Journal of Statistical Physics, Vol. 67, Nos. 3/4, 1992

# Convexity Properties of the Surface Tension and Equilibrium Crystals

**Alain Messager,**[1] **Salvador Miracle-Solé,**[1] **and Jean Ruiz**[1]

*Received November 26, 1991*

We study the thermodynamic limit of the orientation-dependent surface tension. Under general conditions, which we show to hold true for a large class of lattice systems, we prove that the limit exists and that it satisfies some convexity properties related to the pyramidal inequality introduced by R. L. Dobrushin and S. B. Shlosman.[1] We discuss some consequences of these results for the equilibrium crystal shape.

**KEY WORDS:** Surface tension; crystal shapes; pyramidal inequality; Wulff construction; Andreev construction.

## 1. INTRODUCTION

This work is devoted to a study of the surface tension and its dependence on the orientation of the interface in relation to the equilibrium crystal shape. The surface tension is also of a fundamental importance in the study of phase transitions and we refer the reader to ref. 2 for a review of many previous results.

It is well known that the equilibrium crystal shape of one component $a$ inside another component $b$ is obtained by minimizing the surface free energy between $a$ and $b$, and that this shape is given by the Wulff construction, provided one knows the orientation-dependent surface tension between the components. It is therefore important, even if a microscopic derivation of the Wulff construction within statistical mechanics has been proved only for a small class of lattice models,[3,4] to study the properties of the surface tension $\tau(\mathbf{n})$ as a function of the unit vector $\mathbf{n}$ which specifies the orientation of the interface. In particular, the above-mentioned

[1] Centre de Physique Théorique, CNRS-Luminy Case 907, F-13288 Marseille Cedex 9, France.



0022-4715/92/0500-0449$06.50/0 

microscopic derivations need a good knowledge of $\tau(\mathbf{n})$, and Dobrushin *et al.*[3] have proved, for the two-dimensional Ising model, an inequality between the surface tensions at different orientations, called the strong triangular inequality. A consequence this is that the corresponding Wulff shape is a convex body with smooth boundary. It was conjectured[1] that this inequality, in its nonstrict form, holds true in very general situations, as well as its higher dimensional analog called the pyramidal inequality.

In this paper we show, for lattice models in dimension $d \geqslant 2$ and under certain general assumptions, that the thermodynamic limit $\tau(\mathbf{n})$ of the finite-volume surface tension exists, and that it satisfies the pyramidal inequality. The assumptions are shown to hold true for a large class of models, as a consequence of correlation inequalities. The pyramidal inequality is shown to be equivalent to the convexity of a related quantity, namely of the function $f(\mathbf{x}) = |\mathbf{x}|\, \tau(\mathbf{x}/|\mathbf{x}|)$ (for any vector $\mathbf{x}$), and that it implies also the convexity of the projected surface tension $\tau_p = (1/n_d)\, \tau(n_1,..., n_d)$, as a function of $d-1$ variables. We may therefore define the convex conjugate functions or Legendre transforms of $f$ and $\tau_p$. Let us denote them by $\delta$ and $\varphi$, respectively. It turns out that $\delta$ is the indicator function of the equilibrium crystal shape and that the graph of $x_d = \varphi(x_1,..., x_{d-1})$ gives the boundary of this shape. Thus, $\varphi$ is the function used in the Andreev equivalent construction[5] of the equilibrium crystal shape, and we show that it can also be obtained as the free energy associated to an appropriate statistical ensemble.

The paper is organized as follows. In Section 2 we study the thermodynamic limit of the finite-volume surface tension under two general conditions called C1 and C2. We prove the existence of this limit for parallelepipedic and also for more general sequences of boxes. In Section 3 we show that, under the same conditions, the surface tension satisfies the pyramidal inequality and that the pyramidal inequality is equivalent to the convexity of $f(\mathbf{x})$. We also comment on the equilibrium crystal shape, discuss some consequences of the convexity of $f(\mathbf{x})$, and prove the equivalence of the statistical mechanical ensembles whose free energies give, respectively, the projected surface tension and the graph of the crystal shape. Other related results are described in a number of remarks at the end of Section 3. Finally, we prove in the Appendix that conditions C1 and C2 hold true for a general class of lattice systems.

## 2. DEFINITION OF THE SURFACE TENSION

We consider a spin model on a $d$-dimensional regular lattice $\mathscr{L}$, with configuration space $\Omega = S^{\mathscr{L}}$, where $S$ is a finite set of values of the spin $\sigma(i)$ attached at each lattice site $i$, and a finite-range, translation-invariant interaction $\{\phi_A\}$, $A \subset \mathscr{L}$. The functions $\phi_A\colon S^A \to \mathbb{R}$ may be understood as $A$-cylindrical functions on $\Omega$ such that $\phi_A = 0$ if diam $A > R$ and $\phi_{A'}(\sigma') = \phi_A(\sigma)$ if $A' = A + \alpha$ and $\sigma'(i+\alpha) = \sigma(i)$ for any $\alpha \in \mathscr{L}$. Denoting by $\sigma_\Lambda$ the restriction of a configuration $\sigma \in \Omega$ to a subset $\Lambda \subset \mathscr{L}$, $\sigma_\Lambda = \{\sigma(i)\}$, $i \in \Lambda$, and by $\sigma_\Lambda \cup \sigma_{\Lambda^c}$ the configuration (in $\Omega$) whose restrictions to $\Lambda$ and its complement $\Lambda^c = \mathscr{L} \backslash \Lambda$ are $\sigma_\Lambda$ and $\sigma_{\Lambda^c}$, respectively, we introduce the Hamiltonian in $\Lambda$ under a boundary condition $\bar{\sigma} \in \Omega$ by

$$H_\Lambda(\sigma_\Lambda \mid \bar{\sigma}) = \sum_{A \cap \Lambda \neq \varnothing} \phi_A(\sigma_\Lambda \cup \bar{\sigma}_{\Lambda^c}) \tag{1}$$

and the partition function at the inverse temperature $\beta$ by

$$Z^{\bar{\sigma}}(\Lambda) = \sum_{\sigma_\Lambda} \exp[-\beta H_\Lambda(\sigma_\Lambda \mid \bar{\sigma})] \tag{2}$$

We consider two distinct thermodynamic phases $(a)$ and $(b)$ that coexist at the inverse temperature $\beta$, which means two extremal periodic (with respect to the translations of $\mathscr{L}$) Gibbs states. We assume, as usual, that these states are associated with two periodic ground configurations $a = \{a(i)\}$, $i \in \mathscr{L}$, and $b = \{b(i)\}$, $i \in \mathscr{L}$, in such a way that they correspond to the limits, when $\Lambda \to \infty$, of the finite-volume Gibbs measures $Z^{\bar{\sigma}}(\Lambda)^{-1} \exp[-\beta H_\Lambda(\sigma_\Lambda \mid \bar{\sigma})]$ with the boundary conditions $\bar{\sigma}$ respectively equal to $a$ and $b$.

Let $\Lambda$ be a parallelepiped of sides $L_1,\ldots, L_{d-1}$, $M$, parallel to the axes $e_1,\ldots, e_d$, centered at the site $c \in \mathscr{L}$, and let $\mathbf{n} = (n_1,\ldots, n_d) \in \mathbb{R}^d$ be a unit vector such that $n_d = \mathbf{n} \cdot e_d > 0$. We denote by $p_{\mathbf{n}}$ the hyperplane orthogonal to $\mathbf{n}$ and passing through the center $c$ of $\Lambda$, by $S_{\mathbf{n}}(\Lambda)$ the area of the portion of this plane contained inside $\Lambda$, and by $(a, b, \mathbf{n})$ the mixed boundary condition where $\bar{\sigma}(i) = a(i)$ if $i$ is above the plane, i.e., if $(i - c) \cdot \mathbf{n} \geqslant 0$, and where $\bar{\sigma}(i) = b(i)$ if $(i - c) \cdot \mathbf{n} < 0$.

We define the surface tension associated with the interface $(a, b)$ orthogonal to $\mathbf{n}$ by

$$\tau(\mathbf{n}) = \lim_{L_1,\ldots, L_{d-1} \to \infty} \lim_{M \to \infty} \frac{F_{\mathbf{n}}(\Lambda)}{S_{\mathbf{n}}(\Lambda)} \tag{3}$$

where

$$F_{\mathbf{n}}(\Lambda) = -\frac{1}{\beta} \log \frac{Z^{(a,b,\mathbf{n})}(\Lambda)}{[Z^a(\Lambda)\, Z^b(\Lambda)]^{1/2}} \tag{4}$$

This definition is justified by noticing that in this expression the volume terms proportional to the free energy of the coexisting phases, as well as the terms corresponding to the boundary effects, cancel, and only the term that takes into account the free energy of the interface is left. The symmetry of the box and the boundary condition with respect to the center are necessary for the cancelation of the boundary terms. For a nonsymmetric box the numerator in the argument of the logarithm should be replaced by $[Z^{(a,b,\mathbf{n})}(\Lambda)\, Z^{(b,a,\mathbf{n})}(\Lambda)]^{1/2}$.

We shall also consider the projected surface tension defined by

$$\tau_p = \frac{\tau(\mathbf{n})}{n_d} \tag{5}$$

In order to study the existence of the limit (3) and some basic properties of the surface tension it will be useful to consider more general boxes and boundary conditions.

For any $i = (i_1, ..., i_d)$ we write $i' = (i_1, ..., i_{d-1})$ and consider these $i'$ as sites of a $(d-1)$-dimensional lattice $\mathscr{L}'$, the projection of $\mathscr{L}$ along the direction $e_d$. We introduce the vertical cylinders

$$\Lambda = \{i \in \mathscr{L}: i' \in Q,\, m_1(i') \leqslant i_d \leqslant m_2(i')\} \tag{6}$$

where $Q$ is a finite subset of $\mathscr{L}'$ and $x_d = m_k(x_1, ..., x_{d-1})$, $k = 1, 2$, are two hyperplanes in $\mathbb{R}^d$.

We introduce also more general mixed boundary conditions $(a, b, \lambda)$ associated with a smooth, real-valued function $x_d = \lambda(x_1, ..., x_{d-1})$ defined on $\mathbb{R}^{d-1}$, by taking $\bar{\sigma}(i) = a(i)$ if $i_d \geqslant \lambda(i')$ and $\bar{\sigma}(i) = b(i)$ if $i_d < \lambda(i')$. We assume that the normal vector $\mathbf{n}$ to the hypersurface $x_d = \lambda(x_1, ..., x_{d-1})$ satisfies $n_d > \alpha$ for some given $\alpha > 0$ and that the portion inside $\Lambda$ of the hyperplane $m_1$ lies above and at a distance larger than $R$ from this surface. The analogous condition is assumed for the hyperplane $m_2$ lying below $\lambda$.

Then we consider the expression

$$F(\Lambda) = -\frac{1}{\beta} \log \left( \frac{Z^{(a,b,\lambda)}(\Lambda)\, Z^{(b,a,\lambda)}(\Lambda)}{Z^a(\Lambda)\, Z^b(\Lambda)} \right)^{1/2} \tag{7}$$

which gives the residual free energy associated with the corresponding interface.

We remark that the following property holds:

*C.0: If $\Lambda$ and $\Lambda'$ are two disjoint boxes separated by a distance larger than R, then*

$$F(\Lambda \cup \Lambda') = F(\Lambda) + F(\Lambda') \tag{8}$$

This is because the partition functions in (7) factorize.

We assume that the following conditions are satisfied:

*C.1: If $\Lambda$ and $\Lambda'$ are cylindrical boxes with the same basis $Q$ and $\Lambda \supset \Lambda'$, then*

$$0 \leqslant F(\Lambda) \leqslant F(\Lambda') \tag{9}$$

*C.2: If $\Lambda$ and $\Lambda'$ are cylindrical boxes with bases $Q$ and $Q'$ and $\Lambda \supset \Lambda'$, then*

$$F(\Lambda) \leqslant F(\Lambda') + |Q \backslash Q'| \, (K/\alpha) \tag{10}$$

*where $K$ is some positive constant.*

In the Appendix we prove that conditions C1 and C2 are fulfilled for the following situations:

1. Ferromagnetic spin-1/2 systems with pair interactions, where

$$H = -\sum J_A \sigma_A$$

with $J_A \geqslant 0$, $J_A = 0$ if $|A|$ is odd, $\sigma_A = \prod_i \sigma(i)$, and $\sigma(i) \in \{-1, +1\}$. For these systems, which include the ferromagnets with two-body potentials at zero external field, the considered surface tension is that between the $(+)$ and $(-)$ phases respectively associated with the boundary conditions $a(i) = 1$ and $b(i) = -1$.

2. Ferromagnetic $q$-state spins systems of the form

$$H = -\sum J(M) \cos M\theta$$

where $M$ is a multiplicity function, $M\theta = \sum_i M_i \theta(i)$, $J(M) \geqslant 0$, $J(M) = 0$ unless $\sum_i M_i = 0$, $\theta(i) = (2\pi/q)\,\sigma(i)$, and $\sigma(i) \in \{1,..., q\}$. The Potts and clock models belong to this class of systems. For them the considered surface tension is that between two ordered phases $(a)$ and $(b)$ respectively associated with the boundary conditions $a(i) = a$ and $b(i) = b$, where $a, b \in \{1,..., q\}$.

3. Solid-on-solid models of interfaces.

The proof of conditions C1 and C2 given in the Appendix follows from correlation inequalities and is valid for all temperatures. Similar conditions should hold for a large class of spin systems, in particular, in the framework of the Pirogov–Sinaï theory[6] at low temperatures.

**Theorem 1.** Under the hypothesis above, the surface tension $\tau(\mathbf{n})$ defined by the limit (3) exists and equals

$$\inf_{L_1,..., L_{d-1}} \inf_{M} \frac{F_{\mathbf{n}}(\Lambda)}{S_{\mathbf{n}}(\Lambda)} \tag{11}$$

Moreover, $\tau(\mathbf{n})$ is nonnegative, bounded above by $K$, and lower semicontinuous as a function of $\beta$ and the interaction potentials.

*Proof.* First, we establish the monotonicity property

$$F_{\mathbf{n}}(\{L_i\}, M) \leqslant F_{\mathbf{n}}(\{L_i\}, M') \qquad \text{if} \quad M \geqslant M' \tag{12}$$

for $F_{\mathbf{n}}(\Lambda) = F_{\mathbf{n}}(\{L_i\}, M)$ and $M'$ large enough. This shows that the limit $M \to \infty$ exists and

$$\lim_{M \to \infty} F_{\mathbf{n}}(\{L_i\}, M) = \inf_M F_{\mathbf{n}}(\{L_i\}, M) \equiv F_{\mathbf{n}}(\{L_i\}) \tag{13}$$

We shall then prove that $F_{\mathbf{n}}(\{L_i\})$ is bounded

$$F_{\mathbf{n}}(\{L_i\}) \leqslant \prod_{i=1}^{d-1} (L_i + R)(K/n_d) \tag{14}$$

and that it satisfies the following subadditivity property (up to boundary terms)

$$\begin{aligned} &F_{\mathbf{n}}(\{L_1' + L_1'' + R, L_2, ..., L_{d-1}\}) \\ &\quad \leqslant F_{\mathbf{n}}(\{L_1', L_2, ..., L_{d-1}\}) + F_{\mathbf{n}}(\{L_1'', L_2, ..., L_{d-1}\}) \\ &\quad\quad + \sum_{i=1}^{d-1} \frac{2RKL_1 \cdots L_{d-1}}{L_i} + \frac{RKL_2 \cdots L_{d-1}}{\alpha} \end{aligned} \tag{15}$$

The subadditivity (15) together with the bound $F(\Lambda) \geqslant 0$ implies, following standard arguments in the theory of thermodynamic limits (see, for instance, ref. 7), the existence of

$$\lim_{L_i \to \infty} \left( \prod_{i=1}^{d-1} \frac{1}{L_i} \right) \cdot F_{\mathbf{n}}(\{L_i\}) \tag{16}$$

which equals the infimum over $L_1, ..., L_{d-1}$. Since $S_n(\Lambda) = (1/n_d) \prod L_i$, this ends the proof of the first part of Theorem 1.

From $F(\Lambda) \geqslant 0$ it follows that $\tau(\mathbf{n}) \geqslant 0$, the upper bound follows from (14), and the lower semicontinuity from the fact that $\tau(\mathbf{n})$ is the infimum over a set of continuous functions.

We next prove properties (12), (14), and (15).

The monotonicity property (12) follows clearly from condition C1. The upper bound (14) follows from condition C2 by taking $\Lambda' = \varnothing$.

In order to prove the subadditivity property (15), we consider three parallelepipeds $\Lambda'$, $\Lambda''$, and $\Lambda$ of sides $(L_1', L_2, ..., L_{d-1}, M')$, $(L_1'', L_2, ..., L_{d-1}, M'')$, and $(L_1' + L_1'' + R, L_2, ..., L_{d-1}, M)$ placed in such a way that $\Lambda' \cup \Lambda'' \subset \Lambda$, the distance from $\Lambda'$ to $\Lambda''$ is $R$, and the same hyperplane which passes through the center $c \in \mathscr{L}$ of $\Lambda$ passes also through the center of $\Lambda'$ and $\Lambda''$, and defines the $(a, b)$ boundary condition for the three boxes. Now we apply condition C2, taking (8) into account:

$$F_{\mathbf{n}}(\Lambda) \leqslant F_{\mathbf{n}}(\Lambda') + F_{\mathbf{n}}(\Lambda'') + \frac{RKL_2 \cdots L_{d-1}}{\alpha} \tag{17}$$

We notice that the first term on the right-hand side of (17) approximatively coincides with the sum $F_{\mathbf{n}}(\{L_1', L_2,..., L_{d-1}\}) + F_{\mathbf{n}}(\{L_1'', L_2,..., L_{d-1}\})$, when $M'$, $M''$, and $M$ tend to infinity. Some error is made because from the construction the centers of $\Lambda'$ and $\Lambda''$ do not necessarily coincide with a site of the lattice, as is assumed in the definition of $\tau(\mathbf{n})$. This error is bounded, however, by the third term on the left-hand side of (15). This may be seen by using an appropriate function $\lambda$ introduced to compensate the displacement of the center (by a distance less than one) and the fact that the interaction has a finite norm. ∎

We next extend the proof of the existence of the limit to more general sequences of boxes.

We shall consider the boxes $\Lambda$ defined by (6), in which $m_1$ and $m_2$ are two parallel hyperplanes. For these boxes $F(\Lambda)$ will represent the function defined by (7) when the function $\lambda$ specifying the boundary conditions is a hyperplane $x_d = p_{\mathbf{n}}(x_1,..., x_{d-1})$ orthogonal to $\mathbf{n}$. We assume that

$$m_1(i') \leqslant p_{\mathbf{n}}(i') \leqslant m_2(i') \qquad \text{for all} \quad i' \in Q \tag{18}$$

and when the hyperplanes $m_1$ and $m_2$ are orthogonal to $\mathbf{n}$, we denote by $h_1$ and $h_2$ their respective distances to the hyperplane $p_{\mathbf{n}}$.

Let $|Q_\rho|$ be the number of lattice sites at distance less than or equal to $\rho$ to $Q$ and to its complement. We say that the sets $Q$ tend to infinity in the sense of van Hove if $|Q| \to \infty$ and $|Q_\rho|/|Q| \to 0$ for all $\rho \geqslant 0$. We say that the sets $Q$ tend to infinity in the sense of Lanford, $Q \to \mathscr{L}'$, if they become infinitely large in the sense of van Hove and for each $Q$ there is a parallelepiped $P_Q$ which contains $Q$ such that for sufficiently small $\delta > 0$ and all $Q$ we have $|Q|/|P_Q| \geqslant \delta$.

**Theorem 2.** Under the above hypotheses, if the family of sets $Q \subset \mathscr{L}'$ tend to infinity in the sense of Lanford, then the limit defining the surface tension exists

$$\tau(\mathbf{n}) = \lim_{Q \to \mathscr{L}'} \frac{F(\Lambda)}{|Q|} \cdot n_d$$

provided that the heights $h_1 = h_1(Q)$ and $h_2 = h_2(Q)$ tend to infinity when $Q \to \mathscr{L}'$ (as slowly as we wish).

*Proof.* The fact that instead of taking a family of parallelepipeds $Q$ one can choose a family of sets $Q$ tending to infinity in the sense of Lanford is a known result in the theory of the thermodynamic limit. We refer the reader to ref. 7 for this. We thus restrict ourselves to the situation where the basis of the cylinder $\Lambda$ is a parallelepiped $Q$ of sides $L_1,..., L_{d-1}$. To prove the theorem in this case, we shall generalize an argument used in ref. 8 for the analysis of the surface tension in the Ising model.

We deal first with the case in which the hyperplanes $m_1$ and $m_2$ are parallel to $p_{\mathbf{n}}$, and assume that $h_1(Q)$ and $h_2(Q)$ tend to infinity when $Q \to \mathscr{L}'$.

First, we consider a cylinder $\bar{\Lambda}$ of parallelepipedic basis $\bar{Q}$ with sides $L'_1,..., L'_{d-1}$, centered on a lattice site, and defined with two hyperplane at distance $\bar{h}$ from the hyperplane orthogonal to $\mathbf{n}$ and passing through the center of $\bar{\Lambda}$. We take $L'_i = (L_i/r) - (R/2)$, for $i = 1,..., d-1$ and some integer $r$, and put $\bar{h} = \min\{h_1 - 1, h_2 - 1\}$. We notice that it is possible to place $k = r^{d-1}$ translates $\Lambda_j$ of $\bar{\Lambda}$ inside $\Lambda$ in such a way that the mutual distances between two different cylinders is at least $R$ and that the hyperplane orthogonal to $\mathbf{n}$, which defines the boundary condition for $\Lambda$, is at distance less than one from the centers of the $\Lambda_j$. Then conditions C2, with $\Lambda' = \bigcup \Lambda_j$, and C0 give

$$F(\Lambda) \leqslant \sum_{j=1}^{k} F(\Lambda_j) + \left(\frac{|Q|\, R(d-1)}{\inf L'_i}\right) \frac{K}{\alpha}$$

Assume that $F(\bar{\Lambda})$ is computed with the boundary condition determined on $\bar{\Lambda}$ by the hyperplane orthogonal to $\mathbf{n}$ which passes through its center. Then by taking into account condition C1 and the fact that the difference arising from the two boundary conditions, defined with different hyperplanes at distance less than one, is at most $RK/n_d$ multiplied by the perimeter of $\bar{Q}$, we get

$$F(\Lambda_j) \leqslant F(\bar{\Lambda}) + \sum_{i=1}^{d-1} \frac{2RKL'_1 \cdots L'_{d-1}}{n_d \cdot L'_i} \tag{19}$$

for each $\Lambda_j$, and therefore

$$\frac{F(\Lambda)}{|Q|} \leqslant \frac{F(\bar{\Lambda})}{|\bar{Q}|} + \frac{RK(d-1)}{\alpha \min L'_i} + \frac{2RK}{k} \sum_{i=1}^{d-1} \frac{1}{L'_i}$$

Then, by letting $r \to \infty$, we obtain

$$\limsup_{Q \to \mathscr{L}'} \frac{F(\Lambda)}{|Q|} \leqslant \frac{1}{|\bar{Q}|} \lim_{h \to \infty} F(\bar{\Lambda}) + o(|\bar{Q}|) \tag{20}$$

where $o(|\bar{Q}|) \to 0$ when $L_1, \ldots, L_{d-1} \to \infty$.

Next, we prove the converse inequality. We choose $\bar{\Lambda}$ with basis $\bar{Q} = Q$ and $h$ large enough, placed in such a way that $\bar{\Lambda} \supset \Lambda$ and that the two hyperplanes defining the boundary conditions for $\Lambda$ and $\bar{\Lambda}$ are at distance less than one. Then condition C1, together with the bound used in (19), implies

$$F(\Lambda) \geqslant F(\bar{\Lambda}) - \sum_{i=1}^{d-1} \frac{2RKL_1 \cdots L_{d-1}}{n_d \cdot L_i}$$

and therefore

$$\liminf_{Q \to \mathscr{L}'} \frac{F(\Lambda)}{|Q|} \geqslant \lim_{Q \to \mathscr{L}'} \frac{1}{|\bar{Q}|} \lim_{h \to \infty} F(\bar{\Lambda}) \tag{21}$$

The theorem in the considered case now follows from (20) and (21), because for $\bar{Q} \to \mathscr{L}'$, the right-hand sides of both inequalities coincide with $(1/n_d)\,\tau(\mathbf{n})$.

We next deal with the case in which $m_1$ and $m_2$ are not orthogonal to $\mathbf{n}$ and relation (18) is satisfied. We notice that inequality (21) may be proved as above. To prove (20), we proceed by defining the box $\bar{\Lambda}$ and its $k = (d-1)^r$ translates as was done above, the only difference being that now all translates $\Lambda_1, \ldots, \Lambda_k$ of $\bar{\Lambda}$ may be placed inside $\Lambda$, except those whose bases $Q_j$ are at distance less than one from $\mathscr{L}' \backslash Q$. Neglecting these exceptional $\Lambda_j$, whose number is only proportional to $(d-2)^r$, the same argument gives the desired inequality (20) and ends the proof of the theorem. ∎

*Remark 1.* The interface often has large oscillations, with probability one, which are perhaps not permitted inside the box assumed in Theorem 2. Nevertheless, one always obtains the correct surface tension.

*Remark 2.* The surface tension defined by (3) has the same symmetry properties under rotations and reflections of the lattice as the interactions. One easily sees this fact by taking an appropriately symmetric $\Lambda$ and then applying Theorem 2.

*Remark 3.* In this section it has been assumed that $n_d > 0$. It is clear that this is not a real restriction for lattice systems (it is a necessary hypothesis instead for solid-on-solid models), and that by choosing appropriate axes we obtain $\tau(\mathbf{n})$ for all $\mathbf{n}$. Since the surface tension only depends on the orientation of the plane $p_{\mathbf{n}}$, we have $\tau(\mathbf{n}) = \tau(-\mathbf{n})$.

## 3. CONVEXITY PROPERTIES

Let $A_0, A_1, ..., A_d \in \mathbb{R}^d$ be any set of $d+1$ points in general position and, for $i = 0, ..., d$, let $\Delta_i = \Delta(A_0, ..., \hat{A}_i, ..., A_d)$ be the $(d-1)$-dimensional simplex defined by all points $A_0, ..., A_d$, except $A_i$. We denote by $\mathbf{n}_i$ the unit vector orthogonal to $\Delta_i$ and by $|\Delta_i|$ the $(d-1)$-dimensional area of $\Delta_i$. Following ref. 1, we say that $\tau(\mathbf{n})$ satisfies the pyramidal inequality if, for any set $A_0, ..., A_d$,

$$|\Delta_0| \, \tau(\mathbf{n}_0) \leqslant \sum_{i=1}^{d} |\Delta_i| \, \tau(\mathbf{n}_i) \tag{22}$$

We introduce the function on $\mathbb{R}^d$ defined by

$$f(\mathbf{x}) = |\mathbf{x}| \, \tau(\mathbf{x}/|\mathbf{x}|) \tag{23}$$

**Theorem 3.** The following propositions are equivalent:

1. $\tau(\mathbf{n})$ satisfies the pyramidal inequality.
2. $f(\mathbf{x})$ is a positively homogeneous convex function.

Moreover, for the considered systems and under conditions C1 and C2, these propositions hold.

*Proof.* For simplicity, we shall restrict ourselves to the 3-dimensional case. We first prove statement 1 for the systems under consideration.

We introduce the vertices $A_0, ..., A_3$ of the pyramid and their projections $A'_0, ..., A'_3$ on the horizontal plane, and assume that $A'_0$ falls in the interior of the triangle $A'_1, A'_2, A'_3$. We denote by $Q_0$ the set of sites of $\mathscr{L}'$ inside the triangle $A'_1, A'_2, A'_3$ and by $Q_1$ the set of sites of $\mathscr{L}'$ inside the triangle $A'_0, A'_2, A'_3$ whose distance from the sides of this triangle is larger than $R$. Similarly, we define the sets $Q_2$ and $Q_3$ with respect to the triangles $A'_0, A'_1, A'_3$ and $A'_0, A'_1, A'_2$. We introduce $\lambda(x_1, x_2)$ as the function associated with the surface which coincides with the plane $A_1, A_2, A_3$ outside the triangle $A'_1, A'_2, A'_3$ and with the other three faces of the pyramid inside it. Taking into account definition (7) and condition C1, we write $F(Q) = \inf_\Lambda F(\Lambda)$. Then condition C2 and property (8) imply

$$F(Q_0) \leqslant F(Q_1) + F(Q_2) + F(Q_3) + |Q_0 \backslash (Q_1 \cup Q_2 \cup Q_3)| \, (K/\alpha)$$

From this relation the pyramidal inequality follows by using Theorem 2 and passing to the limit when the three triangles tend to infinity.

We shall now prove that statements 1 and 2 are equivalent.

Clearly, from definition (23),

$$f(\alpha \mathbf{x}) = \alpha f(\mathbf{x}) \qquad \text{for any} \quad \alpha > 0 \tag{24}$$

and conversely. In dimension $d = 2$, it is easy to see that the triangular inequality for $\tau(\mathbf{n})$ is equivalent to

$$f(\mathbf{x} + \mathbf{y}) \leqslant f(\mathbf{x}) + f(\mathbf{y}) \tag{25}$$

But properties (24) and (25) just say that $f$ is a positively homogeneous convex function. We shall now show that also in dimension $d = 3$, property (25) is equivalent to the pyramidal inequality for $\tau(\mathbf{n})$. In fact, since

$$|\Delta_0|\, \mathbf{n}_0 = |\Delta_1|\, \mathbf{n}_1 + |\Delta_2|\, \mathbf{n}_2 + |\Delta_3|\, \mathbf{n}_3 \tag{26}$$

the pyramidal inequality says that

$$f(\mathbf{x}_1 + \mathbf{x}_2 + \mathbf{x}_3) \leqslant f(\mathbf{x}_1) + f(\mathbf{x}_2) + f(\mathbf{x}_3) \tag{27}$$

with $\mathbf{x}_k = |\Delta_k|\, \mathbf{n}_k$, $k = 1,..., 3$. To prove (25), it is enough to find pyramids such that

$$|\Delta_1|\, \mathbf{n}_1 \to \mathbf{x}, \qquad |\Delta_2|\, \mathbf{n}_2 \to \mathbf{y}, \qquad |\Delta_3|\, \mathbf{n}_3 \to 0 \tag{28}$$

for all $\mathbf{x}$ and $\mathbf{y}$. This may be done as follows. We place the vertices $A_0$ and $A_1$ on the line of intersection of two planes $p_1$ and $p_2$, respectively, orthogonal to $\mathbf{x}$ and $\mathbf{y}$. We choose $A_2$ on $p_1$ and $A_3$ on $p_2$ in such a way that the angles $A_0A_1A_2$ and $A_0A_1A_3$ are equal and that $\overline{A_2A_1}/\overline{A_3A_1} = |\mathbf{x}|/|\mathbf{y}|$. By letting the distance $\overline{A_0A_1}$ tend to infinity while $\overline{A_0A_2}$ and $\overline{A_0A_3}$ are kept constant, we find that (28) and therefore (25) follow. ∎

*Remark 4.* Since $\tau(\mathbf{n})$ is bounded, the convex function $f(\mathbf{x})$ is everywhere finite and hence (see ref. 9, Theorem 24.7) Lipschitz continuous.

The pyramidal inequality may be interpreted as a thermodynamic stability condition[1,3] and thus also the convexity of $f(\mathbf{x})$. The relevance of this inequality in the Wulff construction of the shape of a drop (equilibrium crystal) has already been discussed in ref. 1.[2] Using the theory of convex functions initiated by Minkowsky,[9,12] we briefly comment on this subject.

[2] More general conditions called ellipticity and semiellipticity appear in the mathematical literature; see ref. 10, Chapter 5, where instead of pyramids one considers more general subspaces of $\mathbb{R}^d$. In particular, the semiellipticity condition implies the pyramidal inequality and the ellipticity condition implies the strict pyramidal inequality.[11]

Let us recall that for any convex set $\mathscr{K}$ in $\mathbb{R}^d$ the support function of $\mathscr{K}$ is the real (or $+\infty$)-valued function defined on $\mathbb{R}^d$ by

$$\delta^*(\mathbf{y} \mid \mathscr{K}) = \sup_{\mathbf{x} \in \mathscr{K}} \mathbf{x} \cdot \mathbf{y} \tag{29}$$

and that the support functions of nonempty convex bodies are the finite, positively homogeneous convex functions (see ref. 9, p. 114). A second function associated with a convex set $\mathscr{K}$, which is also positively homogeneous and convex, is the gauge function, defined by

$$g(\mathbf{y} \mid \mathscr{K}) = \inf_{\lambda > 0,\, \mathbf{y} \in \lambda \mathscr{K}} \lambda$$

It is also known that the support function of a convex set characterizes the set. This fact can be quantitatively expressed with the notion of the indicator function of a convex set

$$\delta(\mathbf{x} \mid \mathscr{K}) = \begin{cases} 0, & \text{if } \mathbf{x} \in \mathscr{K} \\ +\infty, & \text{if } \mathbf{x} \notin \mathscr{K} \end{cases} \tag{30}$$

It then turns out that $\delta$ and $\delta^*$ are conjugate convex functions, i.e., they are related by the Legendre transformations

$$\delta(\mathbf{x} \mid \mathscr{K}) = \sup_{\mathbf{y}} \{\mathbf{x} \cdot \mathbf{y} - \delta^*(\mathbf{y} \mid \mathscr{K})\} \tag{31}$$

$$\delta^*(\mathbf{y} \mid \mathscr{K}) = \sup_{\mathbf{x}} \{\mathbf{x} \cdot \mathbf{y} - \delta(\mathbf{x} \mid \mathscr{K})\} \tag{32}$$

The crystal shape $\mathscr{W}$, which is defined as an intersection of closed half-spaces, namely

$$\mathscr{W} = \{\mathbf{x} \colon \mathbf{x} \cdot \mathbf{n} \leqslant \tau(\mathbf{n})\} \tag{33}$$

is therefore a closed, bounded convex set (i.e., a convex body). It has been established in refs. 1 and 3 that among the functions which through (33) define the same shape $\mathscr{W}$, there is a unique $\tau(\mathbf{n})$ which satisfies the pyramidal inequality.

From (23) and (33) we see that in fact the Wulff construction tells us that $f$ is the support function of the crystal shape $\mathscr{W}$, i.e.,

$$f(\mathbf{y}) = \delta^*(\mathbf{y} \mid \mathscr{W}) \tag{34}$$

Therefore, the indicator function $\delta(\mathbf{x} \mid \mathscr{W})$ of the Wulff crystal shape is the Legendre transform of $f$.

Though nonsymmetric situations are also physically interesting (they appear, for instance, in the case of a sessile drop on a wall), in the case under consideration we have $f(\mathbf{x}) = f(-\mathbf{x})$ and the convex body $\mathscr{W}$ is symmetric with respect to the origin. Now, if $\mathscr{W}$ is a symmetric, closed, bounded, convex set and the origin belongs to the interior of $\mathscr{W}$, then the support function of $\mathscr{W}$ is finite everywhere, symmetric, and strictly positive except at the origin (i.e., it is a norm). See ref. 9, Theorem 15.2.

In this case, the function $f$ may then be interpreted as the gauge function of some convex body $\mathscr{W}^* = \{\mathbf{x}: f(\mathbf{x}) \leqslant 1\}$, the dual of the set $\mathscr{W}$ (the gauge function of $\mathscr{W}$ is $g(\mathbf{x}) = \sup_{\mathbf{y}} [\mathbf{x} \cdot \mathbf{y}/f(\mathbf{y})]$). One can use the convex set $\mathscr{W}^*$ instead of the usual Wulff polar plot of $\tau(\mathbf{n})$ to study the properties of the crystal shape $\mathscr{W}$. This duality tells us, for example, in dimension $d = 3$, that corners and edges on $\mathscr{W}^*$ correspond to plane facets and straight lines in $\mathscr{W}$, and conversely.[3] The strict convexity of $f$ (or the strict pyramidal inequality) implies that the crystal shape has no edges or corners.

Andreev[5] first pointed out that the Wulff construction is simply the geometrical version of a Legendre transformation. He obtained from this fact a function $\varphi$ on $\mathbb{R}^{d-1}$ such that the graph of $x_d = \varphi(x_1,..., x_{d-1})$ for $x_d > 0$ coincides with the boundary of the crystal shape $\mathscr{W}$. Since $\mathscr{W}$ is a convex body, symmetric with respect to the origin, $\varphi$ is a concave function, and

$$\mathscr{W} = \{\mathbf{x} \in R^d: -\varphi(-x_1,..., -x_{d-1}) \leqslant x_d \leqslant \varphi(x_1,..., x_{d-1})\} \tag{35}$$

In the present context this means that $-\varphi$ is the convex conjugate of another convex function. It is not difficult to see that this function is the projected surface tension (5), considered as a function $\tau_p(\mathbf{v})$ on $\mathbb{R}^{d-1}$ by letting $\mathbf{v} = (n_1/n_d,..., n_{d-1}/n_d)$. Then, since

$$\tau_p(x_1,..., x_{d-1}) = f(x_1,..., x_{d-1}, 1) \tag{36}$$

the function $\tau_p$ is convex, and

$$-\varphi(\mathbf{u}) = \tau_p^*(\mathbf{u}) = \sup_{\mathbf{v}} \{\mathbf{u} \cdot \mathbf{v} - \tau_p(\mathbf{v})\} \tag{37}$$

Indeed, from (31) we see that, if $\mathbf{x} \in \mathscr{W}$, then, $\mathbf{x} \cdot \mathbf{y} - f(\mathbf{y}) \leqslant 0$ for any $\mathbf{y}$, and therefore

$$x_d \leqslant f(y_1,..., y_{d-1}, 1) - (x_1 y_1 + \cdots + x_{d-1} y_{d-1}) \tag{38}$$

which together with (36) and with the definition of $\varphi$ implies (35).

[3] Let us illustrate these facts in the simplest example of the Ising ferromagnet at zero temperature. In this case $\tau(\mathbf{n}) = J(|n_1| + \cdots + |n_d|)$ and its polar plot consists of a portion of a sphere in each octant of $\mathbb{R}^d$. The function $f$ is then $f(\mathbf{x}) = J(|x_1| + \cdots + |x_d|)$, which is the support function of a cube, and $g(\mathbf{x}) = J \max\{|x_1|,..., |x_d|\}$ is the associated gauge function.

The crystal shape itself may be regarded as the free energy associated with a statistical mechanical ensemble. This ensemble is defined by expressions (39) and (40) below and, as we shall prove in the next theorem, gives the function $\varphi$ in the thermodynamic limit.

Let $\Lambda$ be a parallelepipedic box of sides $L_1,..., L_{d-1}$, $M$ with basis

$$Q = \{i \in \mathscr{L}': 0 \leqslant i_k \leqslant L_k, k = 1,..., d-1\}$$

For $\mathbf{v} \in \mathbb{R}^{d-1}$, we denote by $(a, b, \mathbf{v})$ the mixed boundary condition $(a, b, \lambda)$ when $\lambda$ is the hyperplane which passes through the origin and the points

$$(L_1, 0,..., 0, v_1), (0, L_2,..., 0, v_2),..., (0, 0,..., L_{d-1}, v_{d-1})$$

For any $\mathbf{u} \in \mathbb{R}^{d-1}$ we define

$$\Xi_Q(\mathbf{u}) = \sum_{\mathbf{v} \in \mathbb{Z}^{d-1}} \{\exp[\beta(\mathbf{u} \cdot \tilde{\mathbf{V}})]\} \sup_M \left(\frac{Z^{(a,b,\mathbf{v})}(\Lambda)\, Z^{(b,a,\mathbf{v})}(\Lambda)}{Z^a(\Lambda)\, Z^b(\Lambda)}\right)^{1/2} \tag{39}$$

and

$$\varphi_Q(\mathbf{u}) = -\frac{1}{\beta\,|Q|} \log \Xi_Q(\mathbf{u}) \tag{40}$$

where the vector $\tilde{\mathbf{V}}$ is related to $\mathbf{v}$ by $\tilde{V}_i = (|Q|/L_i)\, v_i$, for $i = 1,..., d-1$.

We introduce the effective domain of a convex function $f$ on $\mathbb{R}^{d-1}$ to be the set

$$\operatorname{dom} f = \{\mathbf{u}: f(\mathbf{u}) < \infty\}$$

We define $D = \operatorname{dom}(-\varphi)$ and write, respectively, $D^{\text{int}}$, $\bar{D}$, and $\partial D$ for the interior, the closure, and the boundary of the convex set $D$.

**Theorem 4.** Under the above hypothesis, we have the following results.

1. If $\mathbf{u} \in D^{\text{int}}$, then the thermodynamic limit of $\varphi_Q(\mathbf{u})$ exists, and

$$\lim_{Q \to \mathscr{L}'} \varphi_Q(\mathbf{u}) = \varphi(\mathbf{u})$$

2. If $\mathbf{u} \in \mathbb{R}^{d-1} \backslash \bar{D}$, then

$$\lim_{Q \to \mathscr{L}'} \varphi_Q(\mathbf{u}) = -\infty$$

3. If $\mathbf{u} \in \partial D$, then

$$\limsup_{Q \to \mathscr{L}'} \varphi_Q(\mathbf{u}) \leqslant \limsup_{\substack{\mathbf{u}_0 \to \mathbf{u} \\ \mathbf{u}_0 \in \operatorname{int} D}} \varphi(\mathbf{u}_0)$$

*Proof.* We first remark that if we define $F_{\mathbf{v}}(Q) = \inf_M F(\Lambda)$, where $F(\Lambda)$ is the function introduced in (7), we may write

$$\Xi_Q(\mathbf{u}) = \sum_{\mathbf{v} \in \mathbb{Z}^{d-1}} \{\exp[\beta(\mathbf{u} \cdot \tilde{\mathbf{V}})] \exp[-\beta F_{\mathbf{v}}(Q)]\}$$

We introduce

$$\Xi_Q^+(\mathbf{u}) = \sup_{\mathbf{v} \in \mathbb{Z}^{d-1}} \{\exp[\beta(\mathbf{u} \cdot \tilde{\mathbf{V}})] \exp[-\beta F_{\mathbf{v}}(Q)]\}$$

and proceed, as in the Appendix of ref. 13, to study the thermodynamic limit for this quantity.

According to Theorem 1 and definition (37), we have

$$|Q| \ (\mathbf{u} \cdot \mathbf{v}) - F_{\mathbf{v}}(Q) \leqslant |Q| \ \tau_p^*(\mathbf{u})$$

for all $\mathbf{v} \in \mathbb{R}^{d-1}$, so that

$$\Xi_Q^+(\mathbf{u}) \leqslant \exp[\beta \ |Q| \ \tau_p^*(\mathbf{u})] \tag{41}$$

On the other hand, for any $\delta > 0$ and sufficiently large $Q$ one can find, taking into account that $\tau_p(\mathbf{v}) = \inf_{Q \subset \mathscr{L}'} [F_{\mathbf{v}}(Q)/|Q|]$ and definition (37), an orientation $\mathbf{v} \in \mathbb{R}^{d-1}$ such that

$$\begin{aligned}
|Q| \ (\mathbf{u} \cdot \mathbf{v}) - F_{\mathbf{v}}(Q) &= |Q| \left[ (\mathbf{u} \cdot \mathbf{v}) - \frac{F_{\mathbf{v}}(Q)}{|Q|} \right] \\
&= |Q| \ [(\mathbf{u} \cdot \mathbf{v}) - \tau_p(\mathbf{v})] + |Q| \left[ \tau_p(\mathbf{v}) - \frac{F_{\mathbf{v}}(Q)}{|Q|} \right] \\
&\geqslant |Q| \ [\tau_p^*(\mathbf{u}) - \delta]
\end{aligned}$$

and therefore

$$\Xi_Q^+(\mathbf{u}) \geqslant \exp\{\beta \ |Q| \ [\tau_p^*(\mathbf{u}) - \delta]\} \tag{42}$$

Inequalities (41) and (42) imply the statement 1 of the theorem with $\Xi$ replaced by $\Xi^+$.

To prove this statement for $\Xi$, we follow the argument of Theorem 2 in ref. 13. First, it is clear that

$$\Xi_Q^+(\mathbf{u}) \leqslant \Xi_Q(\mathbf{u})$$

Next, let $I$ be the $(d-1)$-dimensional interval

$$I = \{\mathbf{u} \in \mathbb{R}^{d-1} \colon u_i' \leqslant u_i \leqslant u_i'', \ i = 1, \ldots, d-1\}$$

and $J$ the set of the vertices of $I$. Then, the inequality

$$\exp[-\beta F_{\mathbf{v}}(Q)] \leqslant \{\exp[-\beta\, |Q|\, (\bar{\mathbf{u}} \cdot \mathbf{v})]\}\, \Xi_Q^+(\bar{\mathbf{u}})$$

for $\bar{\mathbf{u}} \in J$ implies

$$\Xi_Q(\mathbf{u}) \leqslant \prod_{i=1}^{d-1} \left\{ \sum_{v_i \geqslant 0} \exp[\beta\, |Q|\, v_i(u_i' - u_i)] + \sum_{v_i \leqslant 0} \exp[\beta\, |Q|\, v_i(u_i'' - u_i)] \right\} \cdot \sup_{\bar{\mathbf{u}} \in J} \Xi_Q^+(\bar{\mathbf{u}})$$

so that, for $\mathbf{u} \in I$, we get

$$\Xi_Q(\mathbf{u}) \leqslant \left[ \frac{2}{1 - e^{-\gamma\Delta}} \right]^{d-1} \sup_{\bar{\mathbf{u}} \in J} \Xi_Q^+(\bar{\mathbf{u}})$$

where

$$\Delta = \min_{i=1,\dots,d-1} \min_{\bar{\mathbf{u}} \in J} |u_i - \bar{u}_i|, \qquad \gamma = \min_{i=1,\dots,d-1} (\beta\, |Q|/L_i)$$

Then we conclude the proof of Statement 1 by using the continuity of $\tau_p^*(\mathbf{u})$. Statements 2 and 3 can be proved analogously; see again ref. 13. ∎

*Remark 5.* An interesting application of Theorem 4 comes from the fact that generally $\varphi(u)$ is easier to compute than $\tau(\mathbf{n})$, because the summation on the right-hand side of (39) suppresses a canonical constraint. In particular, in dimension two, for the interface described by the solid-on-solid model (see the Appendix for the definition of this model) the function $\varphi$ is easily computed by summing a geometrical series, and one obtains

$$\varphi(u) = J - \beta^{-1} \log \frac{\sinh \beta J}{\cosh \beta J - \cosh \beta u}$$

where $u \in D^{\text{int}}$ and $D = [-J, J]$.

*Remark 6.* Notice that in dimension two, if $\mathbf{n} = (-\sin\theta, \cos\theta)$ and $\tau(\theta) = \tau(\mathbf{n})$, then $v = -\tan\theta$ and the projected surface tension is

$$\tau_p(v) = \tau(\mathbf{n})/\cos\theta$$

When $\tau_p$ is differentiable, the maximum in (37) is obtained for $v = -\tan\theta$ such that $u = \tau_p'(v)$, i.e., for

$$u = -\sin\theta\, \tau(\theta) - \cos\theta\, \tau'(\theta) \tag{43}$$

which gives

$$\varphi(u) = \cos\theta\, \tau(\theta) - \sin\theta\, \tau'(\theta) \tag{44}$$

$$\varphi'(u) = \tan\theta \tag{45}$$

$$-\varphi''(u) = 1/\tau_p''(v) = 1/\{\cos^3\theta[\tau(\theta) + \tau''(\theta)]\} \tag{46}$$

It has been proposed that the right-hand side of (46) is the mean square vertical displacement per unit length of an interface with slope $\theta$. This has been proved in the cases of solid-on-solid and Ising models.[18] When the denominator of this term is strictly positive (and this was also shown in the above-mentioned cases), then the strong triangular inequality holds and the equilibrium shape has a smooth boundary.

*Remark 7.* For the two-dimensional Ising model with nearest neighbor interactions, with horizontal and vertical coupling constants $J_1$ and $J_2$, it has been shown[14] that the right-hand side of (44) is (up to a factor $\beta^{-1}$) the Onsager function $\hat{\gamma}(\omega)$, while that of (45) is its derivative (up to a factor $-i$). The Onsager function is defined by the equation

$$\cosh\hat{\gamma}(\omega) = \cosh 2K_1 \cosh 2K_2^* - \sinh 2K_1 \sinh 2K_2^* \cos\omega$$

where $K_i = \beta J_i$ for $i = 1, 2$ and $K_i^* = -(1/2)\log\tanh K_i$ are the dual coupling constants. We thus get $\hat{\gamma}(\omega) = \beta\varphi(u)$ and $i\omega = \beta u$, so that the Wulff shape can be obtained from

$$\varphi(u) = \beta^{-1}\hat{\gamma}(-i\beta u)$$

*Remark 8.* Recalling the modified Young relation for a sessile drop of a phase $a$ inside a phase $b$ on a wall $w$, that is,

$$\cos\theta_0\, \tau_{ab}(\theta_0) - \sin\theta_0\, \tau'_{ab}(\theta_0) = \tau_{aw} - \tau_{bw}$$

where $\tau_{\alpha\beta}$ denotes the surface tension between the considered phases, we see that relations (43)–(45) lead directly to the Winterbottom construction[15] and give an easy way to compute the contact angle of the drop with the wall, namely

$$\theta_0 = \arctan\varphi'_{ab}[\varphi_{ab}^{-1}(\tau_{aw} - \tau_{bw})]$$

*Remark 9.* It is also convenient to use the functions $\varphi$ to study the coexistence of three phases, say $a$, $b$, and $c$. In this case, one associates three functions $\varphi_{ab}$, $\varphi_{bc}$, and $\varphi_{ac}$ with the three corresponding interfaces.

The contact angles $\theta_1$ and $\theta_2$ of a meniscus of the phase $b$ inside $a$ and $c$ satisfy the Herring relations.[16] They can be written

$$\varphi_{ab}(u_1) + \varphi_{bc}(u_2) = \varphi_{ac}(0)$$
$$u_1 = u_2$$

where

$$\varphi_{ab}(u_1) = \cos\theta_1\, \tau_{ab}(\theta_1) - \sin\theta_1\, \tau'_{ab}(\theta_1)$$
$$\varphi_{bc}(u_2) = \cos\theta_2\, \tau_{bc}(\theta_2) - \sin\theta_2\, \tau'_{bc}(\theta_2)$$

The meniscus can then be drawn according to the so-called double Winterbottom construction[17] and the solution $u_1 = u_2 = u$ gives the contact angles $\theta_1$ and $\theta_2$ of the meniscus:

$$\tan\theta_1 = \varphi'_{ab}(u)$$
$$\tan\theta_2 = \varphi'_{bc}(u)$$

*Remark 10.* In dimension $d = 3$ our Theorem 4 is much less useful. In fact a modified expression for the partition function (39) has been used to obtain the function $\varphi(x_1, x_2)$, and thus the crystal shape, in some exactly solvable surface models of solid-on-solid type, in which the height differences for nearest-neighbor sites are restricted to have only two possible values. One of these models is the body-centered solid-on-solid model of van Beijeren[19] and another is the triangular Ising solid-on-solid model of Blöte and Hilhorst[20] (see also ref. 21). These two models appear in the description of the ground-state interfaces for the Ising model on a body-centered cubic lattice.[22] The crystal shape associated with these models was obtained from the following partition function, for which, unfortunately, we are not able to prove the corresponding equivalence theorem. One replaces in expression (39) the sum over all $\mathbf{v} \in \mathbb{Z}^2$ by the sum over all integers $w_i$ and $w'_j$, where $i = 1,..., L_1$ and $j = 1,..., L_2$. Then, instead of the boundary condition $(a, b, \mathbf{v})$ one uses the condition $(a, b, \lambda)$, where $\lambda$ is a surface which passes through the points $(i, 0, w_i)$, $(i, L_2, w'_{L_2} + w_i)$, $(0, j, w'_j)$, and $(L_1, j, w_{L_1} + w'_j)$, for $i = 1,..., L_1$ and $j = 1,..., L_2$. Finally, the vector $\tilde{\mathbf{V}} = (\tilde{V}_1, \tilde{V}_2)$ is defined by $\tilde{V}_1 = \sum_{i=0}^{L_1} w_i$ and $\tilde{V}_2 = \sum_{j=0}^{L_2} w'_j$. In this way the van Beijeren model is equivalent to a six-vertex model with polarizations, and the Blöte–Hilhorst model to a zero-temperature triangular Ising antiferromagnet with external fields. The equilibrium shape of the correspond crystals is directly related to the free energy of these models and may be exactly computed. The first model shows facet formation in directions of type (100) and (110), the second, in directions of type

(110). See the original work by Jayaprakash *et al.*[23] and Nienhuis *et al.*[24] for more detailed discussions, including a computation of the boundary of these facets and the study of their roughening transitions.

## APPENDIX

The proof of conditions C1 and C2 for ferromagnetic $q$-state spin systems goes as follows. We let $S_1$ be the set of sites of $\Lambda\backslash\Lambda'$ which are above (or on) the hypersurface defined by the function $\lambda$, and $S_2$ the sites of $\Lambda\backslash\Lambda'$ which are below this surface.

To prove C1, we notice that $F(\Lambda')$ may also be obtained by adding the external fields

$$\begin{aligned}
-h \sum_{i \in S_1 \cup S_2} \delta_{\sigma(i), a} \quad &\text{to} \quad H(\sigma_\Lambda \mid a)\\
-h \sum_{i \in S_1 \cup S_2} \delta_{\sigma(i), b} \quad &\text{to} \quad H(\sigma_\Lambda \mid b)\\
-h \sum_{i \in S_1} \delta_{\sigma(i), a} - h \sum_{i \in S_2} \delta_{\sigma(i), b} \quad &\text{to} \quad H(\sigma_\Lambda \mid (a, b))\\
-h \sum_{i \in S_1} \delta_{\sigma(i), b} - h \sum_{i \in S_2} \delta_{\sigma(i), a} \quad &\text{to} \quad H(\sigma_\Lambda \mid (b, a))
\end{aligned}$$

and letting $h$ tend to infinity. In fact, after this limit the partition functions $Z^{(\bar{\sigma},\lambda)}(\Lambda)$ in (7) are replaced by $Z^{(\bar{\sigma},\lambda)}(\Lambda')$ multiplied by the term $\exp[\sum_{A \cap \Lambda' = \varnothing, A \cap (S_1 \cup S_2) \neq \varnothing} \Phi_A(\bar{\sigma})]$. This last sum decomposes into $\sum_{A \cap \Lambda' = \varnothing, A \cap S_1 \neq \varnothing} \Phi_A(\bar{\sigma})$ and $\sum_{A \cap \Lambda' = \varnothing, A \cap S_2 \neq \varnothing} \Phi_A(\bar{\sigma})$, so that these terms cancel in the ratio in formula (7) because $\Phi_A(a) = \Phi_A(b)$. Then, the Ginibre inequalities[25] and their generalizations[26] tell us that, for any $c$,

$$\begin{aligned}
\langle \delta_{\sigma(i), a} \rangle^a - \langle \delta_{\sigma(i), c} \rangle^{(a,b)} &\geqslant 0\\
\langle \delta_{\sigma(i), b} \rangle^b - \langle \delta_{\sigma(i), c} \rangle^{(b,a)} &\geqslant 0
\end{aligned}$$

where $\langle \cdots \rangle^{\bar{\sigma}}$ denotes the expectation values corresponding to the Gibbs measure $(Z^{\bar{\sigma}})^{-1} \exp[-\beta H(\sigma \mid \bar{\sigma})]$, and show that the derivative with respect to $h$ of the modified $F(\Lambda)$ is positive. From this the second inequality of condition C1 follows. The same inequalities imply that $Z^a$ or $Z^b$ is greater than $Z^{(a,b)}$ or $Z^{(b,a)}$ and give the first inequality of condition C1.

To prove C2, we proceed analogously. Since in this case there can be some subset $A$ of diameter less than $R$ and containing sites of both $S_1$ and

$S_2$, the modified $F(\Lambda)$ gives in the limit $h \to \infty$ the sum of $F(\Lambda')$ with a term which is bounded above by

$$2 \sum_{A} \sup_{\sigma} \phi_A(\sigma)$$

where the sum is over those $A$ satisfying $A \subset S_1 \cup S_2$, $A \cap S_1 \neq \emptyset$, and $A \cap S_2 \neq \emptyset$. This last term is clearly bounded by the second term of the right-hand side of C2 provided that $K/2$ is greater than the norm of the interaction:

$$K \geqslant 2 \sup_{\sigma} \sum_{A \ni 0} |\phi_A(\sigma)|$$

The proof for the ferromagnetic spin-1/2 system appears as the particular case $q = 2$, or can be proved analogously by using Griffiths inequalities.

Notice that conditions C0, C1, and C2 hold also for solid-on-solid models of interfaces. In these cases $F(\Lambda)$ takes the following form:

$$F(\Lambda) = -\frac{1}{\beta} \log \sum_{h(i')} \exp\left\{-\beta \sum_{\langle i', j'\rangle \in Q} P(|h(i') - h(j')|)\right\}$$

where $P(x)$ is some polynomial (positive for $x \geqslant 0$), the $h(i')$ belong to $\mathbb{Z}$, $m_1(i') \leqslant h(i') - \lambda(i') \leqslant m_2(i')$ and $h(i') = \lambda(i')$ in the boundary of $Q$.

The proof of the second inequality of C1 is here obvious, while the proof of C2 follows by restricting the summation to the $h(i')$ such that $h(i') = \lambda(i')$ if $i' \in Q \backslash Q'$. The proof of C0 follows analogously by restricting in the appropriate way the summation over the $h(i')$. The first inequality of C1 ($F(\Lambda) \geqslant 0$) is not always true. However, let us notice that, for the existence of the surface tension, we only need $F(\Lambda) \geqslant -c|Q|$ which follows from the condition

$$\sum_{x \in \mathbb{Z}} e^{-\beta P(|x|)} < +\infty$$

## ACKNOWLEDGMENT

We are grateful to R. L. Dobrushin for helpful and stimulating discussions.

## NOTE ADDED IN PROOF

We notice that Taylor's article [27] contains already the remark that if the surface tension is extended by positive homogeneity to a function on $\mathbb{R}^d$ and it is a convex functional, then it is the support of the convex body W.

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