit

$$\mu = \lim_{V \uparrow \mathbb{L}} \mu_V^{\beta H}(\cdot \mid \bar{\sigma})$$

under a fixed boundary condition $\bar{\sigma}$, we shall call it the *Gibbs state corresponding to a boundary condition* $\bar{\sigma}$.

Now, *ground states* are defined simply as Gibbs states at $\beta = \infty$, i.e., as Gibbs states with the specification

$$\mu_V^{\infty H}(\sigma_V \mid \bar{\sigma}) = \lim_{\beta \to \infty} \mu_V^{\beta H}(\sigma_V \mid \bar{\sigma})$$

Clearly, an explicit formula is

$$\mu_V^{\infty H}(\sigma_V \mid \bar{\sigma}) = \begin{cases} 1/|M_V(\bar{\sigma})| & \text{if} \quad \sigma_V \in M_V(\bar{\sigma}) \\ 0 & \text{if} \quad \sigma_V \notin M_V(\bar{\sigma}) \end{cases}$$

where

$$M_V(\bar{\sigma}) = \{\sigma_V \in \Omega_V \mid H_V(\sigma_V \mid \bar{\sigma}) = \min_{\tilde{\sigma}_V \in \Omega_V} H_V(\tilde{\sigma}_V \mid \bar{\sigma})\}$$

is the set of *ground configurations in* V *under the boundary condition* $\bar{\sigma}$. Occasionally we shall refer to the measure $\mu_V^{\infty H}(\cdot \mid \bar{\sigma})$ on Ω_V as a ground state in V under a boundary condition $\bar{\sigma}$.

If a ground state is supported by a single configuration $\sigma \in \Omega$, i.e., if it is the Dirac measure δ_σ on Ω, we call it a *rigid ground state.* Examples of rigid ground states are the + and − ground states of an Ising ferromagnet. It is easy to see that δ_σ is a rigid ground state if and only if $\sigma_V \in M_V(\sigma)$ and $|M_V(\sigma)| = 1$ for every finite $V \subset \mathbb{L}$. Often the set $M_V(\bar{\sigma})$ is quite rich and it may lead to a nonrigid (or random) ground state, which is a genuine measure supported on a large set of configurations. This is the case of, e.g., the Ising antiferromagnet on a triangular lattice or the Potts antiferromagnet on square or cubic lattices.[3] When describing interfaces in the next section we shall meet ground states of a particular type. The considered boundary condition $\bar{\sigma}$ will lead, in some cases, to a large set $M_V(\bar{\sigma})$ (a set of widely fluctuating interfaces) equivalently described as a set of configurations of a certain SOS model. The fact that a Gibbs state of this SOS model does not exist in the thermodynamic limit (this is possible since the set of one-site configurations of an SOS model is noncompact[9]) then reflects the fact that the ground state under the boundary condition $\bar{\sigma}$ (in the thermodynamic limit) actually turns out to be just a combination $\frac{1}{2}(\delta_+ + \delta_-)$ of rigid, translation-invariant + and − ground states.

Another useful notion is that of a weak ground state. Let us consider an additional finite-range interaction $\{\tilde{\varphi}_A\}$ and the corresponding Hamiltonian $\tilde{H}$ and introduce the specification (a weak ground state in V under the boundary condition $\bar{\sigma}$ corresponding to the direction $\tilde{H}$)

$$\mu_V^{\infty H,\tilde{H}}(\sigma_V \mid \bar{\sigma}) = \lim_{\beta \to \infty} \mu_V^{\beta(H+\tilde{H}/\beta)}(\sigma_V \mid \bar{\sigma})$$

$$= \begin{cases} \dfrac{\exp[-\tilde{H}_V(\sigma_V \mid \bar{\sigma})]}{\sum_{\tilde{\sigma}_V \in M_V(\bar{\sigma})} \exp[-H_V(\tilde{\sigma}_V \mid \bar{\sigma})]} & \text{if} \quad \sigma_V \in M_V(\bar{\sigma}) \\ 0 & \text{if} \quad \sigma_V \notin M_V(\bar{\sigma}) \end{cases}$$

Gibbs states with these conditional probabilities will be called *weak ground states* (*corresponding to the direction* $\tilde{H}$). Again we may have rigid or random weak ground states.

As we shall see in the following sections, the set of (weak) ground states may have quite a rich structure. Even though it may be of interest in itself, the most interesting aspect is what it says about the Gibbs states at nonvanishing temperatures $\beta \neq \infty$. Thus, one is led to the notion of *stable* (weak) ground states, which are defined as those (weak) ground states that are the limit when $\beta \to \infty$ of Gibbs states corresponding to βH [respectively to $\beta(H + \tilde{H}/\beta)$]. Alas, no general criteria of stability are known.

[3] Notice that even the problem of classification of different ground states for the latter models is still not entirely clarified (cf. Ref. 13).

Some particular cases of periodic rigid ground states are covered by the Pirogov–Sinai theory[14] and a class of non-translation-invariant ground states was tackled in Ref. 15. A general criterion of stability for rigid (weak) ground states was conjectured by Dobrushin and Shlosman.[9] Since their paper is not easily available, we shall, for the reader's convenience, review here their conjecture.

To state it, we shall need some additional notions. We shall also suppose that $\mathbb{L}$ is a regular crystal lattice and $\{\varphi_A\}$ a translation-invariant interaction.

The diameter of a set $V \subset \mathbb{L}$ is the supremum of distances of all pair of lattice sites in V, and V is said to be n-connected if for every pair (x, y) of sites in V there is a sequence $\{x_1,..., x_m\} \subset V$ such that $x_1 = x$, $x_m = y$, and the distance from x_k to x_{k+1}, $k = 1,..., m-1$, is not larger than n. Given a configuration σ, we consider its local connected perturbations. We denote by $\Sigma_n(\sigma)$ the set of configurations $\tilde{\sigma} \in \Omega$ for which the set $P(\tilde{\sigma} \mid \sigma) = \{x \in \mathbb{L} \mid \tilde{\sigma}_x \neq \sigma_x\}$ is finite and n-connected. For $\tilde{\sigma} \in \Omega$ we define the excess energy of $\tilde{\sigma}$ with respect to σ by

$$E(\tilde{\sigma} \mid \sigma) = \sum_A [\varphi_A(\tilde{\sigma}) - \varphi_A(\sigma)]$$

We say that a ground configuration σ is nonperturbable[4] if its local perturbations $\Sigma_n(\sigma)$ have bounded excess energy, namely if for all $n > 0$ and $E > 0$, one has

$$\sup\{\text{diam } P(\tilde{\sigma} \mid \sigma) \mid \tilde{\sigma} \in \Sigma_n(\sigma) \text{ and } E(\tilde{\sigma} \mid \sigma) < E\} < \infty$$

The second part of the Dobrushin and Shlosman conjecture (we do not state here the first part, which concerns the rigid weak ground states) is the following statement.

Conjecture.[9] Assume that the set of all periodic rigid ground states is finite and transitive with respect to the group of local symmetries and translations of $\{\varphi_A\}$. Then a rigid ground (not necessarily periodic) state δ_σ is stable if and only if the ground configuration σ is nonperturbable.

Several statements in the following section are actually a proof of this conjecture in some particular cases.

3. ISING MODEL ON A BCC LATTICE: INTERFACES

A bcc lattice L consists of two simple cubic lattices $\mathbb{Z}^3$, to be called sublattices L_1 and L_2, which are mutually shifted by the vector (1/2, 1/2,

[4] We replace here the term nondegenerated used in Ref. 9 by nonperturbable, since the term degenerated is widely used in the physical literature when referring to a ground state that is nonrigid in our terminology.

1/2). A site x in, say the sublattice L_1 has eight nearest neighbors (n.n.), all of them belonging to the sublattice L_2, and six next nearest neighbors (n.n.n.), belonging again to L_1. The configuration space is $\Omega = (-1, +1)^L$ and the energy of the corresponding Ising model is given by

$$H = -J_0 \sum_{\text{nn}} \sigma_x \sigma_y - J \sum_{\text{nnn}} \sigma_x \sigma_y$$

where the first sum runs over all pairs of n.n., and the second over all pairs of n.n.n. We shall restrict ourselves to ferromagnetic n.n. coupling ($J_0 > 0$), bearing in mind that the results may be transformed into the corresponding ones for $J_0 < 0$ by changing the sign of all configurations (as well as the boundary conditions) on, say, the sublattice L_1.

The conjectured phase diagram for this system is discussed in Ref. 16. At low temperatures a first-order transition line, the equation of which may be written as $J/J_0 = f(\beta)$, with $f(\infty) = -2/3$, separates two regions. In the first region, $J/J_0 \geqslant f(\beta)$, two ferromagnetically ordered phases (with positive and negative magnetizations) coexist, while in the second region the phases have an antiferromagnetic order on both sublattices. This fact may actually be proved by applying Pirogov–Sinai theory. Indeed, the periodic ground states of the system are, for $J > -(2/3)\, J_0$, the rigid states δ_+ and δ_-, and for $J < -(2/3)\, J_0$, the four rigid states associated to the ground configurations $\sigma_x = \varepsilon_1(-1)^{x_1 + x_2 + x_3}$ if $x \in L_1$ and $\sigma_x = \varepsilon_2(-1)^{x_1 + x_2 + x_3 + 1/2}$ if $x \in L_2$, the four possibilities being given by choosing ε_1 and ε_2 equal to $+1$ or -1.

We shall consider the region $J > (-2/3)\, J_0$ at low temperatures, where two ferromagnetically ordered phases coexist. Our aim will be to study the behavior of the Gibbs states corresponding to particular interfaces.

To this end, we shall specify a plane by its normal vector $k = (k_1, k_2, k_3)$ and consider the boundary condition $\bar{\sigma}^{(k)}$ (or simply $\bar{\sigma}$) defined to be $\bar{\sigma}_x = +1$ for the lattice sites above or on the considered plane ($xk = x_1 k_1 + x_2 k_2 + x_3 k_3 \geqslant 0$), and $\bar{\sigma}_x = -1$ for x below it ($xk < 0$).

Our claim will be that while the (110) interface is always rigid at low temperatures, there is a roughening transition for the (100) interface around $J = 0$.

3.1. The (100) Interface

When studying the ground states corresponding to the (100) boundary condition, the situation depends significantly on the sign of the n.n.n. coupling J. We shall analyze first the case $J > 0$.

Theorem 1. The ground state corresponding to the (100) boundary condition for $J>0$ is rigid. Moreover, the ground configuration is nonperturbable.

Proof. Let $\bar{\sigma}$ denote in this subsection the boundary condition $\bar{\sigma}^{(100)}$. To see that the ground state is rigid, it is enough to observe that in this case the set $M_V(\bar{\sigma})$ consists for any V of only one configuration, namely $\bar{\sigma}$ itself. We shall skip the formal proof of the nonperturbability of $\bar{\sigma}$, which is slightly cumbersome, though straightforward. Let us only illustrate the nonperturbability with respect to a particular type of excitation. Introducing the orthogonal projection S of the bcc lattice onto the plane $x_1=0$ and taking a set $Q \subset S$, we may consider the configuration $\tilde{\sigma}_V$ corresponding to elevating the interface by 1/2 above Q. Namely,

$$\tilde{\sigma}_x = +1 \qquad \text{if} \quad (x_2, x_3) \in Q \text{ and } x_1 \geqslant 1/2 \quad \text{or} \quad (x_2, x_3) \notin Q \text{ and } x_1 \geqslant 0$$
$$\tilde{\sigma}_x = -1 \qquad \text{otherwise}$$

The energy $H_V(\tilde{\sigma}_V \mid \bar{\sigma})$ of this configuration is larger by about $J\,|\partial Q|$ (with $|\partial Q|$ denoting the length of the boundary of Q) than the energy $H_V(\bar{\sigma}_V \mid \bar{\sigma})$ of the ground configuration. Thus, excitations whose energy does not exceed a given bound may not be constructed on a set Q whose diameter exceeds a certain value. ▌

According to the Dobrushin–Shlosman conjecture, this ground state should be stable. This means the existence at low temperatures of a non-translation-invariant Gibbs state with a rigid interface, i.e., a Gibbs state for which the interface in a typical configuration does not differ much from the ground configuration $\bar{\sigma}$.

Here the conjecture may indeed be proven. One possibility is to use the method introduced by Dobrushin[(17)] for the Ising model on a simple cubic lattice and generalized later to other models.[(15)] Another approach is due to van Beijeren,[(18)] which we follow in the next theorem. We get the same result using the characterization of the roughening transition in terms of the step free energy σ_{step}, defined as the excess of surface free energy per unit length of a single step in an otherwise flat interface[5], indeed, we may adapt the argument due to Bricmont *et al.*[(20)]

Theorem 2. For every $J>0$ there exists $\beta_0(J)$ such that for every $\beta \geqslant \beta_0(J)$ the Gibbs state corresponding to the (100) boundary condition presents a rigid interface. Moreover, the step free energy corresponding to this interface is strictly positive.

[5] It was conjectured in Ref. 19 that the step free energy is vanishing when the interface is rough.

Proof. We associate with every $x=(x_1, x_2, x_3)$ with $x_1 \geqslant 1/2$ its symmetric site $x'=(-x_1, x_2, x_3)$ and the spin variables

$$s_x = \sigma_x + \sigma_{x'}, \qquad t_x = \sigma_x - \sigma_{x'}$$

Rewriting $H_V(\sigma_V \mid \bar{\sigma})$ in terms of these new variables s_x, t_x for $x \in V$ and $x_1 \geqslant 1/2$, and the initial σ_x for $x \in V$ and $x_1 = 0$, the new expression contains only ferromagnetic interactions and positive external fields. Hence, we may apply Lebowitz inequalities,[21] in the same way as in the original van Beijeren proof, to show that the expectation $\langle \sigma_0 \rangle$ of the spin at the origin σ_0 will decrease if we introduce positive fields μ_x acting on all variables t_x that belong to the plane $x_1 = 1/2$, and let this field μ_x tend to infinity. Since this fixes all σ_x in the plane $x_1 = 1/2$ to be equal to $+1$ and simultaneously all σ_x in the plane $x_1 = -1/2$ to be equal to -1, we get

$$\langle \sigma_0 \rangle \geqslant m_2(\beta J)$$

where $\langle \sigma_0 \rangle$ denotes the expectation of σ_0 in the original system and m_2 is the spontaneous magnetization of the two-dimensional Ising model (on the sublattice $x_1 = 0$) as a function of the coupling constant. If $\beta J > \alpha_0$, where $\alpha_0 = \frac{1}{2} \ln(1+\sqrt{2})$ is the critical value for the two-dimensional model, the magnetization m_2 is strictly positive and hence also $\langle \sigma_0 \rangle > 0$. Since symmetric points with respect to the plane $x_1 = -1/2$ have opposite expectations, this implies the presence of a rigid interface.

The argument concerning the step free energy is very close to the preceding one and we shall use the same notations. Let us compute the derivative of σ_{step} in a finite volume (defined as the logarithm of the ratio of the partition functions with appropriate boundary conditions) with respect to the external field μ_x for some $x \in V$, $x_1 = 1/2$. This derivative, when expressed as the difference of correlation functions, is nonpositive, according to, again, Lebowitz inequalities. Hence, the finite-volume σ_{step} decreases when we let $\mu_x \to \infty$ for all $x \in V$ such that $x_1 = 1/2$, and we finally obtain

$$\sigma_{\text{step}} \geqslant \tau_2(\beta J)$$

where τ_2 denotes the surface tension of the two-dimensional Ising model on a square lattice. Thus we prove that the step free energy is nonzero if $\beta J > \alpha_0$. ∎

Remark 1. The arguments above may be applied to any ferromagnetic system with respect to a chosen interface, provided that the following conditions are satisfied: (a) the system is symmetric with respect to the plane of the interface, (b) all bonds crossing this plane are orthogonal to it and join symmetric sites, (c) the two-dimensional system obtained as the restriction to this plane of the original system has a spontaneous magnetization, such as the Ising systems on a simple cubic lattice with nearest and next nearest neighbor attractions considered in Ref. 1.

Remark 2. If $\sigma_{\mathrm{step}} > 0$, then there is a cusp in the Wulf plot in the direction (100). The proof of this fact in our case is the same as that given by Bricmont *et al.*[22] for the Ising ferromagnet on a simple cubic lattice.

In the case $J = 0$ we are confronted with a new situation. The ground state corresponding to the (100) boundary condition is no longer rigid. Actually, many ground configurations belong to the set $M_V(\bar{\sigma})$ and, already at zero temperature, the system is governed by a nontrivial random ground state. To get some information about it we shall notice that it is equivalent to the exactly solvable body-centered solid-on-solid (BCSOS) model introduced by van Beijeren.[5]

Let $\mathbb{S}$ be a two-dimensional square lattice $\mathbb{Z}^2$ and let $\mathbb{S}_1$ and $\mathbb{S}_2$ be its sublattices formed by sites $i = (i_1, i_2)$ for which $i_1 + i_2$ is even and odd, respectively. Consider the set $\Sigma_{\mathbb{S}}$ of height configurations $n = (n_i)$, $i \in \mathbb{S}$, with $n_i \in \mathbb{Z}$ if $i \in \mathbb{S}_1$ and $n_i \in \mathbb{Z} + 1/2$ if $i \in \mathbb{S}_2$, and let $\Sigma^B_{\mathbb{S}}$ be the set of such configurations for which $|n_i - n_j| = 1/2$ whenever i and j are nearest neighbors in $\mathbb{S}$ (their distance $|i - j| = 1$). For a fixed boundary condition $\bar{n} \in \Sigma^B_{\mathbb{S}}$ we denote by $\Sigma^B_\Lambda(\bar{n})$ the set of configurations in $\Lambda \subset \mathbb{S}$ for which $n_\Lambda \cup \bar{n}_{\Lambda^c} \in \Sigma^B_{\mathbb{S}}$. For any $n \in \Sigma^B_{\mathbb{S}}$ and any elementary square s of the lattice $\mathbb{S}$, let us introduce the function $\chi_s(n)$, which equals zero if $n_i = n_j$ for both diagonals (i, j) of the elementary square and equals one in the remaining cases. For every real parameter α we then define the specification of the BCSOS model by

$$\mu^{B,\alpha}_\Lambda(n_\Lambda \mid \bar{n}) = Z^{B,\alpha}_\Lambda(\bar{n})^{-1} \exp\left[-\sum_{s \cap \Lambda \neq \varnothing} \alpha \chi_s(n_\Lambda \cup \bar{n}_{\Lambda^c})\right]$$

with

$$Z^{B,\alpha}_\Lambda(\bar{n}) = \sum_{n_\Lambda \in \Sigma^B_\Lambda(\bar{n})} \exp\left[-\sum_{s \cap \Lambda \neq \varnothing} \alpha \chi_s(n_\Lambda \cup \bar{n}_{\Lambda^c})\right]$$

We may now consider the Gibbs states of the BCSOS model in accordance with the general theory. In connection with the (100) boundary condition of the bcc Ising model, a special role will be given to the boundary configuration $\bar{n} \in \Sigma^B_{\mathbb{S}}$: $\bar{n}_i = 0$ for $i \in \mathbb{S}_1$ and $\bar{n}_i = 1/2$ for $i \in \mathbb{S}_2$. Notice also that if we denote by $\pi(x)$ the orthogoal projection of $x \in L$ onto the plane $x_1 = 0$, the projection $\pi(L)$ of all the lattice L is a square lattice and may be identified with $\mathbb{S}$ by taking for the components of $i = \pi(x)$ the values $i_1 =$

$x_1 + x_2$ and $i_2 = x_1 - x_2$ ($\bar{n}$ and π will always be used in this sense in this subsection; later, when a confusion with projections onto other planes could arise, we shall use the notation $\pi^{(100)}$).

Theorem 3. The ground state corresponding to the (100) boundary condition and $J = 0$ is asociated to a state of the BCSOS model corresponding to the boundary condition $\bar{n}$ and $\alpha = 0$. More precisely, let V be a cylinder orthogonal to the plane $x_1 = 0$ (such that the distances from the plane $x_1 = 0$ to its top and to its bottom are larger than the diameter of its base) and let $\Lambda = \pi(V)$. Then there is a one-to-one correspondence between the ground configurations $M_V(\bar{\sigma})$ and the configurations $\Sigma_\Lambda^B(\bar{n})$ of the BCSOS model which maps the ground specification $\mu_V^{\infty H}(\sigma_V \mid \bar{\sigma})$ into the specification $\mu_\Lambda^{B,0}(n_\Lambda \mid \bar{n})$.

Proof. We consider the particular volume V together with the condition about its top and bottom to prevent the BCSOS surfaces from touching the boundaries of V, which would spoil the stated equivalence. Let Ω_1 be the set of configurations $\sigma \in \Omega$ for which $\sigma_x \geqslant \sigma_y$ whenever $\pi(x) = \pi(y)$ and $x_1 > y_1$. For every $\sigma \in \Omega_1$ and $i \in \mathbb{S}$ introduce the height

$$n_i = \inf\{x_1 \mid \sigma_x = +1 \text{ and } \pi(x) = i\}$$

This defines a one-to-one correspondence between Ω_1 and $\Sigma_{\mathbb{S}}$. The energy corresponding to $H_V(\sigma_V \mid \bar{\sigma})$ in terms of the height variables may be easily computed. Up to an additive constant fixed so that $H_\Lambda(\bar{n}_\Lambda \mid \bar{n}) = 0$, one gets

$$H_\Lambda(n_\Lambda \mid \bar{n}) = \sum_{\text{nn}} 4J_0(|n_i - n_j| - 1/2) + \sum_{\text{nnn}} 2J\,|n_i - n_j|$$

where $n_i = \bar{n}_i$ whenever $i \notin \Lambda$. Clearly, if $J = 0$, the set $M_V(\bar{\sigma})$ corresponds to all height configurations for which $H_\Lambda(n_\Lambda \mid \bar{n}) = 0$, namely the set of height configurations for which $|n_i - n_j| = 1/2$ whenever $|i - j| = 1$. This is just the set $\Sigma_\Lambda^B(\bar{n})$. The equivalence of specifications is then straightforward. ∎

We postpone some comments on this theorem until Theorem 5 and we next analyze the case $J < 0$. It turns out that $\lim_{V \uparrow \mathbb{L}} \mu_V^{\infty H}(\cdot \mid \bar{\sigma})$ now does not exist. However, considering particular sequences of volumes $\{V_n\}$, we may get different ground states corresponding to the boundary condition $\bar{\sigma}$.

Theorem 4. Several different rigid ground states correspond to the (100) boundary condition and $J < 0$. The associated ground configurations are perturbable.

Proof. We first prove that for $J < 0$ the set $M_V(\bar{\sigma})$ is mapped onto a subset of $\Sigma_\Lambda^B(\bar{n})$ by the correspondence introduced in Theorem 3. As in the case $J = 0$, we have $M_V(\bar{\sigma}) \subset \Omega_1$, where Ω_1 is the subset of configurations introduced in the preceding proof. Now, it is useful to rewrite the energy as a sum of contributions of elementary squares s of the lattice $\mathbb{S}$, namely

$$H_\Lambda(n_\Lambda \mid \bar{n}) = \sum_{s \cap \Lambda \neq \varnothing} H_s$$

with

$$H_s = 2J_0 \sum_{\mathrm{nn}} |n_i - n_j| + 2J \sum_{\mathrm{nnn}} |n_i - n_j| - J_0$$

where the sums run over the four vertices of the square s. The minimal value $-2|J|$ of H_s is attained when $|n_i - n_j| = 1/2$ for all n.n. pairs, and $|n_i - n_j| = 1$ for one pair of n.n.n., while $|n_i - n_j| = 0$ for the other pair. Indeed, if $|n_i - n_j| = 1/2$ for all pairs of n.n., then necessarily either $|n_i - n_j| = 1$ for one pair of n.n.n. and $|n_i - n_j| = 0$ for the remaining pair, or $|n_i - n_j| = 0$ for both of them. If, however, $|n_i - n_j| \neq 1/2$ for some n.n., then $|n_i - n_j| \geqslant 3/2$ and $\sum_{\mathrm{nn}} |n_i - n_j| \geqslant 3$. By the triangular inequality, we have

$$\sum_{\mathrm{nn}} |n_i - n_j| \leqslant \sum_{\mathrm{nnn}} |n_i - n_j|, \qquad i, j \in s$$

and therefore

$$\begin{aligned} H_s &\geqslant (2J_0 - 2|J|) \sum_{\mathrm{nn}} |n_i - n_j| - J_0 \\ &\geqslant 3(2J_0 - 2|J|) - J_0 \geqslant 5J_0 - 4|J| - 2|J| \geqslant -2|J| \end{aligned}$$

whenever $|J| \leqslant (2/3) J_0 < (5/4) J_0$. Thus, the ground configurations of $M_V(\bar{\sigma})$ correspond to the configurations of $\Sigma_\Lambda^B(\bar{n})$ for which $|n_i - n_j| = 1$ for one pair of n.n.n. vertices in each elementary square s.

It turns out that $M_V(\bar{\sigma})$ depends on the particular form of V. We examine, for instance, the case in which V is a cylinder orthogonal to the plane $x_1 = 0$ with a projection $\Lambda = \pi(V)$, which is a parallelogram centered at the origin and with edges parallel to the lines $x_2 = x_3$ and $x_2 = -x_3$. Then there are four different cases according to whether the corners of Λ fall into one of the following subsets of $\mathbb{S}$:

$$\mathbb{S}_{0,0} = \{i \in \mathbb{S} \mid i_1 \text{ and } i_2 \text{ even}\}, \qquad \mathbb{S}_{0,1} = \{i \in \mathbb{S} \mid i_1 \text{ even, } i_2 \text{ odd}\}$$

$$\mathbb{S}_{1,0} = \{i \in \mathbb{S} \mid i_1 \text{ odd, } i_2 \text{ even}\}, \qquad \mathbb{S}_{1,1} = \{i \in \mathbb{S} \mid i_1 \text{ and } i_2 \text{ odd}\}$$

In each of these cases we get a unique ground configuration; e.g., in the first case the heights n_i take the values 0, 1/2, 1, and 1/2 for $i \in \mathbb{S}_{0,0}$, $\mathbb{S}_{0,1}$, $\mathbb{S}_{1,0}$, and $\mathbb{S}_{1,1}$, respectively. If we take limits over a sequence $\{V_n\}$ with

$\pi(V_n)$ in one of the above cases, we finally get four rigid ground states supported on the configurations

$$\begin{aligned} &\sigma_x = 1 && \text{whenever} \quad x_1 \geqslant 1/2 - \delta \\ &\sigma_x = \varepsilon(-1)^{x_1 + x_2} && \text{whenever} \quad x_1 = -\delta \\ &\sigma_x = -1 && \text{whenever} \quad x_1 \leqslant -1/2 - \delta \end{aligned}$$

with the four possibilities being given by choosing $\varepsilon = \pm 1$ and $\delta = 0, 1/2$.

Any of these four configurations closely follows the horizontal plane $x_1 = 0$ and it may seem on first view that this interface may still be rigid at low temperatures. However, even low-energy excitations may significantly perturb the interface. Namely, supposing for concreteness that the ground configuration is the one obtained by the choice $\varepsilon = 1$, $\delta = 0$, consider a configuration $\tilde{\sigma}$ corresponding to elevating the interface by 1 above Q, with $Q \subset \Lambda$ any rectangle with corners such that i_1 and i_2 are odd and sides parallel to the axes $i_1 = 0$ and $i_2 = 0$. That is, $\tilde{n}_i = \bar{n}_i + 1$ if $i \in Q$ and $\tilde{n}_i = \bar{n}_i$ if $i \notin Q$. Then $H_V(\tilde{\sigma}_V \mid \bar{\sigma}) - H_V(\sigma_V \mid \bar{\sigma}) = 4J$ independently of the size of the rectangle Q. Thus, this ground configuration is perturbable. ▮

This recalls the case of the interface for the Ising model on a square lattice, which may also be perturbed above large segments by paying only a fixed amount of energy. Recalling that this fact led, for the two-dimensional model, to a proof of the roughness of the interface for all positive temperatures,[23] it is natural to expect that also in our case, for J negative, the interface is rough, in accordance with the conjecture of Dobrushin and Shlosman,[9] which would say that our rigid ground states are not stable. While we do not know how to make the above reasoning into a real proof, we get an additional argument for the roughness of the interface for $J < 0$ from the investigation of the weak ground states in the case of a vanishing n.n.n. coupling.

We shall thus extend Theorem 3 and consider the weak ground states corresponding to a "n.n.n. direction α," namely, to the situation where J_0 is kept fixed and $J = \alpha/\beta$ while $\beta \to \infty$. Inspecting the proof of Theorem 3, it turns out that the corresponding specification $\mu_V^{\infty J_0, \alpha}(\sigma_V \mid \bar{\sigma})$ is equivalent to $\mu_\Lambda^{B,\alpha}(n_\Lambda \mid \bar{n})$ and thus we may control the dependence on α of the weak ground state.

Theorem 5. The weak ground state of the Ising model on a bcc lattice corresponding to the "n.n.n. direction α" and the (100) boundary condition is, by the one-to-one correspondence introduced in Theorem 3, mapped into the Gibbs states of the BCSOS model on a square lattice with parameter α and boundary condition $\bar{n}$.

We may refer to the van Beijeren analysis of the BCSOS model[5] to get a description of this weak ground state in terms of a six-vertex model with the weights $w_1 = w_2 = w_3 = w_4 = e^{-2\alpha}$ and $w_5 = w_6 = 1$. If $\alpha > \alpha_R = \frac{1}{2}\ln 2$, the six-vertex model is in the ferroelectric phase and the interface is rigid; if $\alpha < \alpha_R$, the results about the six-vertex model are usually interpreted as describing a rough interface, which actually should mean that the corresponding infinite-volume Gibbs state of the BCSOS model does not exist and our weak ground state is translation-invariant. Notice that even though one would interpret the parameter α as an inverse temperature of the BCSOS model, the above theorem shows that in the genuine isotropic Ising model it rather plays the role of an angle in the (J, T) plane under which we approach the point $J = 0$, $T = 0$.

Now, an important question arises, that of the stability of these weak ground states, which is a reasonable, but still unproved hypothesis. Under this hypothesis the results above suggest the existence, for any small, positive J, of a roughening transition at a temperature $T_R(J)$ such that $T_R(J) \to 0$ for $J \to 0$ with a slope given by the critical value α_R.[10]

Remark 3. As a consequence of Theorem 2 and the preceding analysis, we get, independently of the exact solution, the existence of an ordered phase for the BCSOS and the six-vertex model for $\alpha < \alpha_0$.

3.2. The (110) Interface

The ground states associated to the (110) interface, unlike those considered in the preceding subsection, behave uniformly in J.

Theorem 6. The ground state corresponding to the (110) boundary condition is rigid for any $J > -\frac{2}{3}J_0$. Moreover, the ground configuration is nonperturbable.

Proof. The boundary condition $\bar{\sigma} = \bar{\sigma}^{(110)}$ associated to the (110) interface belongs to the set Ω_1 introduced in the proof of Theorem 3 and corresponds to the configuration of heights $\bar{n} \in \Sigma_{\mathbb{S}}^B$ defined by $\bar{n}_i = i_1 + i_2$. In this case the set $\Sigma_\Lambda^B(\bar{n})$ reduces to the single configuration $\bar{n}_\Lambda$. This configuration satisfies $|\bar{n}_i - \bar{n}_j| = 1$ for all n.n.n. such that $i_1 - i_2 = j_1 - j_2$ and gives a contribution to the energy $H_s = 2J$ for every elementary square of the lattice. Any other configuration $\sigma \in \Omega_1$ would be associated with a configuration $n \in \Sigma_{\mathbb{S}}$ satisfying $|n_i - n_j| \geqslant 1$ for all the just mentioned n.n.n., in order to be compatible with the boundary condition, and would give a larger energy $H_V(\sigma_V \mid \bar{\sigma})$. This is clear if $J \geqslant 0$ and has already been shown, in the first part of the proof of Theorem 4, when $J < 0$, provided that $|J| < \frac{2}{3}J_0$. Hence $\bar{\sigma}_V$ is the unique ground configuration and therefore the ground state is rigid.

Next we sketch the proof of the nonperturbability of $\bar{\sigma}$. Let Q be a subset of $\Lambda = \pi^{(100)}(V)$ and consider the configuration $\tilde{\sigma} \in \Omega_1$ associated with the height variables $\tilde{n}_i = \bar{n}_i + 1$ if $i \in Q$ and $\tilde{n}_i = \bar{n}_i$ if $i \notin Q$. Only the bonds (i, j) such that $i \in Q$ and $j \notin Q$ contribute to the difference $H_V(\tilde{\sigma}_V \mid \bar{\sigma}) - H_V(\bar{\sigma}_V \mid \bar{\sigma})$ and the amount of this contribution is $4J_0$ if i and j are n.n. and $i_1 > j_1$ or $i_2 > j_2$, and $2J$ if i and j are n.n.n. neighbors and $i_1 + i_2 = j_1 + j_2$. There are exactly $\frac{1}{2} |\partial Q|$ bonds of the first type and at most $|\partial Q|$ bonds of the second type. Hence, even in the worst situation we have

$$H_V(\tilde{\sigma}_V \mid \bar{\sigma}) - H_V(\bar{\sigma}_V \mid \bar{\sigma}) \geqslant |\partial Q| (2J_0 + 2J)$$

Provided that $J > -J_0$, this excess of energy is proportional to $|\partial Q|$ and hence the ground configuration is nonperturbable. ▮

In the same way as for the (100) interface, if $J \geqslant 0$, we can prove the rigidity of the interface (110) at low temperatures.

Theorem 7. For every $J \geqslant 0$ there exists β_0 such that for every $\beta > \beta_0$ the Gibbs state corresponding to the (110) boundary condition presents a rigid interface. Moreover, the step free energy corresponding to this interface is strictly positive.

Proof. The proof is obtained by arguing as in Theorem 1 (Remark 1) and realizing that the intersection of the (110) plane with the bcc lattice yields a two-dimensional Ising model which, even for $J = 0$, has a nonvanishing magnetization if $\beta J_0 > \alpha_0$. ▮

Remark 4. In the preceding proof the hypothesis $J \geqslant 0$ appears as a technical condition for the validity of the Lebowitz inequalities. One expects the same conclusion for any J inside the ferromagnetic phase. The proof of Theorem 6, for which only the condition $J > -J_0$ was required for the rigidity, already suggested this fact, which could be made rigorous by using Dobrushin method.[15,17] On the other hand (see Remark 2) for $J \geqslant 0$ it may be proven that if $\sigma_{\text{step}} > 0$, then there is a cusp in the Wulf plot in the direction (110).

3.3. The (111) Interface

We shall next point out that the ground state associated with the (111) boundary condition $\bar{\sigma}^{(111)}$ (which in this subsection will simply be denoted by $\bar{\sigma}$) can be described in terms of the triangular Ising solid-on-solid (TISOS) model considered by Nienhuis *et al.*[6,7]

Let $\mathbb{T}$ be a triangular lattice. By taking e_1, e_2, e_3 to be three unit vectors on the plane at angles $2\pi/3$, the sites $i \in \mathbb{T}$ may be described by the vectors

$$i = i_1 e_1 + i_2 e_2 + i_3 e_3$$

where i_1, i_2, and i_3 are integers. $\mathbb{T}$ is divided into three triangular sublattices $\mathbb{T}_0$, $\mathbb{T}_1$, and $\mathbb{T}_2$ labeled in such a way that $i_1 + i_2 + i_3$ for i on sublattice $\mathbb{T}_l$ is equal to l plus a multiple of 3 ($l = 0, 1, 2$). Consider the set $\Sigma_{\mathbb{T}}$ of height configurations $n = \{n_i\}$, $i \in \mathbb{T}$, with $n_i \in \mathbb{Z} + l/3$ for $i \in \mathbb{T}_l$, $l = 0, 1, 2$. The configurations $\Sigma_{\mathbb{T}}^T$ of the TISOS model are obtained by restricting the configurations of $\Sigma_{\mathbb{T}}$ to satisfy $|n_i - n_j| \leqslant 2/3$ for all pairs (i, j) of n.n. on $\mathbb{T}$. This is equivalent to the condition that the differences $n_i - n_j$ between n.n. in the oriented lattice (that is, for all n.n. i, j belonging respectively to $\mathbb{T}_0$ and $\mathbb{T}_1$, to $\mathbb{T}_1$ and $\mathbb{T}_2$, and to $\mathbb{T}_2$ and $\mathbb{T}_0$) take the values $-1/3$ or $2/3$. Clearly, in any elementary triangle of $\mathbb{T}$, the difference $n_i - n_j$ takes then the value $-1/3$ on two sides of the triangle and the value $2/3$ on the other side. Therefore a configuration of $\Sigma_{\mathbb{T}}^T$ can equivalently be described by distinguishing one side in each elementary triangle of the lattice $\mathbb{T}$. This shows that $\Sigma_{\mathbb{T}}^T$ is equivalent to the set of ground configurations of the Ising antiferromagnet (or the set of dimer configurations) on a triangular lattice.

For a fixed boundary condition $\bar{n} \in \Sigma_{\mathbb{T}}^T$ we denote by $\Sigma_\Lambda^T(\bar{n})$ the set of configurations in $\Lambda \subset \mathbb{T}$ for which $n_\Lambda \cup \bar{n}_{\Lambda^c} \in \Sigma_{\mathbb{T}}^T$. A special role will be given in this subsection to the boundary condition $\bar{n}$ defined by $\bar{n}_i = l/3$ for $i \in \mathbb{T}_l$, $l = 0, 1, 2$. Notice also that if we denote, for $x \in \mathbb{L}$, by $\pi(x)$ [or more precisely by $\pi^{(111)}(x)$] its orthogonal projection onto the plane $x_1 + x_2 + x_3 = 0$, the projection $\pi(\mathbb{L})$ of all the lattice $\mathbb{L}$ is a triangular lattice, which may be identified with $\mathbb{T}$ by taking

$$i = \pi(x) = x_1 e_1 + x_2 e_2 + x_3 e_3$$

We remark that $\pi(\mathbb{L}_1) = \pi(\mathbb{L}_2) = \pi(\mathbb{L})$.

Theorem 8. Let $\bar{\sigma}$ denote the (111) boundary condition and let V be a cylinder orthogonal to the plane $x_1 + x_2 + x_3 = 0$ (with top and bottom at a distance from this plane larger than the diameter of its base) and let $\Lambda = \pi^{(111)}(V)$. Then, there is a one-to-one correspondence between the ground configurations $M_V(\bar{\sigma})$ and the configurations $\Sigma_\Lambda^T(\bar{n})$ of the TISOS model, for any $J > -\frac{2}{3}J_0$. The ground specification $\mu_V^{\infty H}(\sigma_V \mid \bar{\sigma})$ is mapped into the state $\mu_\Lambda^{T,0}(n_\Lambda \mid \bar{n})$ of the TISOS model with support on the set $\Sigma_\Lambda^T(\bar{n})$ and assigning equal probabilities to the configurations of this set.

Proof. We take $v(x) = \frac{2}{3}(x_1 + x_2 + x_3)$ as a measure of the height of the site $x \in \mathbb{L}$ on the (1, 1, 1) plane and we consider the set Ω_2 of configurations $\sigma \in \Omega$ for which $\sigma_x \geqslant \sigma_y$ whenever $v(x) > v(y)$ and $\pi(x) = \pi(y)$. For every $\sigma \in \Omega_2$ and $i \in \mathbb{T}$ we introduce the variable

$$n_i = \inf\{v(x) \mid \sigma_x = +1 \text{ and } \pi(x) = i\}$$

This defines a one-to-one correspondence between Ω_2 and $\Sigma_{\mathbb{T}}$. The energy $H_V(\sigma_V \mid \bar{\sigma})$ in terms of the height variables may be easily computed. Up to an additive constant fixed so that $H_\Lambda(\bar{n}_\Lambda \mid \bar{n}) = 0$, one gets

$$\begin{aligned} H_\Lambda(n_\Lambda \mid \bar{n}) = 2J_0 \Bigg\{ & \sum_{i \in \mathbb{T}_0, j \in \mathbb{T}_1} (|n_i - n_j + 1/3| - 1/3) \\ & + \sum_{i \in \mathbb{T}_1, j \in \mathbb{T}_2} (|n_i - n_j + 1/3| - 1/3) \\ & + \sum_{i \in \mathbb{T}_2, j \in \mathbb{T}_0} (|n_i - n_j + 1/3| - 1/3) \Bigg\} \\ & + 2J \Bigg\{ \sum_{i \in \mathbb{T}_0, j \in \mathbb{T}_1} (|n_i - n_j - 2/3| - 2/3) \\ & + \sum_{i \in \mathbb{T}_1, j \in \mathbb{T}_2} (|n_i - n_j - 2/3| - 2/3) \\ & + \sum_{i \in \mathbb{T}_2, j \in \mathbb{T}_0} (|n_i - n_j - 2/3| - 2/3) \Bigg\} \end{aligned}$$

where the sums run over all n.n. in $\mathbb{T}$ and $n_i = \bar{n}_i$ whenever $i \notin \Lambda$. For any TISOS configuration, i.e., for any $n \in \Sigma_\Lambda^T(\bar{n})$, we have $H_\Lambda(n_\Lambda \mid \bar{n}) = 0$, since in every elementary triangle of $\mathbb{T}$, for one of the sides $|n_i - n_j + 1/3| = 1$ and $|n_i - n_j - 2/3| = 0$, while for the two other sides $|n_i - n_j + 1/3| = 0$ and $|n_i - n_j - 2/3| = 1$. It is clear that if $J \geqslant 0$, the other configurations of $\Sigma_{\mathbb{T}}$ that do not belong to $\Sigma_{\mathbb{T}}^T$ give an energy strictly larger than zero. Therefore, in this case the set $\Sigma_\Lambda^T(\bar{n})$ corresponds exactly to the set of ground configurations. We shall now show that the same occurs in the case $J < 0$ in the considered interval. Let t be an elementary triangle of $\mathbb{T}$ and let us denote by 0, 1, and 2 its vertices belonging, respectively, to $\mathbb{T}_0$, $\mathbb{T}_1$, and $\mathbb{T}_2$. Then $H_\Lambda(n_\Lambda \mid \bar{n})$ can be written as a sum of contributions

$$\begin{aligned} H_t = {} & J_0\{|n_0 - n_1 + 1/3| + |n_1 - n_2 + 1/3| + |n_2 - n_0 + 1/3| - 1\} \\ & + J\{|n_0 - n_1 - 2/3| + |n_1 - n_2 - 2/3| + |n_2 - n_0 - 2/3| - 2\} \end{aligned}$$

associated to the elementary triangles of $\mathbb{T}$. If we write $m_1 = n_0 - n_1 + 1/3$ and $m_2 = n_1 - n_2 + 1/3$, which for $n \in \Sigma_{\mathbb{T}}$ can be arbitrary integers, then

$$\begin{aligned} H_t = {} & J_0\{|m_1| + |m_2| + |m_1 + m_2 - 1| - 1\} \\ & + J\{|m_1 - 1| + |m_2 - 1| + |m_1 + m_2| - 2\} \end{aligned}$$

Now

$$H_t = -J_0 + 2|J| + (J_0 - |J|)\{|m_1| + |m_2| + |m_1 + m_2 - 1|\}$$
$$+ |J|\{|m_1| - |m_1 - 1| + |m_2| - |m_2 - 1|$$
$$+ |m_1 + m_2 - 1| - |m_1 + m_2|\} > 0$$

because

$$|m_1| + |m_2| + |m_1 + m_2 - 1| > 1$$

if $n \notin \Sigma_{\mathbb{T}}^{T}$ and

$$|m_1| - |m_1 - 1| + |m_2| - |m_2 - 1| + |m_1 + m_2 - 1| - |m_1 + m_2| \geqslant -1$$

since $|m_1| - |m_1 - 1| = 1$ if $m_1 \geqslant 1$ and $|m_1| - |m_1 - 1| = -1$ if $m_1 \leqslant 0$. Therefore $H_t > 0$ when $n \in \Sigma_{\mathbb{T}}$ does not belong to $\Sigma_{\mathbb{T}}^{T}$ also in the case $J < 0$. This shows the one-to-one correspondence between $M_V(\bar{\sigma})$ and $\Sigma_{\Lambda}^{T}(\bar{n})$. The other statements of the theorem are straightforward. ∎

From the analysis of the TISOS model[6,7] it follows that the surface is rough in the present situation and hence the ground state on the bcc lattice is translation-invariant.

3.4. General (k_1, k_2, k_3) Interfaces

The equivalences discussed in Sections 3.1 and 3.3 between ground states of our Ising system and SOS models are actually valid also for other boundary conditions $\bar{\sigma}^{(k)}$, $k = (k_1 k_2 k_3)$. We observe that by relabeling the axes and their orientations we may always suppose

$$0 \leqslant k_3 \leqslant k_2 \leqslant k_1$$

We shall distinguish two regions according to whether $k_2 + k_3 \leqslant k_1$ or $k_2 + k_3 \geqslant k_1$, the boundary condition (110) being included in both of them. In the first region and using the notations of Theorem 3, we have:

Theorem 9. Assume that $k_2 + k_3 \leqslant k_1$, and define the BCSOS configuration $\bar{n}^{(k)} \in \Sigma_{\mathbb{S}}^{B}$ by

$$\bar{n}_i^{(k)} = \inf\{x_1 \mid x \in \mathbb{L},\ x_1 k_1 + x_2 k_2 + x_3 k_3 \geqslant 0 \text{ and } \pi^{(100)}(x) = i\}$$

Suppose also that V is a cylinder as in Theorem 3, and let $\Lambda = \pi^{(100)}(V)$. Then there is one-to-one correspondence between the ground configurations $M_V(\bar{\sigma}^{(k)})$ and the BCSOS configurations $\Sigma_{\Lambda}^{B}(\bar{n}^{(k)})$ which maps the ground state $\mu_V^{\infty H}(\sigma_V \mid \bar{\sigma}^{(k)})$ into the state $\mu_{\Lambda}^{B,0}(n_\Lambda \mid \bar{n}^{(k)})$.

Under the hypothesis of the theorem, the boundary condition $\bar{\sigma}^{(k)}$ belongs to the set Ω_1, considered in Theorem 3, and is associated with the configuration $\bar{n}^{(k)} \in \Sigma_{\mathbb{S}}^B$. The proof then follows using the one-to-one correspondence between Ω_1 and $\Sigma_{\mathbb{S}}$ as that of Theorem 3. Notice also that the weak ground states $\mu_V^{\infty J_0, \alpha}(\sigma_V \mid \bar{\sigma}^{(k)})$ of Theorem 5 are mapped by this correspondence into the states $\mu_\Lambda^{B,\alpha}(n_\Lambda \mid \bar{n}^{(k)})$, and that the cases $J>0$ or $J<0$ can be considered as the limiting situations where $\alpha = \infty$ and $\alpha = -\infty$, respectively (see the proof of Theorem 4).

Similarly, in the complementary region $k_2 + k_3 \geqslant k_1$, we have, using the notations of Theorem 8, for any $J \geqslant -\frac{2}{3} J_0$, the following result.

Theorem 10. Assume that $k_2 + k_3 \geqslant k_1$ and let $\tilde{n}^{(k)} \in \Sigma_{\mathbb{T}}^T$ be the TISOS configuration

$$\tilde{n}_i^{(k)} = \inf\{ v(x) \mid x \in \mathbb{L},\ x_1 k_1 + x_2 k_2 + x_3 k_3 \geqslant 0 \text{ and } \pi^{(111)}(x) = i \}$$

Suppose also that V is as in Theorem 8 and let $\Lambda = \pi^{(111)}(V)$. Then, there is a one-to-one correspondence between the ground configurations $M_V(\bar{\sigma}^{(k)})$ and the TISOS configurations $\Sigma_\Lambda^T(\tilde{n}^{(k)})$ which maps the ground state $\mu_V^{\infty H}(\sigma_V \mid \bar{\sigma}^{(k)})$ into the state $\mu_\Lambda^{T,0}(n_\Lambda \mid \tilde{n}^{(k)})$.

This shows how in the study of these ground states we are always led to consider the BCSOS and TISOS models with boundary conditions. Without going further into their study, let us only mention that we expect rough interfaces for the ground states under these general boundary conditions.

4. ISING MODEL ON A BCC LATTICE: EQUILIBRIUM CRYSTAL SHAPES

We shall now consider the Wulf construction of the equilibrium crystal shape of a droplet of opposite phase. We are again led to BCSOS and TISOS models. The formation of facets, including a computation of their form, based on these two models was discussed in detail by Jayaprakash *et al.*[24,25] and Nienhuis *et al.*[6,7] and we are not going to repeat their calculations here. Instead, we shall stress the unity of the description by showing how both BCSOS and TISOS models appear naturally when considering the low-temperature asymptotic behavior of a single model, that is, the Ising model on a bcc lattice. Namely, as we saw already in Theorems 9 and 10, taking the boundary condition $\bar{\sigma}^{(k)}$ corresponding to an interface of an arbitrary orientation k (without loss of generality we always suppose $0 \leqslant k_3 \leqslant k_2 \leqslant k_1$), the ground configurations from $M_V(\bar{\sigma}^{(k)})$ are configurations satisfying the BCSOS condition whenever $k_2 + k_3 \leqslant k_1$, while they satisfy the TISOS condition if $k_2 + k_3 \geqslant k_1$. Thus, when computing the low-temperature asymptotic behavior of the orientation-dependent surface tension $\tau(k)$ (interface free energy), the main ingredient of the Wulf construction,[1,2] we may for all orientation rely on either the BCSOS or the TISOS models.

The surface tension $\tau(k)$ is defined by

$$\tau(k)=\lim_{V\uparrow\mathbb{L}}\left(-\frac{1}{\beta}\frac{1}{|S\cap V|}\log\frac{Z_V(\bar{\sigma}^{(k)})}{Z_V(\sigma^+)}\right)=\lim_{V\uparrow\mathbb{L}}\tau_V(k)$$

where $|S\cap V|$ is the area of the intersection of the surface $k_1x_1+k_2x_2+k_3x_3=0$ with V (thinking of V for a while as a subset of $\mathbb{R}^3$) and we recall that $Z_V(\bar{\sigma}^{(k)})$ [resp. $Z_V(\sigma^+)$] is the partition function in V under the boundary condition $\bar{\sigma}^{(k)}$ (resp. σ^+: $\sigma_x^+=+1$ for every $x\in\mathbb{L}$). The limit is over suitably chosen finite volumes V such that $|S\cap V|\to\infty$. Unfortunately, we are in general not able to control this limit and thus we shall consider only the asymptotic behavior of $\tau_V(k)$, believing that it also remains valid after the thermodynamic limit is performed.

First, let us consider the Wulf plot at zero temperature, where the only contribution to the surface tension is the excess of energy of the interface over the energy of a translation-invariant ground state σ^+, normalized to the unit of area:

$$e(k)=\lim_{|S\cap V|\to\infty}E_V(k)/|S\cap V|$$

with

$$E_V(k)=H_V(\bar{\sigma}_V^{(k)}\mid\bar{\sigma}^{(k)})-H_V(\sigma_V^+\mid\sigma^+)=|S\cap V|\,e_V(k)$$

Theorem 11. The excess of energy of the $(k_1k_2k_3)$ interface per unit area is, for $k_2+k_3\leqslant k_1$,

$$e(k)=8(J_0+J)\,k_1 \qquad \text{if} \quad J\leqslant 0$$

$$e(k)=8J_0k_1+4J(k_1+k_2+k_3) \qquad \text{if} \quad J\geqslant 0$$

and, for $k_2+k_3\geqslant k_1$

$$e(k)=4(J_0+J)(k_1+k_2+k_3)$$

(we suppose that k is normalized to unity).

Proof. Let us denote by $\omega(k)$ the inverse of the ratio (in the limit $|S\cap V|\to\infty$) of the area $|S\cap V|$ to the area $|\Lambda_1|$ of its orthogonal projection $\Lambda_1=\pi^{(100)}(S\cap V)$ for $k_2+k_3\leqslant k_1$:

$$\omega(k)=\lim(|\Lambda_1|/|S\cap V|)=(k,(1,0,0))=k_1$$

and to the area $|\Lambda_2|$ of the projection $\Lambda_2 = \pi^{(111)}(S \cap V)$ for $k_2 + k_3 \geqslant k_1$:

$$\omega(k) = (k, (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})) = (1/\sqrt{3})(k_1 + k_2 + k_3)$$

We first compute $e(k)$ for $k_2 + k_3 \leqslant k_1$. Let us denote by $N_s(\Lambda_1)$ the number of elementary squares of the lattice $\mathbb{S}$ inside Λ_1, and notice that $2\,|\Lambda_1| = N_s(\Lambda_1)$. If $e_s(k)$ denotes the average excess energy per elementary square, we have (up to boundary terms)

$$E_V(k) = N_s(\Lambda_1)\, e_s(k) = 2\,|\Lambda_1|\, e_s(k)$$

and thus

$$e(k) = 2\omega(k)\, e_s(k) = 2k_1 e_s(k)$$

Now, in the case $J < 0$, we have seen in the proofs of Theorems 4 and 9 that $e_s(k)$ is independent of the boundary condition, since the ground configurations always satisfy the condition $|n_i - n_j| = 1$ for one pair of n.n.n. in each square. Hence, if $J < 0$, we have

$$e_s(k) = -2\,|J| + 4J_0 - 2\,|J|$$

with the first term corresponding to the energy of the BCSOS configuration and the last two, $4J_0 - 2\,|J|$, taking into account its normalization. Thus we get the first formula of the theorem.

In the case $J > 0$, the energy of the ground configurations depends on the boundary condition $\bar{\sigma}^{(k)}$. We shall have $|n_i - n_j| = 1$ for the minimum possible number of n.n.n. compatible with $\bar{\sigma}^{(k)}$, and $|n_i - n_j| = 0$ for the remaining n.n.n. Since the increase of height of the plane $k_1 x_1 + k_2 x_2 + k_3 x_3 = 0$ above Λ_1 along the diagonals of a square of the lattice $\mathbb{S}$ is $-k_2/k_1$ in the direction x_2 and $-k_3/k_1$ in the direction x_3, we must have (think of Λ_1 as a rectangle)

$$\sum_{\substack{\text{nnn} \\ i_1 + j_1 = i_2 + j_2}} |n_i - n_j| = N_s(\Lambda_1)(k_2/k_1)$$

$$\sum_{\substack{\text{nnn} \\ i_1 - j_1 = i_2 - j_2}} |n_i - n_j| = N_s(\Lambda_1)(k_3/k_1)$$

and therefore

$$e_s(k) = 2J(k_2/k_1 + k_3/k_1) + 4J_0 + 2J$$

Then, from $e(k) = 2k_1 e_s(k)$, the second formula of the theorem follows.

Finally we consider the case $k_2 + k_3 \geqslant k_1$. Let $N_t(\Lambda_2)$ be the number of elementary triangles of the lattice $\mathbb{T}$ inside Λ_2, and let $e_t(k)$ be the average energy per triangle. Since the area of each triangle in Λ_2 is $1/(2\sqrt{3})$ (observe that the projection of a cube of side one of the lattice $\mathbb{L}$ is an hexagon of area $\sqrt{3}$ and contains six triangles), we have

$$\begin{aligned} e(k) &= E_V(k)/|S \cap V| = [N_t(\Lambda_2)/|S \cap V|]\, e_t(k) \\ &= 2\sqrt{3}\,\omega(k)\, e_t(k) = 2(k_1 + k_2 + k_3)\, e_t(k) \end{aligned}$$

From Theorems 8 and 10 we know that the ground configurations contribute the same value to $e_t(k)$, independently of the boundary condition (for all $J > -\frac{2}{3}J_0$), namely, that of the TISOS model. Hence, we get

$$e_t(k) = 2J_0 + 2J$$

This proves the third formula of the theorem. ∎

The Wulf plot, that is, the set of points $m = \tau(k).k$, is in the region $0 \leqslant k_3 \leqslant k_2 \leqslant k_1$ the external envelope of the following two spheres:

$$m_1^2 + m_2^2 + m_3^2 - 4(J_0 + J)(m_1 + m_2 + m_3) = 0 \qquad \text{for all} \quad J > -\tfrac{2}{3}J_0$$

and

$$m_1^2 + m_2^2 + m_3^2 - 8(J_0 + J)\, m_1 = 0 \qquad \text{if} \quad J < 0$$

$$m_1^2 + m_2^2 + m_3^2 - (8J_0 + 4J)\, m_1 - 4Jm_2 - 4Jm_3 = 0 \qquad \text{if} \quad J \geqslant 0$$

We complete the Wulf plot by rotating twice the diagram by an angle $2\pi/3$ around the (111) axis and then taking the symmetries with respect to the coordinate planes.

It is easy to observe that the Wulf construction yields a complete faceted shape. For $J < 0$ it has 12 facets of type (110), and passing from negative to positive values of J, six new facets of the type (100) develop.

Let us inspect more closely the region around $J = 0$ at nonvanishing temperatures. The ground configurations are not unique and one should thus take into account also the contribution of the entropy of the ground states. Our claim generically is that this entropy may be described in terms of an SOS model. Namely,

$$\lim_{\beta \to \infty} [\beta\tau_V(k) - \beta e_V(k)] = -(1/|S \cap V|) \log Z^{\text{SOS}}_{\pi(V)}$$

with $Z^{\text{SOS}}_{\pi(V)}$ denoting (according to the orientation k) either the BCSOS or the TISOS model partition function under the boundary condition corresponding to k (i.e., respectively, $\bar{n}^{(k)}$ or $\tilde{n}^{(k)}$ of Theorems 9 and 10).

Indeed, referring briefly to Theorems 9 and 10 and observing that every excitation brings an energy at least of order J_0, we get the following result.

Theorem 12.

I. Suppose that V is a cylinder satisfying the conditions of Theorem 3, with base $\Lambda = \pi^{(100)}(V)$, and let k be such that $0 \leqslant k_3 \leqslant k_2 \leqslant k_1$ and $k_2 + k_3 \leqslant k_1$. Then the surface tension $\tau_V(k)$ at the inverse temperature β and with n.n.n. coupling $J = \alpha/\beta$ may be expressed by

$$\tau_V(k) = e_V^{J=0}(k) - \frac{1}{\beta}\frac{1}{|S \cap V|}\log[e^{2\alpha N_s(\Lambda)} Z_\Lambda^{B,\alpha}(\bar{n}^{(k)})] + O(e^{-\beta J_0})$$

where $e_V(k)$ is taken at $J = 0$ and $N_s(\Lambda)$ is the number of lattice sites in Λ.

II. Suppose that V is a cylinder satisfying the conditions of Theorem 8 with base $\Lambda = \pi^{(111)}(V)$, and let k be such that $0 \leqslant k_3 \leqslant k_2 \leqslant k_1$ and $k_2 + k_3 \geqslant k_1$. Then the surface tension $\tau_V(k)$ at the inverse temperature β and with n.n.n. coupling $J > -\frac{2}{3}J_0$ may be expressed by

$$\tau_V(k) = e_V(k) - \frac{1}{\beta}\frac{1}{|S \cap V|}\log Z_\Lambda^{T,0}(\bar{n}^{(k)}) + O(e^{-\beta J_0})$$

Let us notice that while the ground-state entropy term is proportional to the temperature $1/\beta$, the rest is of the order $e^{-\beta J_0}$ and thus much smaller at low temperatures. Unfortunately, we do not have a bound on the rest uniform in $|S \cap V|$ and thus we can only conjecture that the first two terms yield the leading asymptotic behavior also in the thermodynamic limit.

This conjecture may actually be supported by the following arguments. First, one introduces the description of configurations in terms of contours separating completely ordered areas. Observing that the configurations contributing to $Z_V(\bar{\sigma}^{(k)})$ always contain a large interface contour λ separating the region of the $(+)$ phase above λ from the region of the $(-)$ phase below λ, one may evaluate[6]

$$\left| \log \left\{ \frac{Z_V(\bar{\sigma}^{(k)})}{Z_V(\sigma^+)} \exp[\beta\, |S \cap V|\, e_V(k)] \right\} - \log Z_{\pi(V)}^{\mathrm{SOS},\alpha} \right|$$

by

$$\log \frac{\sum_\lambda \exp[-\beta H_V(\lambda) - \beta H_V(\bar{\sigma}_V \mid \bar{\sigma})]}{\sum_{\lambda,\mathrm{SOS}} \exp[-\beta H_\alpha(\lambda)]}$$

Here the sum in the numerator is over all interfaces λ compatible with the boundary condition with energy contribution $H_V(\lambda)$, while the sum in the denominator is only over the interfaces of SOS type with $H_\alpha(\lambda)$ the

[6] In the case $k_2 + k_3 \leqslant k_1$ we take $e_V^{J=0}(k)$ and include into $Z_{\pi(V)}^{\mathrm{SOS},\alpha}$ the term $e^{2\alpha N_S(\Lambda)}$.

corresponding energy {from Section 3, it equals $H_A(n_A|\bar{n}) - H_A(\bar{n}_A|\bar{n})$ [resp. $H_A(n_A|\tilde{n}) - H_A(\tilde{n}_A|\tilde{n})$] with a suitable n_A corresponding to λ}. In this evaluation we disregarded the terms that follow from standard low-temperature cluster expansions applied to the (+) phase in the region above λ, to the (−) phase below λ, and to the partition function $Z_V(\sigma^+)$. These terms would eventually lead to an error of order $|\pi(V)|\, e^{-\beta J_0}$, which is compatible with our claim. Now, mimicking the standard treatment given in Refs. 17, 15, and 26, we may consider those parts of the interface λ that are locally [over an elementary square (resp. triangle) of the projection $\pi(V)$] not of the SOS type as excitations—walls, in the terminology of the works just quoted. The remaining parts of λ are surfaces of an SOS type and play the role of the ceilings of Refs. 17, 15, and 26. The idea, then, is that for introducing a wall one pays by an energy proportional to its area [compared with $H_V(\bar{\sigma}_V|\bar{\sigma})$], a fact that would with not much effort finally lead to an estimate of the order $|\pi(V)|\, e^{-\beta J_0}$. The only obstacle is that, even though when introducing a wall one certainly loses in energy, one may gain in entropy at the same time. Namely, let us consider, for instance, an interface λ corresponding to the configuration $\bar{\sigma}^{(110)}$. Such an interface λ is completely inflexible in the sense that keeping it fixed outside some region, it has only one prolongation inside compatible with the SOS conditions. One may however, consider a wall, the projection of which has the form of a crown, joining this inflexible interface with the region inside the wall made of interfaces of type (1, 0, 0) with their rich flexibility within SOS configurations. The gain of entropy is proportional to the area of the inside region, while the loss of energy linked with the considered wall corresponds to its area which may be in principle only of the order of the boundary of the inside region. One may however argue that a wall joining the horizontal inside with the steeply inclined outside have necessarily an area proportional to the area of its interior and thus the gain in entropy will not overweight the loss of energy following the introduction of a wall. However the evaluations involved may be quite tricky and we shall not attemt here to present a complete proof.

Supposing the validity of the above conjecture, we shall now briefly discuss the Wulf plot and the corresponding equilibrium crystal shape. The interface free energy is approximated by

$$e(k) - (1/\beta)\, \omega(k)\, p^{\mathrm{SOS}}(k)$$

where (provided that the limits exist) for $k_2 + k_3 \leqslant k_1$ it is

$$p^{\mathrm{SOS}}(k) = \lim_{A \uparrow \mathbb{S}} (1/|A|) \log[e^{2\alpha N(A)} Z_A^{B,\alpha}(\bar{n}^{(k)})]$$

and we put $e(k) = e^{J=0}(k)$, and for $k_2 + k_3 \geqslant k_1$ it is

$$p^{\mathrm{SOS}}(k) = \lim_{\Lambda \uparrow \mathbb{T}} (1/|\Lambda|) \log Z_{\Lambda}^{T,0}(\tilde{n}^{(k)})$$

The function $p^{\mathrm{SOS}}(k)$ may further be rewritten. Considering the above two cases separately, we have the following results.

First Case: For $k_2 + k_3 \leqslant k_1$. Using the equivalence of the BCSOS model with the six-vertex model,[5] one gets

$$p^{\mathrm{SOS}}(k) = 2p_{6\mathrm{v}}^{\alpha}(x, y)$$

Here,

$$p_{6\mathrm{v}}^{\alpha}(x, y) = \lim[1/|N(\Lambda)] \log Z_{\Lambda,6\mathrm{v}}^{\alpha}(x, y)$$

and $N(\Lambda)$ denotes the number of lattice sites in Λ [i.e., $N(\Lambda) = N_s(\Lambda) = 2\,|\Lambda|$], $Z_{\Lambda,6\mathrm{v}}^{\alpha}(x, y)$ is the (canonical) partition function of the six-vertex model with the weights $w_1 = w_2 = w_3 = w_4 = 1$ and $w_5 = w_6 = e^{2\alpha}$, and the polarizations x and y (defined as the difference between the number of up and down arrows divided by the number of all arrows along the respective axes of the six-vertex model) are those that correspond to the configuration $\bar{n}^{(k)}$.[7] Realizing that x and y equal the height increments of the plane $kx = 0$ above the plane $x_1 = 0$ along the sides of elementary squares of the lattice $\mathbb{S}$, we get

$$x = (k_2 + k_3)/k_1, \qquad y = (k_2 - k_3)/k_1$$

The surface tension is thus approximated by

$$8k_1 J_0 - (2k_1/\beta)\, p_{6\mathrm{v}}^{\alpha}(x, y)$$

(By symmetry these formulas may also be extended to other regions of k.) The parameter Δ considered in the six-vertex theory takes the value $\Delta = \frac{1}{2}(2 - e^{4\alpha})$ and thus for $\alpha > \alpha_R$ we have $\Delta < -1$. Then there is a conical singularity at $x = y = 0$ (Ref. 28, Section 6). It corresponds to $k = (1, 0, 0)$ and leads, via the Wulf construction, to the existence of the facet (100). See Ref. 24 for a more detailed discussion, including a computation of the shape of the boundary of this facet. If $\alpha < \alpha_R$, then $\Delta \in (-1, 1)$ and the facet (100) disappears (see Fig. 1 for a schematic view). Adapting the computation of the shape of the (111) facet for the fcc model from Ref. 25, which corresponds here to the point $x = y = 1$, one might study the shape of the (110) facets in our case.

[7] In the following we shall disregard certain problems, such as the very existence of the limit defining $p_{6\mathrm{v}}^{\alpha}$ (cf. Ref. 27, Section III.C) and rely on results announced in Ref. 28.

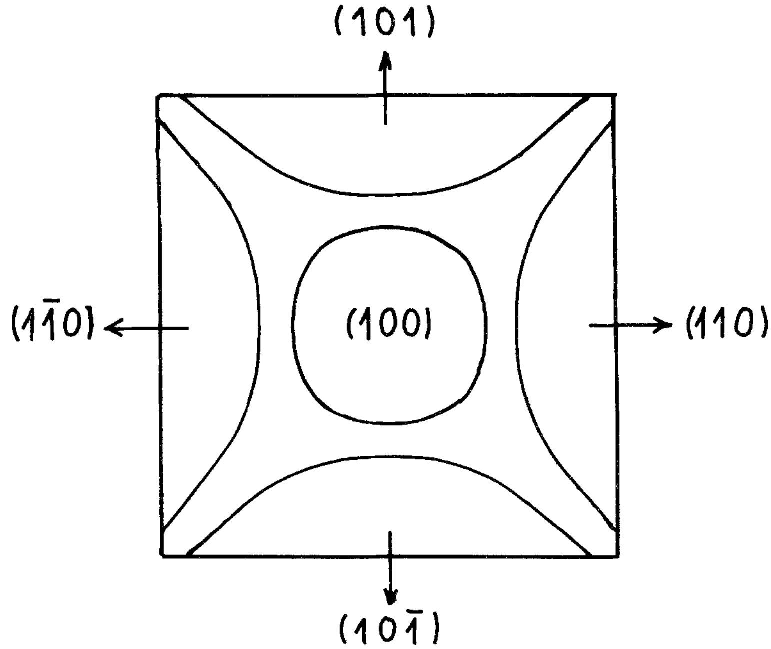

Fig. 1. The crystal viewed along the (100) direction. The central facet is the (100) facet, which disappears when the temperature T grows over $T_R(J)$ ($\sim J/\alpha_R$), while the four remaining facets are of type (110). The areas where the four facets of type (110) meet the facet (100) are rounded for $T>0$.

Second Case: For $k_2+k_3 \geqslant k_1$. The function $p^{\text{SOS}}(k)$ is now given in terms of the TISOS model.[6,7] There are three (not independent) polarizations

$$x=\tfrac{2}{3}[1-3k_1/(k_1+k_2+k_3)]$$

$$y=\tfrac{2}{3}[1-3k_2/(k_1+k_2+k_3)]$$

$$z=\tfrac{2}{3}[1-3k_3/(k_1+k_2+k_3)]$$

which for $k_2+k_3 \geqslant k_1$ fall into the interval $(-1/3, 2/3)$. The exact solution of Nienhuis *et al.*[7] is, however, not formulated in terms of the polarizations; the authors introduce three conjugate "electric fields" instead, and consider the Legendre transformation of the model, which is directly linked with the equilibrium shape of the crystal.[29] We shall not be concerned with detailed calculations and we only present a schematic view along the axis (111) of the resulting crystal (Fig. 2).

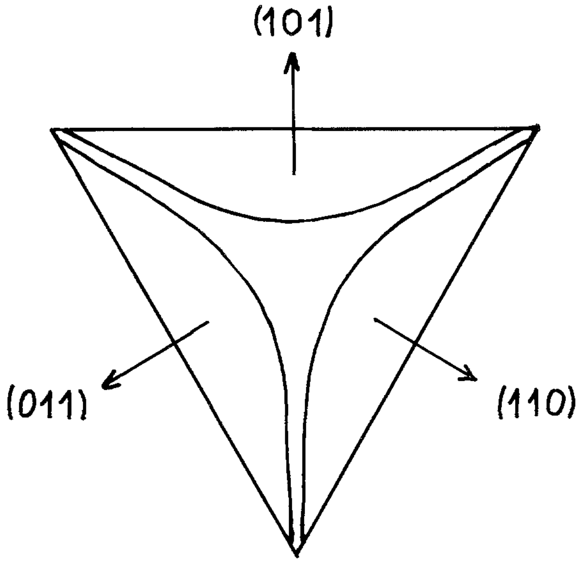

Fig. 2. The crystal viewed along the (111) direction. The area around this direction where the three facets of type (110) meet is rounded for $T > 0$.

Finally, let us notice that in both figures, the same facets of type (110) appear. One could thus in principle compare their shape calculated, in the considered approximation, with the help of the BCSOS[25] and the TISOS[7] models.

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NOTE ADDED IN PROOF

We have recently learned that Miekisz[30] has found a counterexample to the Dobrushin–Shlosman conjecture. However, this counterexample does not seem to be related to the models discussed in this paper.

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