Centre de Physique Théorique*- CNRS - Luminy, Case 907
F–13288 Marseille Cedex 9 - France

SURFACE TENSION, STEP FREE ENERGY AND FACETS IN THE EQUILIBRIUM CRYSTAL

Salvador Miracle-Sole

Abstract

Some aspects of the microscopic theory of interfaces in classical lattice systems are developed. The problem of the appearance of facets in the (Wulff) equilibrium crystal shape is discussed, together with its relation with the discontinuities of the derivatives of the surface tension $\tau(\mathbf{n})$ (with respect to the components of the surface normal $\mathbf{n}$) and the role of the step free energy $\tau^{\text{step}}(\mathbf{m})$ (associated to a step orthogonal to $\mathbf{m}$ on a rigid interface). Among the results are, in the case of the Ising model at low enough temperatures, the existence of $\tau^{\text{step}}(\mathbf{m})$ in the thermodynamic limit, the expression of this quantity by means of a convergent cluster expansion, and the fact that $2\tau^{\text{step}}(\mathbf{m})$ is equal to the value of the jump of the derivative $\partial\tau/\partial\theta$ (when θ varies) at the point $\theta = 0$ (with $\mathbf{n} = (m_1 \sin\theta, m_2 \sin\theta, \cos\theta)$). Finally, using this fact, it is shown that the facet shape is determined by the function $\tau^{\text{step}}(\mathbf{m})$.

Key-Words : Surface tension, step free energy, crystal shapes, roughening transition, Wulff construction.

October 1994
CPT-94/P.3083

anonymous ftp or gopher : cpt.univ-mrs.fr

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* Unité Propre de Recherche 7061

1. Introduction

It is known that the equilibrium shape of a crystal is obtained, according to the thermodynamic theory, by minimizing the total surface free energy associated to the crystal-medium interface, and that this shape is given by the Wulff construction, provided one knows the anisotropic surface tension (or interfacial free energy per unit area). It is therefore important, even if a microscopic derivation of the Wulff construction within Statistical Mechanics has been proved only for some two-dimensional lattice models (see the recent work by Dobrushin *et al.* [1]), to study the properties of the surface tension $\tau(\mathbf{n})$, as a function of the unitary vector $\mathbf{n}$ which specifies the orientation of the interface, with respect to the crystal axes. A first analysis on this subject was reported in Ref. 2. It is the object of the present work to pursue this study and, in particular, to discuss the problem of the appearance of plane facets in the equilibrium crystal shape. For this purpose several aspects of the microscopic theory of interfaces are developed, and another important quantity in this theory, the step free energy, is investigated.

Background. A standard way to define the surface tension between two coexisting phases, in a classical lattice system, is to consider particular boundary conditions which enforce, inside a given volume, an interface orthogonal to the vector $\mathbf{n}$. One expects that the thermodynamic limit $\tau(\mathbf{n})$, of the interfacial free energy per unit area, exits, and that (as a function of $\mathbf{n}$) it satisfies the pyramidal inequality. A proof of these facts, under appropriate assumptions, was given in Ref. 2. Let us mention that the pyramidal inequality, introduced in Ref. 1 for the two-dimensional Ising model, was conjectured to hold true in very general situations, from thermodynamic arguments, in Ref. 3. It is equivalent (as shown in Ref. 2) to the convexity of the function $f(\mathbf{x}) = |\mathbf{x}|\tau(\mathbf{x}/|\mathbf{x}|)$, for any vector $\mathbf{x}$.

The step free energy plays, also, an important role in the problem under consideration. It is defined (again using the appropriate boundary conditions) as the free energy (per unit length) associated with the introduction of a step of height 1 on the interface, and can be regarded as an order parameter for the roughening transition.

Let us consider, as an illustrative example, the Ising ferromagnet in $d = 3$ dimensions. At a low temperature $T > 0$ we expect the interface orthogonal to the direction $\mathbf{n}_0 = (0, 0, 1)$, which is flat at $T = 0$, to be modified by deformations (called walls). The corresponding Gibbs probability of interfaces may be interpreted as a "gas of deformations", a certain two-dimensional system for these walls. Using the Peierls method, Dobrushin [4] proved the dilute character of this gas at low temperatures, which means that the interface is essentially flat (or rigid). Furthermore, cluster expansion techniques have been applied by Bricmont *et al.* [5], to study the surface tension $\tau(\mathbf{n}_0)$ and the interface structure (see also Ref. 6).

It is believed, that at higher temperatures, but before reaching the critical temperature T_c, the fluctuations of the considered interface become unbounded when the volume tends to infinity. The interface undergoes a roughening phase transition at a temperature $T = T_R$. Approximate methods, used by Weeks *et al.* [7], suggest $T_R \sim 0.53\ T_c$, a temperature slightly higher then $T_c^{d=2}$ (the critical temperature of the two-dimensional Ising model), and actually van Beijeren [8] proved, using correlation inequalities, that $T_R \geq T_c^{d=2}$. The analogous result for the step free energy, i. e., that $\tau^{\text{step}} > 0$ if $T < T_c^{d=2}$, was proved in Ref. 9, as well as that $\tau^{\text{step}} = 0$ if $T \geq T_c$. Since then, however, it appears to be no proof of the fact that $T_R < T_c$. At present one is able to study rigorously the roughening transition only for some simplified models of the interface. Thus, Fröhlich and Spencer [10] have proved this transition for the SOS (solid-on-solid) model, and several restricted SOS models, which are exactly solvable, have also been studied in this context (these models are reviewed in Refs. 11 and 12).

The roughness of an interface should be apparent when considering the shape of the equilibrium crystal associated with the system. One knows that a typical equilibrium crystal at low temperatures has smooth plane facets linked by rounded edges and corners. The area of a particular facet decreases as the temperature is raised and the facet finally disappears at a temperature characteristic of its orientation. The reader will find information and references on equilibrium crystals in the review articles Refs. 11, 12, 13 and 14.

It can be argued, as discussed below, that the roughening transition corresponds to the disappearance of the facet whose orientation is the same as that of the considered interface. The exactly solvable SOS models mentioned above, for which the function $\tau(\mathbf{n})$ has been computed, are interesting examples of this behaviour (this subject has been reviewed in Ref. 12, Chapter VII). For the three-dimensional Ising model, Bricmont *et al.* [15] have proved a correlation inequality which establish τ^{step} as a lower bound to the one-sided derivative $\partial\tau(\theta)/\partial\theta|_{\theta=0^+}$, where $\tau(\theta) = \tau(0, \sin\theta, \cos\theta)$. Thus $\tau^{\mathrm{step}} > 0$ implies a kink in $\tau(\theta)$ at $\theta = 0$ and, according to the Wulff construction, a facet is expected.

In fact, it is believed that τ^{step} should be equal to this derivative, and we shall return to this question below. This is reasonable, since the increment in surface tension of an interface tilted by an angle θ, with respect to the surface tension of the rigid interface, can be approximately identified, for θ small, with the free energy of a “gas of steps” (the density of the steps being proportional to θ). And, again, if the interaction between the steps can be neglected, the free energy of this gas can be approximated by the sum of the individual free energies of the steps.

Outline of the present work. In Section 2, some macroscopic properties of the equilibrium crystal shape, given by the Wulff construction, are discussed. We assume that the surface tension satisfies the pyramidal inequality (to be defined in Section 2, equation 3). We prove (Theorem 1) that a facet orthogonal to the direction $\mathbf{n}_0$ appears in the Wulff equilibrium crystal shape if, and only if, the derivative $\partial\tau(\theta,\phi)/\partial\theta$ is discontinuous at the point $\theta = 0$, for all ϕ. Here, the function $\tau(\mathbf{n}) = \tau(\theta,\phi)$ is expressed in terms of the spherical coordinates $0 \le \theta \le \pi$, $0 \le \phi \le 2\pi$ of $\mathbf{n}$, the vector $\mathbf{n}_0$ being taken as the polar axis. Moreover, the one-sided derivatives $\partial\tau(\theta,\phi)/\partial\theta$, at $\theta = 0^+$ and $\theta = 0^-$, exist, and determine the shape of the facet.

In Section 3 we introduce the microscopic theory. The surface tension and the step free energy are defined in the case of a classical lattice gas. Some previous results, based mainly on correlation inequalities, are reviewed and extended. Theorems 2 and 4 concern the properties of the two quantities just mentioned, and Theorem 3 is about the result quoted from Ref. 15. It is clear, from Theorem 1, that the quoted correlation inequality is a sufficient condition for the formation of a facet in the Ising model, if

$\tau^{\text{step}} > 0$. Several applications and examples are discussed at the end of the Section.

In Sections 4, cluster expansions techniques for studying the step free energy at low temperature are developed. For the Ising ferromagnet at $T = 0$, the step parallel to a lattice axis, on the rigid interface orthogonal to $\mathbf{n}_0 = (0, 0, 1)$, is a perfectly rectilinear step of height 1. At a low temperature $T > 0$ we expect some deformations to appear, connected by straight portions of height 1. The step structure, in the corresponding Gibbs state, can then be described as a one-dimensional "gas" of these deformations (to be called step-jumps), which mutually interact through the effect of the rest of the system. This description, somehow similar to the description of the interface of the two-dimensional Ising model used by Gallavotti [16], is valid, in fact, for any orientation of the step, defined by the vector $\mathbf{m} = (\cos\phi, \sin\phi)$ on the plane of the rigid interface. It can be seen that the gas of deformations is a dilute gas at low temperatures and can, also, be studied by using cluster expansion techniques.

As a consequence of this analysis we show that the step free energy per unit length, $\tau^{\text{step}}(\mathbf{m})$, exists in the thermodynamic limit (a question that could not be solved with correlation inequalities), and satisfies the pyramidal inequality in its strict form, provided that the temperature is low enough. Moreover, the step free energy, $\tau^{\text{step}}(\mathbf{m})$, can be expressed in terms of an analytic function of the temperature, for which a convergent series expansion is found (Theorems 5 and 6).

Finally, we study the statistical mechanics of the "gas of steps" which appears in the description of an interface titled by a very small angle with respect to the rigid interface. We consider the three dimensional Ising model at sufficiently low temperature, and apply the results of Section 4 on the step structure. The heuristic argument about the free energy of such interfaces, explained above, can be developed into a proof of the following relation

$$\partial\tau(\theta, \phi)/\partial\theta|_{\theta=0^+} = \tau^{\text{step}}(\phi) \tag{1}$$

This is the content of Theorem 7 in Section 5. This relation, together with Theorem 1, implies that one obtains the shape of the facet by means of the two-dimensional Wulff construction applied to the step free energy $\tau^{\text{step}}(\mathbf{m})$. The facet has a smooth boundary without straight segments.

The results mentioned in the last paragraph are stated in Section 5. Section 6 is devoted to the proof of Theorem 7.

For the reader's convenience we include an Appendix with a brief account of low temperature expansions. Notice that one needs the cluster expansion, in terms of walls, for the rigid interface, in order to describe the interaction between the step jumps and to study the step structure and the associated cluster expansion.

2. Macroscopic properties

According to the Wulff construction, the equilibrium shape of a crystal is given by

$$\mathcal{W} = \{ \mathbf{x} \in I\!\!R^d \ : \ \mathbf{x} \cdot \mathbf{n} \le \tau(\mathbf{n}) \} \tag{2}$$

where the inequality is assumed for each unit vector $\mathbf{n} \in I\!\!R^d$ and $\tau(\mathbf{n})$ is the surface tension of the interface orthogonal to $\mathbf{n}$. One obtains in this way the shape which has the minimum surface free energy for a given volume. Being defined as the intersection of closed half-spaces, $\mathcal{W}$ is a closed bounded convex set (i. e., a convex body) and, since $\tau(\mathbf{n}) = \tau(-\mathbf{n})$, it has a centre at the origin.

Let $A_0, \ldots, A_d \ \in \ I\!\!R^d$ be any set of $d+1$ points in general position and, for $i = 0, \ldots, d$, let Δ_i be the $(d-1)$-dimensional simplex defined by all points $A_0, \ldots, A_d$, except A_i. Let $\mathbf{n}_i$ be the unit vector orthogonal to Δ_i and $|\Delta_i|$ the $(d-1)$-dimensional area of Δ_i. Following Ref. 3 we say that $\tau(\mathbf{n})$ satisfies the *pyramidal inequality* if

$$|\Delta_0| \, \tau(\mathbf{n}_0) \le \sum_{i=1}^{d} |\Delta_i| \, \tau(\mathbf{n}_i) \tag{3}$$

for any set $A_0, \ldots, A_d$. We introduce the function on $I\!\!R^d$ defined by

$$f(\mathbf{x}) = |\mathbf{x}| \, \tau(\mathbf{x}/|\mathbf{x}|) \tag{4}$$

It was proved in Ref. 2 that the pyramidal inequality for $\tau(\mathbf{n})$ is equivalent to the condition that $f(\mathbf{x})$ is a *positively homogeneous convex* function. This means that

$$f(\alpha \mathbf{x}) = \alpha f(\mathbf{x}) \tag{5}$$

$$f(\mathbf{x} + \mathbf{y}) \le f(\mathbf{x}) + f(\mathbf{y}) \tag{6}$$

for any $\alpha > 0$ and any $\mathbf{x}$ and $\mathbf{y}$ in $I\!R^d$. Since $\tau(\mathbf{n})$ is bounded, the convex function $f(\mathbf{x})$ is everywhere finite and hence, Lipschitz continuous.

The pyramidal inequality may be interpreted as a thermodynamic stability condition and thus also the convexity of $f(\mathbf{x})$. If one supposes that $|\Delta_0|\,\tau(\mathbf{n}_0)$ is greater than the right hand side of inequality (3) this would make the interface bounded by the sides of Δ_0 unstable and difficult to realize.

Some consequences of properties (3), (5) and (6) have already been discussed in Refs. 1, 2 and 3. Let us mention that among the functions which through (2) define the same shape $\mathcal{W}$, there is a unique $\tau(\mathbf{n})$ which satisfies the pyramidal inequality. Moreover, see Ref. 2, it turns out that $f(\mathbf{x})$ is the Minkowski's support function of the convex body $\mathcal{W}$ (i. e., $f(\mathbf{x}) = \sup_{\mathbf{y}\in\mathcal{W}}\ \mathbf{x}\cdot\mathbf{y}$).

Other consequences of the convexity properties, which will next be discussed, concern the formation of facets in the equilibrium crystal. The facets of a crystal have certain particular orientations. Let $\mathbf{n}_0$ be one of the corresponding normals and place the coordinate axes $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ in such a way that $\mathbf{n}_0 = (0, 0, 1)$.

Theorem 1. *Consider the surface tension $\tau(\mathbf{n})$ in dimension $d = 3$, and write $\tau(\theta, \phi) = \tau(\mathbf{n})$ for $\mathbf{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. Assume that, using (4), $\tau(\mathbf{n})$ extends by positive homogeneity to a convex function on $I\!R^3$. Then, the following one-sided derivative, exists*

$$\mu(\phi) = (\partial/\partial\theta)_{\theta=0^+}\ \tau(\theta, \phi) \tag{7}$$

and, as a function $\mu(\mathbf{m})$ of the unit vector $\mathbf{m} = (\cos\phi, \sin\phi)$, extends by positive homogeneity to a convex function on $I\!R^2$. Moreover, if $\mu(\phi+\pi) \neq -\mu(\phi)$, then the equilibrium crystal presents a facet, perpendicular to the (0,0,1) direction, whose shape is given by

$$\mathcal{F} = \left\{\mathbf{x} \in I\!R^2\ :\ \mathbf{x}\cdot\mathbf{m} \leq \mu(\mathbf{m})\right\} \tag{8}$$

i. e., by the Wulff construction applied to μ.

Proof. In terms of the function f defined by (4), the Wulff shape (2) is the set of all $\mathbf{x} \in I\!R^3$ such that

$$x_1y_1 + x_2y_2 + x_3y_3 \leq f(\mathbf{y}) \tag{9}$$

for all $\mathbf{y}$. The plane $x_3 = \tau(0)$, where $\tau(0)$ is the value of τ for $\theta = 0$, is a tangent plane to $\mathcal{W}$. The facet $\mathcal{F}$ is the portion of this plane contained in $\mathcal{W}$. These facts follow from the convexity of f, which implies that f is the support function of $\mathcal{W}$ (otherwise, for a general τ, it could happen that the plane does not touch this set). According to (9), the facet $\mathcal{F}$ consists of the points $(x_1, x_2, \tau(0)) \in I\!R^3$ such that

$$x_1 y_1 + x_2 y_2 \leq f(y_1, y_2, y_3) - y_3 \tau(0) = f(y_1, y_2, y_3) - y_3 f(0, 0, 1)$$

for all $\mathbf{y}$. Or, equivalently, such that

$$x_1 y_1 + x_2 y_2 \leq f^{\mathrm{s}}(y_1, y_2) = \inf_{y_3} \left[f(y_1, y_2, y_3) - y_3 f(0, 0, 1) \right] \tag{10}$$

Restricting the infimum to $y_3 = 1/\lambda \geq 0$ and using the positive homogeneity and the convexity of f one obtains

$$g(y_1, y_2) = \lim_{\lambda \to 0, \lambda \geq 0} (1/\lambda) \left[f(\lambda y_1, \lambda y_2, 1) - f(0, 0, 1) \right] \tag{11}$$

Formula (11) implies that g is positively homogeneous and, taking into account the convexity of f, that g is a convex function on $I\!R^2$. Define

$$\mu(\phi) = g(\cos\phi, \sin\phi) \tag{12}$$

From (11) and taking $\lambda = \tan\theta$, one gets

$$\begin{aligned} \mu(\phi) &= \lim_{\theta \to 0, \theta \geq 0} (1/\sin\theta) \left[f(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) - \cos\theta f(0, 0, 1) \right] \\ &= \lim_{\theta \to 0, \theta \geq 0} (1/\theta) \left[\tau(\theta, \phi) - \tau(0) \right] \end{aligned}$$

and therefore the stated expression (7). This, together with the properties of g and definition (12), proves the first part of the Theorem.

To prove the second part, observe that, because of definition (12), condition (10) is equivalent to (8), which gives the facet shape. On the other side, from the convexity of g, it follows that

$$-\mu(-\mathbf{m}) \leq \mu(\mathbf{m}) \tag{13}$$

Thus, the hypothesis $\mu(\phi+\pi) \neq -\mu(\phi)$ implies the strict inequality in (13) and shows, using (8), that the convex set $\mathcal{F}$ has a non-empty interior. This ends the proof of the Theorem.

Remark 1. It is enough to know that the condition $\mu(\phi+\pi) \neq -\mu(\phi)$, is satisfied for two different directions ϕ to conclude that $\mathcal{F}$ has a non-empty interior, i. e., that it is a facet. Then, in fact, the strict inequality in (13) holds for any $\mathbf{m}$, because of the convexity of g. There are two other possibilities for the set $\mathcal{F}$, considered as the intersection of $\mathcal{W}$ and the tangent plane $x_3 = \tau(0)$. Observe that $-\mu(-\mathbf{m})$ coincides with the left derivative of the surface tension, i. e.,

$$\mu(-\mathbf{m}) = \mu(\phi_0+\pi) = -(\partial/\partial\theta)_{\theta=0^-}\tau(\theta,\phi)$$

Therefore, if $\tau(\theta,\phi)$, has a continuous derivative with respect to θ, at $\theta = 0$, for some $\phi = \phi_0$, then, the set $\mathcal{F}$ reduces to a segment. It reduces to a point if this derivative exists for any ϕ.

Remark 2. If $\tau(\theta,\phi) = \tau(\pi-\theta,\phi)$ the crystal shape is reflection symmetric with respect to the plane $x_3 = 0$. Then $\mu(\mathbf{m}) = \mu(-\mathbf{m})$ and the facet $\mathcal{F}$ has a centre at the point $P_0 = (0,0,\tau(0))$. In the general case, however, the point P_0 is not the centre of the facet. P_0 can also be outside $\mathcal{F}$ and in this case the range of $\mu(\mathbf{m})$ includes positive and negative values.

3. Microscopic theory: Some definitions and results

We consider a lattice spin system on a three-dimensional regular lattice $\mathcal{L}$, with configuration space $\Omega = \{-1,1\}^{\mathcal{L}}$. For any $A \subset \mathcal{L}$ we write $\sigma(A) = \prod_{i\in A}\sigma(i)$, where $\sigma(i)$ is the spin at the site i. The interaction is a real valued function on the finite subsets of $\mathcal{L}$. The energy of a configuration $\sigma_\Lambda = \{\sigma(i)\}, i \in \Lambda$, in a finite subset $\Lambda \subset \mathcal{L}$, under the boundary condition $\bar\sigma \in \Omega$, is

$$H_\Lambda(\sigma_\Lambda \mid \bar\sigma) = -\sum_{A\cap\Lambda\neq\emptyset} J(A)\sigma(A) \qquad (14)$$

where $\sigma(i) = \bar{\sigma}(i)$ if $i \notin \Lambda$. The partition function, at the inverse temperature β, is given by

$$Z^{\bar{\sigma}}(\Lambda) = \sum_{\sigma_\Lambda} \exp\,[-\beta H_\Lambda(\sigma_\Lambda \mid \bar{\sigma})]. \tag{15}$$

We assume that J is an even, finite range, translation invariant and ferromagnetic interaction, i. e., $J(A) = 0$ if A has an odd number of sites or if its diameter is larger than some give length, $J(A) = J(A + \alpha)$ for all $\alpha \in \mathcal{L}$, and $J(A) \geq 0$.

We consider the case in which two distinct thermodynamic phases $(+)$ and $(-)$ coexist at the inverse temperature β. This means two extremal translation invariant Gibbs states, associated to the ground configurations $(+)$ and $(-)$, for which $\bar{\sigma}(i) = 1$ and $\bar{\sigma}(i) = -1$ for all $i \in \mathcal{L}$. They correspond to the limits, when $\Lambda \to \infty$, of the finite volume Gibbs measures $Z^{\bar{\sigma}}(\Lambda)^{-1} \exp\,[-H_\Lambda(\sigma_\Lambda \mid \bar{\sigma})]$ with the boundary conditions $\bar{\sigma}$ respectively equal to $(+)$ and $(-)$.

Consider a parallelepiped Λ of sides L_1, L_2, L_3, parallel to the axes and centred at the origin of $\mathcal{L}$. Let $\mathbf{n} = (n_1, n_2, n_3)$ be a unit vector in $\mathbb{R}^3$ such that $n_3 > 0$, $p_{\mathbf{n}}$ the plane orthogonal to $\mathbf{n}$ and passing through the centre of Λ, and $S_{\mathbf{n}}(\Lambda)$ the area of the portion of this plane contained inside Λ. Introduce the mixed boundary conditions $(\pm, \mathbf{n})$ for which $\bar{\sigma}(i) = +1$ if i is above the plane $p_{\mathbf{n}}$, i. e., if $i \cdot \mathbf{n} \geq 0$, and $\bar{\sigma}(i) = -1$ if $i \cdot \mathbf{n} < 0$. The *surface tension* associated to the interface orthogonal to $\mathbf{n}$ is defined by

$$\tau(\mathbf{n}) = \lim_{L_1, L_2 \to \infty} \lim_{L_3 \to \infty} -\frac{1}{\beta S_{\mathbf{n}}(\Lambda)} \ln \frac{Z^{(\pm, \mathbf{n})}(\Lambda)}{Z^{+}(\Lambda)} \tag{16}$$

Such a definition is justified by noticing that in (16) the volume contributions proportional to the free energy of the coexisting phases, as well as the boundary effects, cancel, and only the contributions to the free energy of the interface are left.

The boundary conditions $(\pm, \mathbf{n})$ enforce an interface inside the box Λ. However, with a probability distribution given by the Gibbs measure $Z^{(\pm, \mathbf{n})}(\Lambda)^{-1} \exp\,[-H_\Lambda(\sigma_\Lambda \mid \pm, \mathbf{n})]$, this interface may undergo large fluctuations, so that the corresponding Gibbs state in the thermodynamic limit is translation invariant. On the other side, for some particular directions $\mathbf{n}_0$, it is possible that the interface remains rigid at low temperatures and then, the boundary condition $(\pm, \mathbf{n}_0)$ yield indeed a non translation invariant Gibbs state. In this case, it is generally believed that at higher temperatures, but still before reaching the critical temperature β_c of the system, the interface does not stay rigid anymore. The system comes over the so-called *roughening* transition at a roughening inverse temperature $\beta_R > \beta_c$. There is a quantity, called the *step free energy*, which is expected to play, in the roughening transition, a similar role to that played by the surface tension in the phase transitions.

In order to define this quantity let us place the coordinate axes in such a way that $\mathbf{n}_0 = (0,0,1)$. Denote simply by $(\pm)$ the $(\pm, \mathbf{n}_0)$ boundary condition. Introduce the $(\text{step}, \mathbf{m})$, or simply (step), boundary conditions, associated to the unit vectors $\mathbf{m} = (\cos\phi, \sin\phi) \in \mathbb{R}^2$, by

$$\bar{\sigma}(i) = \begin{cases} 1 & \text{if } i > 0 \text{ or if } i_3 = 0 \text{ and } i_1 m_1 + i_2 m_2 \geq 0 \\ -1 & \text{otherwise} \end{cases} \tag{17}$$

The *step free energy*, for a step orthogonal to $\mathbf{m}$ (such that $m_2 \neq 0$), is

$$\tau^{\text{step}}(\phi) = \lim_{L_1\to\infty} \lim_{L_2\to\infty} \lim_{L_3\to\infty} -\frac{a\cos\phi}{\beta L_1} \ln \frac{Z^{\text{step}}(\Lambda)}{Z^{\pm}(\Lambda)} \tag{18}$$

where the constant a is the distance between the lattice layers orthogonal to $\mathbf{n}_0$.

Clearly, expression (18) represents the residual free energy due to the considered step, per unit length and unit height. Although, the steps orthogonal to $\mathbf{m}$ and $-\mathbf{m}$ have the same orientation, they are not identical (if one is "going up" the other is "going down") and, hence, the corresponding free energies, $\tau^{\text{step}}(\mathbf{m})$ and $\tau^{\text{step}}(-\mathbf{m})$, do not necessarily coincide.

We next review some results proved in Refs. 2, 9 and 15. First, it is shown that the surface tension exists and that it satisfies the stability condition considered in Section 2. The other results concern the step free energy and the facet formation.

Theorem 2. *Under the hypothesis of this Section, the surface tension $\tau(\mathbf{n})$, defined by limit (16), exists, and coincides with the infimum over L_1, L_2, L_3. Moreover, $\tau(\mathbf{n})$ is bounded, non negative and extends, through (4), to a positively homogeneous convex function on $\mathbb{R}^3$.*

Proof. These statements have been proved in Ref. 2 (Theorems 1 and 3) using Griffiths correlation inequalities.

Theorem 3. *In the case of two body attractive interactions, the one-sided angular derivative (7), of the surface tension and the step free energy (18), satisfy*

$$(\partial/\partial\theta)_{\theta=0^+}\ \tau(\theta,\phi) \geq \tau^{\text{step}}(\phi) \tag{19}$$

Proof. Inequality (19) was proved in Ref. 15 (Appendix 1) for the Ising model. With some small changes, needed for adapting it to our notations, the same proof applies to the present case. Let $Z^{\pm}(u)$, where u is a non-negative integer, be the partition functions $Z^{\bar\sigma}(\Lambda)$ associated to the boxes

$$\Lambda = \{i \in \mathcal{L} : 0 \leq i_1 m_1 - i_2 m_2 \leq L_1, 0 \leq i_1 m_1 + i_2 m_2 \leq L_2, -L_3 \leq i_3 \leq L_3\}$$

with $L_3 \geq au$, and to the boundary conditions $\bar\sigma(i) = 1$ if $p_u(i) \geq 0$, $\bar\sigma(i) = -1$ if $p_u(i) < 0$, where $p_u(i) = i_1 m_1 + i_2 m_2 + i_3 \tan\theta$ and $\tan\theta = au/L_2$. For the same Λ, let $Z_u^{\pm}(1)$ be the partition function associated to the boundary conditions $\bar\sigma(i) = 1$ if $i_3 \geq a(u-1)$ and $p_u(i) \geq 0$, $\bar\sigma(i) = -1$ otherwise, and let $Z_u^{\pm}(0)$ be that associated to the condition $\bar\sigma(i) = 1$ if $i_3 \geq a(u-1)$, $\bar\sigma(i) = -1$ if $i_3 < a(u-1)$. Following Ref. 15, we prove that

$$Z^{\pm}(u)/Z^{\pm}(u-1) \leq Z_u^{\pm}(1)/Z_u^{\pm}(0) \tag{20}$$

Observe that if we change, in the right hand side of this expression, the boundary spins $\bar\sigma(i) = 1$ for $i_3 \geq u-1$, into $\bar\sigma(i) = -1$ we obtain the left hand side. As a consequence of Fortuin-Kasteleyn-Ginibre inequalities, the ratio of partition functions increases and thus, inequality (20) follows. From it we get

$$Z^{\pm}(u)/Z^{\pm}(0) \leq \prod_{v=1}^{u} [Z_v^{\pm}(1)/Z_v^{\pm}(0)] \tag{21}$$

We take logarithms in both sides of (21), multiply by $-(1/\beta)(\cos\theta/L_1 L_2)$ and let L_1, L_2 and L_3 tend to infinity. Noticing that $-(a/\beta L_1)\ln[Z_v^{\pm}(1)/Z_v^{\pm}(0)]$ should then tend to τ^{step} (see also Remark 4 below), we obtain

$$\tau(\theta,\phi) - \tau(0) \geq \sin\theta\ \tau^{\text{step}}(\phi)$$

for $\theta \geq 0$, from which the stated inequality (19) follows. The Theorem is proved.

From Theorem 2 it follows that the conditions on the surface tension, needed in Theorem 1, are satisfied. Then, if $\tau^{\text{step}}(\mathbf{m})$ is strictly larger than $-\tau^{\text{step}}(-\mathbf{m})$, Theorem 3 can be applied to show the existence of a facet orthogonal to $\mathbf{n}_0$ in the equilibrium crystal.

The next Theorem concerns the case in which the system is reflection symmetric with respect to the plane $x_3 = 0$. In this case, $\tau^{\text{step}}(\mathbf{m}) = \tau^{\text{step}}(-\mathbf{m})$ and, taking inequality (19) into account, a facet is formed if $\tau^{\text{step}}(\mathbf{m}) > 0$.

Theorem 4. *Consider the case of two body interactions and, for $i = (i_1, i_2, i_3)$, let $i' = (i_1, i_2, -i_3)$. Assume that $J(i,j) \geq 0$, $J(i,j) = J(i',j')$ and that $J(i,j) \geq J(i,j')$ for $i_3, j_3 \geq 0$. Then,*

$$\tau^{\text{step}}(\mathbf{m}) \geq \tau_{d=2}(\mathbf{m}) \tag{22}$$

where $\tau_{d=2}(\mathbf{m})$ is the surface tension of the two dimensional system on the sublattice $i_3 = 0$, interacting through the same $J(i,j)$ restricted to this sublattice.

Proof. Inequality (22) was proved in Ref. 9 (Section 6.2) for the Ising model. The following proof, nearer to the method of Ref. 8, uses only Lebowitz inequalities of the first kind. Let $\sigma'(i)$ be the spin variables for the system restricted to the two-dimensional box $Q = \{i \in \Lambda : i_3 = 0\}$ and associate with every $i \in \Lambda$, with $i_3 \geq 0$, the spin variables $s(i)$ and $t(i)$ defined by

$$\begin{cases} s(i) = \sigma(i) + \sigma(i'), \quad t(i) = \sigma(i) - \sigma(i'), \quad \text{if } i_3 > 0 \\ s(i) = \sigma(i) + \sigma'(i), \quad t(i) = \sigma(i) - \sigma'(i), \quad \text{if } i_3 = 0 \end{cases}$$

Rewriting the products $Z_1 = Z^{\pm}(\Lambda) Z^{(\pm,\mathbf{m})}(Q)$ and $Z_2 = Z^{\text{step}}(\Lambda) Z^{+}(Q)$ as two partition functions in terms of these new variables, the first Lebowitz inequalities can be applied to show that $Z_1 \geq Z_2$, or, equivalently, that

$$Z^{\text{step}}(\Lambda)/Z^{\pm}(\Lambda) \leq Z^{(\pm,\mathbf{m})}(Q)/Z^{+}(Q)$$

This shows the validity of inequality (22).

Remark 3. The above method can also be used to show the non translation invariance of the Gibbs state associated to the $(\pm)$ boundary conditions, at low temperatures, and the rigidity of the corresponding interface (Ref. 5, Part II, Appendix B).

Remark 4. Similar arguments to those used in the proof of Theorem 4 show that $Z^{\text{step}}(\Lambda)/Z^{\pm}(\Lambda)$ is, under the same conditions, an increasing function of L_3 and L_2. and, therefore, that the first two limits in the definition (18) of τ^{step}, exist. The same increasing property holds for non centred boxes, provided that one is included inside the other (like those used in the proof of Theorem 3).

Finally, we comment on some applications of these results.

Example 1. Let us consider the simple cubic lattice gas model (Ising model) with nearest neighbour attractions. At zero temperature, the Wulff crystal shape of this model presents 6 facets of type (001). In fact, one sees that, for $\mathbf{n}_0 = (0, 0, 1)$, the conditions of Theorem 4 are satisfied. Hence $\tau^{\text{step}}(\mathbf{m}) > 0$ for all $\beta > \beta_{c,d=2}$ (the critical inverse temperature of the two-dimensional model), since then $\tau_{d=2}(\mathbf{m}) > 0$. Indeed, one believes that $\tau^{\text{step}}(\mathbf{m}) > 0$ for all temperatures below the roughening transition point. This last inequality, according to Theorems 1 and 3, shows the existence of a facet orthogonal to the direction $\mathbf{n}_0$.

Example 2. The Wulff crystal shape of the body centred cubic lattice gas model, with nearest neighbour and next nearest neighbour attractions presents, at low temperatures, 6 facets of type (100) and 12 facets of type (110). These facts follow, as above, from Theorems 1 to 4. A discussion on the roughening transition in this model may be found in Ref. 17.

Example 3. The last example is the simple cubic lattice gas model with nearest neighbour and next nearest neighbour attractions discussed in Refs. 13 and 18. The Wulff crystal shape of this model presents, at zero temperature, 6 facets of type (100), 12 facets of type (110) and 8 facets of type (111). The existence, at low temperatures, of the first and second kind of facets can be proved as before, although for $\mathbf{n}_0 = (1, 1, 0)$ the two-dimensional model considered in Theorem 4 has anisotropic coupling constants. For $\mathbf{n}_0 = (1, 1, 1)$, the system is not reflection symmetric and our results, and in particular Theorem 4, cannot be directly applied. Of course, at zero temperature it is easy to see that the (111) facets exist and, in fact, playing with the values of the coupling constants, we may obtain, in this case, examples of all situations described in Remark 2.

Actually, some more precise properties of the Wulff crystal shape can be stated. Let us explain this in the case of the first example. Let $\mathcal{W}_{d=2}$ be the equilibrium crystal shape for the two-dimensional Ising model, and let $\mathcal{F}$ be the facet, orthogonal to $\mathbf{n}_0$, of the equilibrium crystal $\mathcal{W}$ associated to the three-dimensional system. Then, inequalities (22) and (19), imply that the facet $\mathcal{F}$ includes in its interior the set $\mathcal{W}_{d=2}$, drown in the plane of $\mathcal{F}$, at the same scale and with the same centre and orientation.

4. The step free energy and its low temperature expansion

In the following we shall consider the Ising model on the simple cubic lattice ($\mathcal{L} = \mathbb{Z}^3$) with nearest neighbour attractions, since the notion of contour, a basic notion for describing the system at low temperatures, is more transparent in this case. However, all considerations can be generalized to other ferromagnetic systems, like those considered in the examples of Section 3. It seems, also, that the main technique can be extended, after some additional work, to a more general class of systems covered by the Pirogov-Sinai theory. In the Appendix, we review a number of results on low temperature cluster expansions that will be needed in the following discussion. We refer also to the Appendix for the precise definitions of some notions used in this Section.

Let Λ be a parallelepipedic box with sides L_1, L_2, L_3, parallel to the axes, and let $\bar{\sigma}$ be, either the $(\pm) = (\pm, \mathbf{n}_0)$, or the $(\text{step}) = (\text{step}, \mathbf{m})$ boundary conditions, introduced in Section 2. To any configuration inside Λ we associate, as explained in the Appendix, the set of *faces* (or closed unit squares) separating opposite spins and decompose this set into an *interface* $\mathcal{I}$ and a family of *contours*. By using the theory of cluster expansions, one can rewrite the partition functions $Z^{\bar{\sigma}}(\Lambda)$, respectively, by means of expressions (A5) and (A6) in the Appendix.

The method for studying the statistics of the interface, in the case of the boundary conditions $\bar{\sigma} = (\pm)$, is also explained in the Appendix. We distinguish two types of faces in the interface $\mathcal{I}$, the *wall-faces* and the *ceiling-faces*, and denote by $W(\mathcal{I})$ the set of wall-faces. A subset w of $W(\mathcal{I})$, whose orthogonal projection $p(w)$ on the horizontal plane $i_3 = -1/2$ is a maximally connected set, is called a *wall*. By a vertical displacement these walls are then referred to a standard position. Taking the two-dimensional projections of these *standard walls* for "polymers" the interface may then be studied by cluster expansion techniques.

Let us now consider the interfaces associated to the boundary conditions $\bar{\sigma} =$ (step). When we decompose, as above, the projection of $W(\mathcal{I})$ into maximally connected components, there is exactly one of these components which is infinite and all other components are bounded. The subset of $W(\mathcal{I})$ which projects into this infinite component will be called S, the *step.* The complementary set of S, in $W(\mathcal{I})$, can be described as a family of walls. In this way we associate to every interface $\mathcal{I}$, a step S and an *admissible* family W of standard walls, compatible with the step (i. e., their projections and the projection of the step are disjoint). The converse is also true: For any step S (compatible with the boundary conditions) and any admissible family W of standard walls, such that $p(S) \cap p(W) = \emptyset$, one can reconstruct in a unique way the interface. This interface will be denoted by $\mathcal{I}(S, W)$.

Consider the system in an infinite cylinder Λ_p of base $L_1 \times L_2$ by taking the limit $L_3 \to \infty$, and introduce the ratio of partition functions

$$e^{-2\beta J L_1 L_2} Q^{\text{step}}(\Lambda_p) = \lim_{L_3 \to \infty} [Z^{\text{step}}(\Lambda)/Z^{+}(\Lambda)] \tag{23}$$

Following the same computations that lead to formula (A6) in the Appendix, one gets:

Proposition 1. *The partition function in (23) is*

$$Q^{\text{step}}(\Lambda_p) = \sum_{S} e^{-2\beta J \|S\|} \sum_{\substack{W \\ p(W) \cap p(S) = \emptyset}} \prod_{w \in W} \psi_2(w) \exp\Big(\sum_{\substack{\Gamma \\ \Gamma \cap \mathcal{I}(S,W) = \emptyset}} \psi_1^{\mathrm{T}}(\Gamma) \Big) \tag{24}$$

In this expression, the first sum runs over all steps, associated to the given boundary conditions, and $\|S\|$ is the excess area of the step (number of faces of S, inside Λ, minus number of faces of $p(S)$). The second sum runs over admissible families W of standard walls and ψ_2 is the activity of a wall. The sum in the exponential runs over clusters of contours Γ and ψ_1^{T} are the corresponding truncated functions.

The purpose now is to write a new expression for the partition function $Q^{\text{step}}(\Lambda_p)$ using the notion of *aggregates* of walls and contours. In the case of the boundary conditions $\bar{\sigma} = (\pm)$ this notion, as explained in the Appendix, allows one to reduce the analysis of the interfaces to the study of a polymer system. Let us first develop Q^{step} in terms of *decorated* interfaces, as one does for $Q^{\pm}$. In the present case, however, a new special aggregate, including the step, has to be introduced. We shall call it the *extended step.* The extended step is a triplet $\xi = (S, \xi', \xi'')$ made with the step S itself, the set ξ', of all walls, and the set ξ'', of all clusters of the decorated interface, such that their projections $p(S)$, $p(\xi')$ and $p(\xi'')$ form a connected set (on $\mathbb{R}^2$). We extend the definition of the function ψ_3 (the activity in the case of aggregates) to the extended step, by putting

$$\psi_3(\xi) = e^{-2\beta J \|S\|} \prod_{w \in \xi'} \psi_2(w) \prod_{\Gamma \in \xi''} \Phi_1(\Gamma)$$

where Φ_1 is given by definition (A9). Then, the following expression

$$\begin{aligned} Q^{\text{step}}(\Lambda_p) &= \sum_{\xi} \psi_3(\xi) \Big(\sum_{\substack{A \\ p(A) \cap p(\xi) = \emptyset}} \prod_{\alpha \in A} \psi_3(\alpha) \Big) \\ &= \sum_{\xi} \psi_3(\xi) \exp \Big(\sum_{\substack{A \\ p(A) \cap p(\xi) = \emptyset}} \psi_3^{\mathrm{T}}(A) \Big) \end{aligned} \tag{25}$$

follows. Here the first sum, after the first and second equality, runs over all extended steps associated to the given boundary condition, the second sum, in the first equality, runs over admissible families of standard aggregates and, the second sum, in the second equality, runs over clusters of standard aggregates. The ψ_3^{T} represent the truncated functions for these clusters. Then, from (25) and (A14), the following proposition follows.

Proposition 2. *With the above notations, we have*

$$Q^{\text{step}}(\Lambda_p)/Q^{\pm}(\Lambda_p) = \sum_{\xi} \psi_3(\xi) \exp \Big(- \sum_{\substack{A \\ p(A) \cap p(\xi) \neq \emptyset}} \psi_3^{\mathrm{T}}(A) \Big) \tag{26}$$

In order to develop the analysis of the step free energy, we shall consider the system in an infinite band Λ_q, of width L_1, by taking the limits L_2 and L_3 tending to infinity.

The absolute convergence of the series $\sum_{A \ni t_0} \psi_3^{\mathrm{T}}(A)$, discussed in the Appendix, implies the existence of the following limit

$$\lim_{L_2 \to \infty} [Q^{\mathrm{step}}(\Lambda_p)/Q^{\pm}(\Lambda_p)] = e^{-2\beta J L_1} \Omega^{\mathrm{step}}(\Lambda_q) \tag{27}$$

The proof of this fact is analogous to the proof, in Ref. 5, concerning the existence of (A7). Limit (27) is given by the same expression (26) where the implicit restriction $A \subset \Lambda_p$, in the second sum, is replaced by $A \subset \Lambda_q$.

Expression (26) is the starting point of the analysis of the step free energy by cluster expansion techniques. We remark the similarity between expressions (26) and (A8) and, like in the previous discussion on the $(\pm)$ interface, we are going to introduce a description of the extended step in terms of elementary excitations, analogous to the walls. These excitations will be called step-jumps.

For this purpose we distinguish two types of faces on the extended step ξ, the *excited* and the *non-excited* faces. Given a face f, whose horizontal projection is $p(f)$, let $\lambda(f)$ be the orthogonal projection of $p(f)$ on the line $i_2 = -1/2$, $i_3 = -1/2$. For any face, $\lambda(f)$ is either a point or a unit segment on this line. A face $f \in \xi$ is a non-excited face if the following condition is fulfilled: f belongs to the step S associated to the extended step ξ, f is parallel to the (i_2, i_3) plane, and there is no other face $g \in \xi$ such that $\lambda(g) = \lambda(f)$. The other faces of ξ are said to be excited. The set of all excited faces is denoted by $J(\xi)$.

A subset j of $J(\xi)$, such that $\lambda(j)$ is a maximally connected set (on $\mathbb{R}$), is called a *step-jump*. Since $\lambda(j)$ is a segment (or reduces to a point), there are always two non-excited faces, f_1 and f_2, belonging to S, such that the unit segments $\lambda(f_1)$ and $\lambda(f_2)$ are adjacent to $\lambda(j)$. Assume that $\lambda(f_1)$ and $\lambda(f_2)$ are ordered according to their i_1-coordinates. The horizontal projections $p(f_1)$ and $p(f_2)$, of these faces, are two unit segments parallel to the i_1-axis, on the plane $i_3 = -1/2$. Let $i_2(f_1)$ and $i_2(f_2)$ be the values of the i_2-coordinate of these segments. The difference $h(j) = i_2(f_1) - i_2(f_2)$, will be called the *height* of the step-jump j. By translating the step-jump along the i_2 direction, in such a way that $i_2(f_1)$ becomes equal to $-1/2$, one obtains the associated *standard* step-jump.

For any extended step ξ, whose excited faces form the set $J(\xi)$, let us decompose the one-dimensional projection $\lambda(J(\xi))$ into maximally connected components. The subsets of $J(\xi)$ which, by means of λ, apply into these components, are the step-jumps associated to ξ. Let $J = \{j_1, ..., j_n\}$ be the set of the corresponding step-jumps. In this way, to every extended step, a family J of standard step-jumps with pair wise disjoint λ-projections (also called an *admissible* family), is associated. Moreover, if the boundary condition is (step) = (step,$\mathbf{m}$), with $\mathbf{m} = (\cos\phi, \sin\phi)$, these families satisfy

$$h(J) = h(j_1) + ... + h(j_2) = N \tag{28}$$

where N is the largest integer not exceeding $L_1 \tan\phi$ (the integer part of $L_1 \tan\phi$). Conversely, for any admissible family of standard step-jumps, satisfying condition (28), one may reconstruct in a unique way the extended step. This extended step will be denoted by $\xi(J)$.

Recall that a step-jump j is a triplet, consisting of a set of faces $j \cap S$ on the step, a set j' of walls and, a set j'' of clusters of standard aggregates. Let $\|j\|$ be the number of faces in $j \cap S$, minus the number of faces in $p(j \cap S)$, minus the length of $\lambda(j \cap S)$. Define the activity of the step-jump j by

$$\psi_4(j) = e^{-2\beta J \|j\|} \prod_{w \in j'} \psi_2(w) \prod_{\Gamma \in j''} \Phi_1(\Gamma)$$

Using the above description of the steps, the following proposition follows.

Proposition 3. *The partition function in (27) is*

$$\Omega^{(\mathrm{step},\mathbf{m})}(\Lambda_q) = \sum_{\substack{J \\ h(J)=N}} \prod_{j \in J} \psi_4(j) \exp\Big(- \sum_{\substack{A \\ p(A) \cap p(\xi) \neq \emptyset}} \psi_3^{\mathrm{T}}(A)\Big) \tag{29}$$

where the first sum runs over admissible families of standard step-jumps and the second over clusters of aggregates.

Therefore, $\Omega^{(\mathrm{step},\mathbf{m})}$, also to be denoted by Ω_N^{step}, can be interpreted as the partition function of a "gas of particles", on a one-dimensional lattice. The "particles" are described by some three-dimensional objects (the step-jumps j), and interact through the exclusion of their one-dimensional projections $\lambda(j)$, and through an effective energy given by the argument of the exponential. Expression (29) is formally identical to the partition function which can be associated with the surface tension of the two-dimensional Ising model, first studied by Gallavotti [19], and more recently in the work by Dobrushin *et al.* [1] (see Section 7.5 in the Appendix). The interfaces of the two-dimensional Ising model can also be described by a one-dimensional "gas of particles", though these "particles" are two-dimensional, instead of three-dimensional objects, and the activities and interactions differ. It may be expected, however, that the same methods apply to the present case.

We are going to follow the method used in Ref. 1. First, a new notion of aggregates, which will be called *step-aggregates*, is introduced. They consist of step-jumps and the already considered aggregates of walls and clusters, and are made in such a way that the λ-projection of a step-aggregate is a connected set (in $\mathbb{R}$). To any step-aggregate ϑ, one associates an activity $\psi_5(\vartheta)$, obtained in the standard way (Appendix, Section 7.4), from the activities ψ_4 of the step-jumps and the truncated functions ψ_3^{T} for the clusters of the old aggregates (of walls and contours). One associates also, to any step aggregate, a height $h(\vartheta)$, defined as the sum of the heights $h(j)$ of the step-jumps belonging to ϑ.

Proposition 4. *With the above definitions, expression (29) becomes*

$$\Omega_N^{\mathrm{step}}(\Lambda_q) = \sum_{\substack{\Theta \\ h(\Theta)=N}} \prod_{\vartheta\in\Theta} \psi_5(\vartheta) \tag{30}$$

where the sum runs over admissible families Θ of standard step-aggregates, $h(\Theta) = \sum_{\vartheta\in\Theta} h(\vartheta)$ and N is the integer part of $L_1 \tan\phi$.

The essential point, which has to be verified in order to apply the method of Ref. 1, is the convergence of the sum $\sum_{t_0\in\vartheta} |\psi_5(\vartheta)|$ over all step-aggregates that contain a given point. Define the order of a step-aggregate ϑ, as the degree of $\psi_5(\vartheta)$ in the variable $z = e^{-2\beta J}$. From the definitions above, and the connexity of the step-aggregates, it is not difficult to verify that the number of step-aggregates of order n (modulo translations) is bounded by a combinatorial factor of the form K^n, where K is a given number. This implies the convergence of the above considered sum for β sufficiently large.

Now, most of the results and proofs in Ref. 1 (Chapter 4), concerning the surface tension in the two-dimensional Ising model, can be extended to the problem of the step free energy, considered here. We shall not repeat all the proofs, which can easily be translated to the present case. Let us mention, however, how the cluster expansions and the truncated functions are introduced. One defines a new partition function, depending on the parameter $u \in \mathbb{R}$, by

$$\tilde{\Omega}_u^{\text{step}}(\Lambda_q) = \sum_{N \in \mathbb{Z}} e^{\beta u N} \Omega_N^{\text{step}}(\Lambda_q) = \sum_{\Theta} \prod_{\vartheta \in \Theta} \psi_5(\vartheta) e^{\beta u h(\vartheta)} \tag{31}$$

We can interpreted (31) as a "grand canonical" partition function, with respect to the step boundaries, and the restriction in the sum (30), as a "canonical" constrain. Since the partition function (31) describes a system of "polymers" interacting only through exclusion, the standard cluster expansion techniques can be applied. One introduces, as usual, the activities $\psi_6(\vartheta) = \psi_5(\vartheta) e^{\beta u h(\vartheta)}$ of these polymers, the Boltzmann factors and, by means of formula (A4) in the Appendix, the truncated functions $\psi_6^{\mathrm{T}}(\Theta)$ for clusters of standard step-aggregates. Then

$$\tilde{\Omega}_u^{\text{step}}(\Lambda_q) = \exp\Big(\sum_{\Theta} \psi_6^{\mathrm{T}}(\Theta)\Big) \tag{32}$$

where the sum runs over all clusters inside Λ_q. The main result of the theory implies that the power series (in the variable $z = e^{-2\beta J}$) defined by the sum $\sum_{t_0 \in \Theta} \psi_6(\Theta)$ is absolutely convergent, provided that $\beta > \beta_0$, where $\beta_0 > 0$ is some constant. This result implies, in particular, the existence of the free energy associated to the grand canonical partition function

$$g(u) = \lim_{L_1 \to \infty} -\frac{1}{\beta L_1} \ln\left[e^{2\beta J L_1} \tilde{\Omega}_u^{\text{step}}(\Lambda_q)\right] \tag{33}$$

and leads to the following results.

Theorem 5. *If the temperature is low enough, i. e., if $\beta \geq \beta_0$, where $\beta_0 > 0$ is a given constant, then the step free energy τ^{step}, defined by limit (18), exists, is strictly positive, and is given by*

$$\tau^{\text{step}}(\phi) = [g(u_\phi) + u_\phi \tan\phi] \cos\phi \tag{34}$$

where $g(u)$ is defined in (33) and u_ϕ is the (unique) solution of the equation $\tan\phi + \partial g/\partial u = 0$. *Moreover,*

$$\tau^{\text{step}}(\mathbf{m}) = \quad 2J(|m_1| + |m_2|) - (1/\beta)\big((|m_1| + |m_2|)\ln(|m_1| + |m_2|) \\ - |m_1|\ln|m_1| - |m_2|\ln|m_2|\big) - (1/\beta)\varphi_{\mathbf{m}}(\beta) \qquad (35)$$

where $\varphi_{\mathbf{m}}$ is an analytic function of $z = e^{-2\beta J}$, for $|z| \le e^{-2\beta_0 J}$, whose corresponding power series can be computed by cluster expansion techniques.

Proof. The Theorem is proved analogously to Proposition 4.12 of Ref. 1.

Notice that the function $\tau_p^{\text{step}}(v) = \lim_{L_1\to\infty} -(1/\beta L_1)\ln\left[e^{2\beta J L_1}\Omega_N^{\text{step}}(\Lambda_q)\right]$, where N is the integer part of $L_1 v$, can be obtained, according to the equivalence theory of canonical and grand canonical ensembles, as the Legendre transform of $g(u)$. On the other hand, from the above definitions, one gets $\tau^{\text{step}}(\phi)/\cos\phi = \tau_p^{\text{step}}(\tan\phi)$. From these facts expression (34) follows.

The first two terms in (35), which represent the main contributions for $\beta \to \infty$, come from the ground state of the system under (step) boundary conditions. The first term can be recognized as the residual energy of the step at zero temperature and, the second term, as $-(1/\beta)$ times the entropy of this ground state. The same two terms occur in the surface tension of the two dimensional Ising model (see Ref. 19) and, though the analogous expression is not given in Ref. 1, it is a consequence of the method developed there. This method can also be applied to our case and consists in splitting up the set of step jumps into those that are typical for low temperatures (called in Ref. 1 "tame animals") and those that can be interpreted as excitations appearing at not vanishing temperatures ("wild animals"). This distinction is also useful for computing, by means of relations (32), (33) and (34), the coefficients of the series $\varphi_{\mathbf{m}}$.

By considering the lowest energy excitations, it can easily be seen that $\varphi_{\mathbf{m}}$ is $O(e^{-4\beta J})$, because the series begins with the term in z^2, and also, that the first term in which this series differs from the series associated to the surface tension of the two-dimensional Ising model, is $O(e^{-12\beta J})$.

Theorem 6. *Under the conditions of Theorem 5, the function $f^{\text{step}}(\mathbf{x}) = \tau^{\text{step}}(\mathbf{x}/|\mathbf{x}|)$, defined for all $\mathbf{x} \in I\!R^2$, is positively homogeneous and convex.*

Proof. The convexity of $g(u)$, which can be proved from (31) and (33), implies the convexity of its Legendre transform $\tau_p(v)$, and from this the Theorem follows. See Ref. 1 (Theorem 4.21) for a detailed analogous proof.

Remark 5. In fact, under the same conditions, the function $f^{\text{step}}(\mathbf{x})$ is strictly convex. This means that $\tau^{\text{step}}(\mathbf{m})$ satisfies the pyramidal inequality (or, in $d = 2$, the triangular inequality) in its sharp form, i. e., the equality occurs in (3) only for degenerated triangles of zero area. See also Ref. 1 (Theorem 4.21).

Remark 6. The thermodynamic limit of the step free energy can also be obtained under more general conditions (on the way in which the boxes tend to infinity) than those specified in definition (18). See Ref. 1 (Theorem 2.2) for an analogous result.

Remark 7. Another consequence of the above analysis is that the step S, even for $\mathbf{m} = (0, 1)$, undergoes large fluctuations at non zero temperatures. See Refs. 16 and 1 (Propositions 4.9 and 4.10) for analogous results on the interface of the two-dimensional model. It follows from this fact that the Gibbs states, associated to the (step) boundary conditions, are invariant under the translations parallel to the (i_1, i_2) plane.

5. The step free energy and the facet shape

A serious difficulty facing the attempts to generalize the work by Dobrushin *et al.* to the three-dimensional Ising model, is the fact that one needs a very accurate description of the partition functions yielding the surface tension, for any orientation $\mathbf{n}$. This is comparatively easy in the two-dimensional case in which the walls are on a one-dimensional lattice. (Appendix, Section 7.5). In the three-dimensional case the same approach leads to difficult problems of random surfaces. The exception is the case of an interface oriented along the axes of the lattice, which has been proved to be rigid at low temperatures. Only in this case, say for $\mathbf{n} = \mathbf{n}_0 = (0, 0, 1)$, the surface tension $\tau(\mathbf{n})$ admits a low temperature expansion (Appendix, Section 7.3). Nevertheless, the methods developed in Section 4 can be used to control, in some sense, the interfaces whose orientations are close to the orientation of this rigid interface. This allows us to derive the following result, with which we come back to the initial problem of describing the equilibrium shape predicted by the Wulff construction.

Theorem 7. *Under the conditions of Theorem 5,*

$$\tau^{\text{step}}(\phi) = (\partial/\partial\theta)_{\theta=0^+}\tau(\phi,\theta) \tag{36}$$

i. e., the step free energy equals the one-sided angular derivative of the surface tension considered in Theorem 1.

Proof. The proof will be given in Section 6.

An intuitive argument for this result has been described in the Introduction. The observation made in Remark 6, provides a new ingredient which will be important for the proof.

It is natural to expect that the equality (36) is true for any β larger than β_R (the roughening inverse temperature), and that for $\beta \leq \beta_R$, both sides in (36) vanish. Since in this last case, the angular derivative of $\tau(\phi,\theta)$ is continuous at $\theta = 0$, the disappearance of the facet is involved†. However, the condition that the inverse temperature β is large enough is important in our discussion. Only when it is fulfilled we have the full control on the equilibrium probabilities that is needed in the proofs.

It has been shown in Theorem 1 that the facet $\mathcal{F}$ in the Wulff equilibrium crystal, is determined, through (8), by the one-sided angular derivative of the surface tension. We see, taking Theorem 7 into account, that the shape of the facet is obtained by applying the two-dimensional Wulff construction to the step free energy. Namely,

$$\mathcal{F} = \left\{ \mathbf{x} \in I\!\!R^2 \ : \ \mathbf{x} \cdot \mathbf{m} \leq \tau^{\text{step}}(\mathbf{m}) \right\} \tag{37}$$

Here the inequality is assumed for each unit vector $\mathbf{x} \in I\!\!R^2$. As a consequence of Remark 5 it follows that $\mathcal{F}$ has a smooth boundary (with a continuous tangent) without straight segments. Therefore, the equilibrium crystal has necessarily rounded edges and corners.

† These facts can be proved for certain solid-on-solid models of interfaces using correlation inequalities [20].

Moreover, according to Theorem 5, we may use a convergent expansion to compute the function $\tau^{\text{step}}(\mathbf{m})$, for all $\mathbf{m}$, and hence to determine the facet shape (at any given temperature $\beta \geq \beta_0$). From the observation made after Theorem 5, it follows that the difference between $\mathcal{F}$ and the equilibrium shape of the two-dimensional Ising model, at the same temperature, is of order $O(e^{-12\beta J})$. Actually, the computation is easier using the "grand canonical" free energy $g(u)$, defined in (33). The graph of this function, as noticed by Andreev for the usual Wulff construction (see Refs. 13 and 2, Theorem 4), coincides with the shape of the facet boundary.

6. Proof of Theorem 7

In order to simplify the notations, Theorem 7 will be proved in the particular case $\phi = 0$. Using the appropriate geometrical setting, the proof extends without any difficulty to the general case. The main observation is the fact that Theorem 4.2 of Ref. 1, which we shall borrow at some point of the proof, can also be applied when $\phi \neq 0$. For $\phi = 0$, we write $\tau(\theta) = \tau(\theta, 0)$, $\tau^{\text{step}} = \tau^{\text{step}}(0)$, $\mathbf{n} = (\cos\theta, 0, \sin\theta)$, and introduce the notation

$$\tau(\theta; L_1, L_2) = -\frac{\cos\theta}{\beta L_1 L_2} \ln \frac{Q^{(\pm,\mathbf{n})}(\Lambda_p)}{Q^{+}(\Lambda_p)} \tag{37}$$

for the surface tension of the finite system. The proof comprises four steps.

Part 1. The convexity properties of the surface tension (see the proof of Theorem 1) imply that

$$(\partial\tau/\partial\theta)_{\theta=0^+} = \inf_{\theta\geq 0} \, (1/\tan\theta)[(\tau(\theta)/\cos\theta) - \tau(0)]$$

Moreover, as mentioned in Theorem 2, the infinite volume limit $\tau(\theta)$ coincides with the infimum over (L_1, L_2) of $\tau(\theta; L_1, L_2)$. From these facts, one obtains

$$\begin{aligned}(\partial\tau/\partial\theta)_{\theta=0^+} \leq \; & (1/\tan\theta)[(\tau(\theta; L_1, L_2)/\cos\theta) - \tau(0; L_1, L_2)] \\ & + (1/\tan\theta)[\tau(0; L_1, L_2) - \tau(0)]\end{aligned} \tag{38}$$

The factor in the first term of (38) is

$$\frac{\tau(\theta; L_1, L_2)}{\cos\theta} - \tau(0; L_1, L_2) = -\frac{1}{\beta L_1 L_2} \ln \frac{Q^{(\pm,\mathbf{n})}(\Lambda_p)}{Q^{\pm}(\Lambda_p)}$$

The factor in the second term may be bounded (for $\beta > \beta_0$) using the convergent cluster expansion of $\tau(0)$. Indeed, expression (A14), in the Appendix, implies that

$$|\tau(0; L_1, L_2) - \tau(0)| \leq \frac{L_1 + L_2}{L_1 L_2} K \tag{39}$$

where $K = K(\beta) > 0$ does not depend on L_1 or L_2.

Part 2. After these observations we are going to analyse the partition function $Q^{(\pm,\mathbf{n})}(\Lambda_p)$ and the associated interfaces. First, let us consider the simplest case $\beta = \infty$. In this case, the interface, which has the minimal area, looks like a perfectly regular stair with rectilinear steps of height one. There are k steps, with k equal to the integer part of $L_2 \tan\theta$, separated by a distance b, nearly equal to $1/\tan\theta$. For $\beta > 0$ some deformations will appear, either in the flat portions of the interface, or on the steps, and also several steps may merge into a larger one. In fact, the situation can again be described by the method used in Section 4, a description which will make sense for large β and very small θ. Let $W(\mathcal{I})$ be the set of wall-faces of the interface $\mathcal{I}$ under consideration, and let $p(W(\mathcal{I}))$ be the projection of this set on the plane π. Decompose $p(W(\mathcal{I}))$ into maximally connected components (in $I\!R^2$). A number k' of these components, with $1 \leq k' \leq k$, are infinite, and the other are bounded. The infinite components are the projections of certain subsets, $S_1, ..., S_{k'}$, of $W(\mathcal{I})$ which will be called steps. The bounded components are the projections of walls. Using the above notations we may write

$$Q^{(\pm,\mathbf{n})}(\Lambda_p) = \sum_{k'=1}^{k} \sum_{S_1,\ldots,S_{k'}} e^{-2\beta J(\|S_1\|+\ldots+\|S_{k'}\|)} \sum_{\substack{W \\ p(W)\cap p(S_l)=\emptyset, l=1,\ldots,k'}} \prod_{w\in W} \psi_2(w)$$
$$\times \exp\Big(\sum_{\substack{\Gamma \\ \Gamma\cap\mathcal{I}(S_1,\ldots,S_{k'},W)=\emptyset}} \psi_1^{\mathrm{T}}(\Gamma) \Big) \tag{40}$$

The first sums in (40) run over all sets of steps with pair wise disjoint projections. We use $\mathcal{I}(S_1, ..., S_{k'}, W)$ to denote the interface, associated to the considered steps and the admissible family W of standard walls.

Part 3. Since all terms are positive, the value of (40) decreases if the sum is restricted to the terms containing exactly k steps and, moreover, it is required that these steps do not go too far from the corresponding steps $S_1^0,\ldots,S_k^0$, at $\beta=\infty$. Namely, if $\Delta_l(b')$ is the set of points (in $I\!R^3$) whose projection on π is at a distance less than b' from $p(S_l^0)$, it is required that $S_l \subset \Delta_l(b/4)$, for every $l=1,...,k$. Next one introduces, as it was done before for $Q^{\rm step}$, the aggregates of walls and contours and the extended steps. Let $\xi_1,...\xi_k$ be the associated extended steps. A similar restriction to that required on the steps is now required on the extended steps. Namely, we require that $\xi_l \subset \Delta_l(b/3)$, for every $l=1,...,k$. Taking into account that the extended steps which do not fulfill this condition are such that

$$|\psi_3(\xi)| \le \exp(-2\beta J\|S\|)\exp(-2\beta J(b/12)) \tag{41}$$

one obtains, for the ratio of partition functions,

$$\frac{Q^{(\pm,\mathbf{n})}(\Lambda_p)}{Q^{\pm}(\Lambda_p)} \ge \sum_{\substack{\xi_1,\ldots,\xi_k \\ \xi_l\subset\Delta_l(b/3), l=1,\ldots,k}} \psi_3(\xi_1)\ldots\psi_3(\xi_k)\exp\Big(-\sum_{\substack{A \\ \exists l, p(A)\cap p(\xi_l)\neq\emptyset}} \psi_3^{\rm T}(A)\Big)$$
$$\times \exp\big(-kL_1 O(e^{-(1/6)\beta Jb})\big) \tag{42}$$

The first sum in (42) runs over the extended steps satisfying the condition above. The last factor is a bound on the error, derived by using (41) and summing over all remaining extended steps. Next, the sum in the exponential in (42) is restricted to the aggregates A for which there is some l such that $A\subset\Delta_l(b/2)$. This means that some large aggregates are neglected, but the error is still bounded by a term of the same order as before. After that, expression (42) factorizes and, again up to an error of the same order, one gets,

$$\frac{Q^{(\pm,\mathbf{n})}(\Lambda_p)}{Q^{\pm}(\Lambda_p)} \ge \left[\frac{Q^{\rm step}(\Lambda'_p)}{Q^{\pm}(\Lambda'_p)}\right]^k \exp\big(-kL_1 O(e^{-(1/6)\beta Jb})\big)$$

where Λ'_p is an infinite cylinder of base $L_1\times b$. By taking logarithms in both sides of this expression, using formula (37), and replacing k by its value $L_2\tan\theta$, it follows that

$$\frac{\tau(\theta;L_1,L_2)}{\cos\theta} - \tau(0;L_1,L_2) \le -\frac{\tan\theta}{\beta L_1}\ln\frac{Q^{\rm step}(\Lambda'_p)}{Q^{\pm}(\Lambda'_p)} + \frac{\tan\theta}{\beta}O(e^{-(1/3)\beta Jb}) \tag{43}$$

Part 4. Now, using inequalities (38), (39) and (43), we obtain

$$(\partial\tau/\partial\theta)_{\theta=0^+} \le -\frac{1}{\beta L_1}\ln\frac{Q^{\rm step}(\Lambda'_p)}{Q^{\pm}(\Lambda'_p)} + \frac{1}{\beta}O(e^{-(1/3)\beta Jb}) + \frac{L_1+L_2}{L_1L_2}Kb \tag{44}$$

The right hand side of this inequality is a function of L_1, L_2 and $b = 1/\tan\theta$ which will be replaced by its minimum value. According to Theorem 5, the first term tends to $\tau^{\rm step}$, in the limit when, first b, and after L_1, tend to infinity. However, as noticed in Remark 6, the same statement is true under more general conditions and, in particular, by adapting to the preset case the proof of Theorem 4.2 in Ref. 1, one sees that the same limit is obtained if one takes $b = L_1^{\frac{1}{2}+\epsilon}$, with $\epsilon > 0$, and then let $L_1 \to \infty$. By choosing $0 < \epsilon < 1/2$, and taking, successively, the limits $L_2 \to \infty$ and $L_1 \to \infty$ in (44), the last two terms in the right hand side vanish, and one obtains

$$(\partial\tau/\partial\theta)_{\theta=0^+} \leq \tau^{\rm step}$$

This inequality, together with Theorem 3, ends the proof of Theorem 7.

We notice that the arguments above have some similarities with those used in Ref. 21 to show Antonov's rule, though, instead of a large number of steps, only two interfaces had to be considered for this purpose.

ACKNOWLEGMENTS : The author acknowledges useful discussions with J. Bricmont, M. Cassandro, G. Gallavotti, R. Kotecky and J. Ruiz. He warmly thanks G. Gallavotti and G. Benfatto for their kind invitation, and the members of the Institute of Physics of the University of Rome "La Sapienza", for the hospitality extended to him during the preparation of this work.

7. Appendix

We summarize here some basic results, mainly adapted form Refs. 22, 5 (part III), 6 and 16, which are needed in Sections 5, 6 and 7. We consider the Ising model on the simple cubic lattice $\mathcal{L} = \mathbb{Z}^3$. Two nearest neighbour spins $\sigma(i)$ and $\sigma(j)$ interact with attractive energy $-J(\sigma(i)\sigma(j) - 1)$ and $J > 0$. Considering $\mathcal{L}$ as a set of points in $\mathbb{R}^3$, we associate to each pair $\langle i, j\rangle$ of nearest neighbour sites the closed unit square (also called *face*) orthogonal to the segment i, j and passing through the middle of this segment. Let $\mathcal{F}_c$ be the set of the non empty connected (in the sense of $\mathbb{R}^3$) sets of faces.

Given a configuration $\sigma_\Lambda = \{\sigma(i)\}$, $i \in \Lambda$, in a box Λ with boundary conditions $\bar\sigma \in \Omega$ we define $X^{\bar\sigma}(\sigma_\Lambda)$ as the the set of faces associated to the nearest neighbours $\langle i,j\rangle$ with opposite spins, the configuration being extended to the whole lattice by using the boundary condition (i. e., $\sigma(i) = \bar\sigma(i)$ if $i \notin \Lambda$). We assume that Λ contains the face associated to $\langle i,j\rangle$ if, and only if, at least one of the two sites belongs to Λ. Then the energy $H_\Lambda(\sigma_\Lambda, \bar\sigma)$ is equal to $-2\beta J$ times the number of faces in $X^{\bar\sigma}(\sigma_\Lambda) \cap \Lambda$.

7.1. *Contours*

Consider the system in the box Λ with (+) boundary conditions. A finite set $\gamma \in \mathcal{F}_c$ is a *contour* if there exists a configuration σ_Λ in Λ (which then is unique) such that $\gamma = X^+(\sigma_\Lambda)$. An *admissible* family of contours is a set of pair wise disjoint contours. For any configuration σ_Λ in Λ, the set $X^+(\sigma_\Lambda)$ splits into maximally connected components $\gamma_1, ..., \gamma_n$, which are pair wise disjoint contours. Therefore, there is a bijection between such configurations and the admissible families of contours inside Λ.

Let the *area* $|\gamma|$ of a contour be the number of faces of γ and let its *activity* be $\psi_1(\gamma) = \exp(-2\beta J|\gamma|)$. Then, the partition function becomes

$$Z^+(\Lambda) = \sum_\Gamma \prod_{\gamma\in\Gamma} \psi_1(\gamma) \tag{A1}$$

where the sum runs over all admissible families of contours in Λ. Expression (A1) shows that the system is equivalent to a *polymer* system, i. e., to a gas of several "species of particles" (all contours modulo translations), interacting only through hard-core exclusion and having the activities $\psi_1(\gamma)$. The properties of polymer systems may, under appropriate conditions, be studied with the help of cluster expansions. They lead to convergent expansions in the small activity region. To develop the theory of these expansions we shall use the method of Ref. 21.

For this purpose we consider also non-admissible families of contours, including families in which a contour occurs several times, identified with the non-negative integer valued functions Γ on the set of contours, such that $\sum_\gamma \Gamma(\gamma) < \infty$ ($\Gamma(\gamma)$ is the multiplicity of the contour γ in the family). Let $\mathcal{M}$ be the set of all these functions, and define $(\Gamma_1 + \Gamma_2)(\gamma) = \Gamma_1(\gamma) + \Gamma_2(\gamma)$. We shall also use the notation Γ, when no confusion arises, for $\gamma_1 \cup ... \cup \gamma_n$, considered as a subset of $I\!R^3$, where $\gamma_1, ..., \gamma_n$ are all the contours for which $\Gamma(\gamma_i) \neq 0$.

The Boltzmann factor is extended to $\mathcal{M}$, by putting

$$\psi_1(\Gamma) = \prod_{\gamma \in \Gamma} \psi_1(\gamma) \tag{A2}$$

if Γ is admissible, and $\psi_1(\Gamma) = 0$, otherwise. The *truncated* functions are defined, on $\mathcal{M}$, by

$$\psi_1^{\mathrm{T}}(\Gamma) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sum{}' \prod_{i=1}^{n} \psi_1(\Gamma_i) \tag{A3}$$

where $\sum'$ represents the sum over all $\Gamma_1, ..., \Gamma_n$ such that $\Gamma_i \neq \emptyset$ and $\sum \Gamma_i = \Gamma$.

A first important consequence of definition (A3) is that $\psi_1^{\mathrm{T}}(\Gamma) \neq 0$ only if Γ is connected. A second consequence is the expression

$$Z^+(\Lambda) = \sum_{\Gamma} \psi_1(\Gamma) = \exp\big(\sum_{\Gamma} \psi_1^{\mathrm{T}}(\Gamma)\big) \tag{A4}$$

The connected Γ will be called *clusters* (of contours). The expansions in terms of the functions $\psi_1^{\mathrm{T}}(\Gamma)$ are the cluster expansions. The main theorem of the theory states that there exists $\beta_0 > 0$, such that if the inverse temperature β is larger than β_0, then the sum $\sum_{t_0 \in \Gamma} \psi_1^{\mathrm{T}}(\Gamma)$, which runs over all clusters containing the point $t_0 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (considered as a power series of the variable $z = e^{-2\beta J}$), is absolutely convergent. This implies the existence and analyticity of the free energy $\varphi_\beta = \lim_{\Lambda \to \infty} -(1/\beta|\Lambda|) \ln Z^{(+)}(\Lambda)$, as well as analyticity and cluster properties for the correlation functions.

7.2. *Interfaces*

Consider the system in a box Λ with mixed $(\pm, \mathbf{n})$ boundary conditions. Given a configuration σ_Λ in Λ we decompose the set $X^{(\pm,\mathbf{n})}(\sigma_\Lambda)$ into maximally connected components. There is exactly one component which is infinite, when the configuration is extended to the whole lattice using the boundary conditions. We call this component $\mathcal{I}$, the *interface*. All other components are contours.

The possible interfaces are the sets $\mathcal{I} \in \mathcal{F}_c$, for which there exits a σ_Λ such that $\mathcal{I} = X^{(\pm,\mathbf{n})}(\sigma_\Lambda)$. A contour γ and the interface $\mathcal{I}$ are compatible if they do not intersect.

Let $|\mathcal{I}|$ be the number of faces of $\mathcal{I}$ (inside Λ). Taking (A4) into account, one obtains the following expressions for the partition function

$$Z^{(\pm,\mathbf{n})}(\Lambda) = \sum_{\mathcal{I}} e^{-2\beta J|\mathcal{I}|}\big(\sum_{\Gamma\cap\mathcal{I}=\emptyset}\psi_1(\Gamma)\big) = \sum_{\mathcal{I}} e^{-2\beta J|\mathcal{I}|}\exp\big(\sum_{\Gamma\cap\mathcal{I}=\emptyset}\psi_1^{\mathrm{T}}(\Gamma)\big) \qquad (A5)$$

where the first sum runs over all interfaces $\mathcal{I}$ compatible with the boundary conditions. Then, from (A1) and (A5), it follows

$$Z^{(\pm,\mathbf{n})}(\Lambda)/Z^{+}(\Lambda) = \sum_{\mathcal{I}} e^{-2\beta J|\mathcal{I}|}\exp\big(-\sum_{\Gamma\cap\mathcal{I}\neq\emptyset}\psi_1^{\mathrm{T}}(\Gamma)\big) \qquad (A6)$$

In order to analyse the interface, we consider the system in an infinite cylinder Λ_p of base $L_1\times L_2$, by taking the limit $L_3\to\infty$. The absolute convergence of the series of truncated functions implies the existence of the following limit for the ratio of partition functions

$$\lim_{L_3\to\infty}[Z^{(\pm,\mathbf{n})}(\Lambda)/Z^{+}(\Lambda)] = e^{-2\beta J(L_1L_2/n_3)}Q^{(\pm,\mathbf{n})}(\Lambda_p) \qquad (A7)$$

(see the proof in Ref. 5, Part III). The limit is given by the same expression (A6), where the implicit restriction $\Gamma\subset\Lambda$, in the second sum, is replaced by $\Gamma\subset\Lambda_p$.

7.3. *Walls*

Consider the case $\mathbf{n}=\mathbf{n}_0=(0,0,1)$, which defines the $(\pm)$ boundary conditions. Let π be the horizontal plane $i_3=-1/2$ and $p(.)$ the orthogonal projection on this plane. The projection $p(f)$ of a face f is either a face or an edge. There are two types of faces in an interface $\mathcal{I}$: The *ceiling-faces*, which are the horizontal faces f such that there is no other face g in $\mathcal{I}$ such that $p(f)=p(g)$, and the *wall-faces*, which are all other faces in $\mathcal{I}$. The set of wall-faces is denoted by $\mathcal{W}(\mathcal{I})$.

A set w of wall faces whose projection $p(w)\in\mathcal{F}_c$ is called a *standard wall*, if there exits an interface $\mathcal{I}$ such that $w=\mathcal{W}(\mathcal{I})$. A family of standard walls is *admissible* if the projections on π of these walls are pair wise disjoint. It will be seen that the interfaces can equivalently be described by the admissible families of standard walls.

We observe that any interface $\mathcal{I}$ decomposes into *walls*, which are the subsets of $W(\mathcal{I})$ which are projected into the maximally connected components of the projection

$p(\mathcal{W}(\mathcal{I}))$, and *ceilings*, or connected sets of ceiling-faces. Given a wall w, consider the set B, of faces on π, which do not belong to $p(w)$, and decompose B into connected components. To each component there corresponds one ceiling adjacent to w which projects into this component. The ceiling which projects into the unique infinite component of B is called the *base* of w. Since the base of a standard wall lies on π, one can associate, to any wall w, the standard wall which is just the vertical translate of w with base on π. In this way, one associates to every interface a family of standard walls, having disjoint projections on π. The converse is also true: For any family W of standard walls with pair wise disjoint projections one can reconstruct, in a unique way, the interface. This interface will be denoted by $\mathcal{I}(W)$.

Let $\|w\|$, the *excess area* of a wall, be the number of faces of w, minus the number of faces of $p(w)$, and let $\psi_2(w) = \exp(-2\beta J\|w\|)$ be the *activity* of w. Given an admissible family W of standard walls we denote by $\mathcal{I}(W)$ the corresponding interface and observe that $|\mathcal{I}(W)| = L_1 L_2 + \sum_{w\in W} \|w\|$. Then, expression (A6) becomes

$$Q^{\pm}(\Lambda_p) = \sum_{W} \prod_{w\in W} \psi_2(w) \exp\big(- \sum_{\Gamma\cap\mathcal{I}(W)\neq\emptyset} \psi_1^{\mathrm{T}}(\Gamma)\big) \tag{A8}$$

where the first sum runs over all admissible families of standard walls in Λ_p.

In expression (A8) the interface has been rewritten in terms of a gas of walls and, thus, can be viewed as a model over a two-dimensional lattice. The second factor in (A8) gives an effective interaction between walls. A theory of cluster expansions may be developed for this system either directly, as in Ref. 5, or, equivalently, by transforming it into a polymer system. This last method, which was used in Ref. 6, will be described in the following paragraph.

7.4. *Aggregates*

We are going to rewrite $Q^{\pm}(\Lambda_p)$ as a sum of certain elements, which we call *decorated interfaces*, and are defined as the pairs $(\mathcal{I}, T)$, where $\mathcal{I}$ is an interface and T a finite set of clusters, such that $\Gamma \cap \mathcal{I} \neq \emptyset$ for every $\Gamma \in T$.

Given an interface $\mathcal{I}$ or, what is the same, an admissible family of standard walls

W such that $\mathcal{I} = \mathcal{I}(W)$, we consider the corresponding term in the sum (A8). We define

$$\Phi_1(\Gamma) = e^{-\psi_1^{\mathrm{T}}(\Gamma)} - 1 \tag{A9}$$

and expand

$$\exp\Big(-\sum_{\Gamma\cap\mathcal{I}\neq\emptyset} \psi_1^{\mathrm{T}}(\Gamma)\Big) = \prod_{\Gamma\cap\mathcal{I}\neq\emptyset} (1+\Phi_1(\Gamma)) = \sum_T \prod_{\Gamma\in T} \Phi_1(\Gamma) \tag{A10}$$

where the last sum runs over all sets T of clusters such that all elements Γ of T intersect $\mathcal{I}(W)$. This leads to the expression of the partition function as a sum over the above defined pairs

$$Q^{\pm}(\Lambda_p) = \sum_{(W,T)} \prod_{w\in W} \psi_2(w) \prod_{\Gamma\in T} \Phi_1(\Gamma) \tag{A11}$$

Let $(\mathcal{I}, T)$ be a decorated interface and let α be a pair $\alpha = (\alpha', \alpha'')$, where α' is a subset of the set of walls of $\mathcal{I}$ and α'' is a subset of T. We shall also use the notation $\alpha = \alpha' \cup \alpha''$ for the union (as sets in $I\!\!R^3$) of the walls in α' and the clusters in α''. Such a pair α is called an *aggregate* if its projection $p(\alpha)$ on π is a connected set (in $I\!\!R^2$). If there exists a decorated interface $(\mathcal{I}, T)$, such that α is the unique aggregate of $(\mathcal{I}, T)$, it is said that α is a *standard aggregate.* We observe that the following geometrical property holds: For any aggregate α, there is a standard aggregate which is just the vertical translate of α. A set of standard aggregates with pair wise disjoint projections is called an *admissible* family.

Given a decorated interface $(\mathcal{I}, T)$, one says that α is an aggregate of $(\mathcal{I}, T)$, if $p(\alpha)$ is a connected component of $p(\mathcal{I} \cup T)$. The mapping that associates to a decorated interface its aggregates in standard position is a bijection onto the admissible families of standard aggregates.

The activity of an aggregate is defined by

$$\psi_3(\alpha) = \prod_{w\in\alpha'} \psi_2(w) \prod_{\Gamma\in\alpha''} \Phi_1(\Gamma) \tag{A12}$$

Finally, the partition function (A8) is expressed as a sum over all admissible families of standard aggregates

$$Q^{\pm}(\Lambda_p) = \sum_A \prod_{\alpha\in A} \psi_3(\alpha) \tag{A13}$$

Taking the two-dimensional projections of the aggregates for polymers, the system may now be studied by the standard cluster expansion techniques. One introduces, as was done before for the contours, the admissible, and the non admissible families with multiplicities, of standard aggregates. By using expressions analogous to (A1) and (A2), one defines the Boltzmann factors $\psi_3(A)$ and the *truncated* functions $\psi_3^{\mathrm{T}}(A)$ on the set of such families. Then, one gets

$$Q^{\pm}(\Lambda_p) = \exp\big(-\sum_A \psi_3^{\mathrm{T}}(A)\big) \tag{A14}$$

where the sum runs over *clusters* A, of standard aggregates inside Λ_p.

The main theorem of the theory ensures the absolute convergence of the power series (in the variable $z = e^{-2\beta J}$) defined by the sum $\sum_{t_0 \in A} \psi_3^{\mathrm{T}}(A)$, provided that $\beta > \beta_0$, where $\beta_0 > 0$ is some constant. From this fact it follows, in particular, that the surface tension $\tau(\mathbf{n}_0)$ exists, at low temperatures, and is given by $\tau(\mathbf{n}_0) = 2J - (1/\beta)\varphi_1$, where $\varphi_1(\beta) = \lim_{\Lambda_p \to \infty}(1/\beta L_1 L_2) \ln Q^{\pm}(\Lambda_p)$ is an analytic function.

7.5. *The two-dimensional case*

The theory discussed in this Appendix can be adapted, with the natural modifications, to any dimension $d \geq 3$. The two-dimensional case differs in some particular but important points. First, we notice that contours and interfaces can be defined as above (a face is now a unit segment), and that all results in Sections 7.1 and 7.2 follow in the same way. To describe the interface, walls and ceilings can be introduced as in Section 7.3, but the notion of base of a wall does not subsist. In fact, the set B being one-dimensional, it has two infinite components, instead of one, and there are two ceilings, adjacent to each wall, which play the role of bases. The wall can be seen as a jump over a height equal to the difference between the ordinates of these ceilings.

Then, the sum over admissible families of standard walls, in expression (A8), has to be restricted to the families W such that $h(W) = \sum_{w \in W} h(w) = 0$, where $h(w)$ is the height of the wall w. A similar expression can be written for interfaces in any orientation, namely

$$Q^{(\pm,\mathbf{n})}(\Lambda_p) = \sum_{h(W)=N} \prod_{w \in W} \psi_2(w) \exp\big(-\sum_{\Gamma \cap \mathcal{I}(W) \neq \emptyset} \psi_1^{\mathrm{T}}(\Gamma)\big) \tag{A15}$$

where N is the integer part of $L_1(n_2/n_1)$. The fact that all interfaces can be described in terms of independent jumps, leads to a very different situation from that found in the three-dimensional case, where the elementary excitations can only be described for a rigid horizontal interface. This analysis for the two-dimensional model was developed by Gallavotti [16] and further studied in Ref. 23.

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