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A Microscopic Justification of the Wulff Construction

R. L. Dobrushin,[1] R. Kotecký,[2] and S. B. Shlosman[1]

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We report results about a rigorous microscopic justification of the Wulff construction for the two-dimensional Ising model at low temperatures and under periodic boundary conditions. The idea of the proof is sketched.

KEY WORDS: Wulff construction; equilibrium crystal shapes; Ising model.

1. INTRODUCTION

The theory of equilibrium crystal shapes and crystal growth dates back to Gibbs article,(1) "On the equilibrium of heterogeneous substances." In that paper Gibbs shows the role of surface tension,[3] depending on the orientation of the surface with respect to the axes of crystallization, for the determination of an equilibrium crystal shape. He also points out the complexities of the actual growth of a crystal and suggests that only very minute crystals have an ideal equilibrium form, while large crystals "will generally be bounded by those surfaces alone on which the deposit of new matter takes place least readily."

These problems were further discussed by Curie.(2) A geometric way to find the optimal crystal shape, for a given orientation-dependent surface tension, was presented by Wulff(3) in 1901 (a Russian version of this paper appeared in 1895). Ironically, though the contribution of Wulff's paper is

[1] Institute for Information Problems, Russian Academy of Sciences, Ermolovoy 19, 103051 Moscow, Russia.

[2] Department of Theoretical Physics and Center for Theoretical Study, Charles University, 116 36 Prague 1, Czechoslovakia.

[3] One should rather call it interface free energy, as it is defined, in Gibbs words, "not by stretching the surface but by the work spent in forming the surface."

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the determination of equilibrium crystal shapes, his point of departure was a study of crystal growth (relating the rate of growth in various directions to the corresponding surface tension). The full proof of Wulff's optimalization result was presented by von Laue,[(4)] Herring,[(5)] and others.

It turns out, as predicted by Gibbs, that it is not easy to bring a crystal into equilibrium with the surrounding vapor or melt. The relaxation times are very long. Only very small crystals have been successfully equilibrated,[(6,7)] with an exceptional case being that of helium crystal, where the transport of matter is facilitated by surrounding superfluid helium and this circumstance allows one to study equilibrium crystals whose sizes are of the order of centimeters.[(8–11)] For more detailed information about theoretical as well as experimental aspects of equilibrium crystal shapes see, e.g., the reviews in refs. 12–14.

While the Wulff construction is a solution of a macroscopic optimalization problem based on an *a priori* knowledge of the orientation-dependent surface tension, it would be interesting to justify the equilibrium crystal shape yielded by the Wulff construction directly from a microscopic theory. It turns out that even in a simple case, when the crystal is modeled by a lattice gas,[4] a mathematically rigorous justification of the Wulff construction involves a detailed discussion of technical results about the statistical behavior of deviations of the average magnetization, about the orientation-dependent surface tension and its finite-volume approximations, and about the stability of the Wulff solution of the optimalization problem. Thus, our fully developed efforts to justify microscopically the Wulff construction resulted in a book.[(16)] Here we state our main result and present some ideas of the proof. In doing so, we restricted ourselves to the simplest case. Namely, we discuss the shape of a droplet for a two-dimensional Ising model in a canonical ensemble.

2. SETTING AND RESULTS

We consider an Ising ferromagnet on a torus T_N, i.e., an $N \times N$ square under periodic boundary conditions, and with the Hamiltonian

$$H(\sigma) = -\tfrac{1}{2} \sum_{\langle s,t \rangle} J\sigma_s \sigma_t - h \sum_t \sigma_t \tag{1}$$

The first sum is over pairs of nearest neighbors, J is a positive coupling constant, and $h \in \mathbb{R}$ is an external field.

[4] A two-dimensional lattice gas model was first used by Burton *et al.*[(15)] to study the growth of a layer at the crystal surface.

For $h \neq 0$ the Gibbs state $\langle \cdot \rangle_{N,\beta,h}$ converges to a unique thermodynamic limit $\langle \cdot \rangle_{\beta,h}$, while for $h=0$ the limit yields the combination $\frac{1}{2}(\langle \cdot \rangle_{\beta,+} + \langle \cdot \rangle_{\beta,-})$ of states with nonvanishing magnetizations[17,18] $\pm m(\beta) > 0$, once $\beta > \beta_{\text{cr}}$.

Our aim is to discuss the asymptotic behavior of this model in the (*small*) *canonical ensemble* determined by fixing the number of sites with positive and negative spins. Namely, for any R of the same parity as N^2, $-N^2 \leqslant R \leqslant N^2$, we consider the probability

$$\hat{P}_{N,\beta,R}(\sigma) = \begin{cases} \hat{Z}(N,\beta,R)^{-1} \exp\{-\beta H_0(\sigma)\} & \text{whenever} \quad \sum_{t \in T_N} \sigma_t = R \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

Here

$$\hat{Z}(N,\beta,R) = \sum_{\sigma \in \Omega_{N,R}} \exp\{-\beta H_0(\sigma)\} \tag{3}$$

T_N is the considered torus, Ω_N the corresponding configuration space $\{-1,+1\}^{T_N}$, and $\Omega_{N,R} = \{\sigma \partial \Omega_N : \sum_{t \in T_N} \sigma_t = R\}$.

Our aim is to study the asymptotics of a sequence of canonical ensembles characterized by the values R_N such that R_N/N^2 converges to a constant ρ as $N \to \infty$. In particular, we are interested in a description of typical configurations in these canonical ensembles.

Locally, the asymptotics is described by the principle of equivalence.[19–24] Namely, if $\beta \leqslant \beta_{\text{cr}}$, or $\beta > \beta_{\text{cr}}$ and $\rho \geqslant m(\beta)$, then for any local observable (cylindrical function) $f(\sigma_V)$, $V \subset \mathbb{Z}^2$, $|V| < \infty$, one has

$$\lim_{N \to \infty} \langle f \rangle_{N,\beta,R_N} = \langle f \rangle_{\beta,h} \tag{4}$$

with h determined by the condition

$$\langle \sigma_t \rangle_{\beta,h} = \rho \tag{5}$$

If $\beta > \beta_{\text{cr}}$ and $\rho \in (-m(\beta), m(\beta))$, the limit is a combination of pure phases with vanishing external field,

$$\lim_{N \to \infty} \langle f \rangle_{N,\beta,R_N} = (1-\lambda)\langle f \rangle_{\beta,+} + \lambda \langle f \rangle_{\beta,-} \tag{6}$$

with the coefficient λ determined by

$$(1-\lambda)\, m(\beta) + \lambda(-m(\beta)) = \rho \tag{7}$$

In other words, choosing randomly a location on the torus, it is with high probability inside of a region of a pure phase—with probability λ the behavior in its close neighborhood is governed by the minus phase.

However, we would like to understand also the global behavior—the probability distribution of different shapes of the separation line between regions of pure phases. One such statement about the canonical ensemble is proved in pioneering papers by Minlos and Sinai.[25,26] Their result can be stated in the following way. Consider a square covering the volume λN^2 and take a strip along its boundary of thickness of the order $e^{-\beta}N$. Then, with probability asymptotically approaching 1, there exists a unique "large contour" separating phases such that it can be confined, shifting it appropriately, inside the considered strip.

It is known that for the Ising ferromagnet in the limit of vanishing temperature, the optimal Wulff shape is actually a square. Thus, the Minlos–Sinai result means that, for a typical configuration and at very low temperatures, the separation line is following closely the zero-temperature Wulff shape. The disadvantage, however, is that one is comparing the separation line with the zero-temperature shape also for nonvanishing temperatures and as a consequence one has to consider a rather broad strip whose thickness is proportional to N.

Our aim is to sharpen this result in such a way that the Wulff shape corresponding to the particular considered temperature becomes relevant. Let us begin by describing the Wulff construction in our case. It is based on the notion of orientation-dependent *surface tension* introduced in a standard way. Namely, considering the set

$$V = V_{N,M} = \{t = (t^1, t^2) \in \mathbb{Z}^2 \colon -N \leqslant t^1 \leqslant N,\ -M \leqslant t^2 \leqslant M\} \subset \mathbb{Z}^2 \tag{8}$$

and fixing a direction $\mathbf{n} \in \mathbb{S}^1$ (where $\mathbb{S}^1 \subset \mathbb{R}^2$ is the unit circle with the center at 0), we introduce the boundary condition $\bar{\sigma}^{\mathbf{n}}$, to enforce an interface perpendicular to $\mathbf{n}$, by taking

$$\bar{\sigma}_t^{\mathbf{n}} = \begin{cases} 1 & \text{if} \quad (t, \mathbf{n}) > 0 \\ -1 & \text{if} \quad (t, \mathbf{n}) \leqslant 0 \end{cases} \tag{9}$$

We introduce also the boundary conditions $\bar{\sigma}^+$ such that

$$\bar{\sigma}^+ = 1 \qquad \text{for all} \quad t \in \mathbb{Z}^2 \tag{10}$$

The surface tension with respect to an interface orthogonal to a vector $\mathbf{n} \in \mathbb{S}^1$ is now defined as the limit

$$\tau_\beta(\mathbf{n}) = -\lim_{N \to \infty} \lim_{M \to \infty} \frac{1}{\beta d(N, \mathbf{n})} \log \frac{Z(V, \beta, \bar{\sigma}^{\mathbf{n}})}{Z(V, \beta, \bar{\sigma}^+)} \tag{11}$$

Here $d(N, \mathbf{n})$ is the length of the segment

$$\{t \in \mathbb{R}^2 \colon (t, \mathbf{n}) = 0,\ t^1 \in [-N, N]\} \tag{12}$$

and

$$Z(V, \beta, \bar{\sigma}) = \sum_{\sigma \in \Omega_V} \exp\{-\beta H(\sigma \mid \bar{\sigma})\} \tag{13}$$

is the partition function in V under fixed boundary conditions $\bar{\sigma}$. The Hamiltonian $H(\sigma \mid \bar{\sigma})$ under a fixed boundary condition $\bar{\sigma}$ is given by

$$H(\sigma \mid \bar{\sigma}) = -\tfrac{1}{2} \sum_{\substack{\langle s,t \rangle \\ s,t \in V, s \neq t}} J\sigma_s \sigma_t - \sum_{\substack{\langle s,t \rangle \\ s \in V, t \in \mathbb{Z}^2 \setminus V}} J\sigma_s \bar{\sigma}_t \tag{14}$$

Once the surface tension $\tau_\beta(\mathbf{n})$ is defined (known), we can ignore, for the moment, all microscopic details and, considering a macroscopic droplet with a boundary given by a closed self-avoiding rectifiable curve γ in $\mathbb{R}^2$, we can pose the problem of a minimalization of an overall surface tension

$$\mathscr{W}_\beta(\gamma) = \int_\gamma \tau_\beta(\mathbf{n}_s)\, ds \tag{15}$$

Here $\mathbf{n}_s \in \mathbb{S}^1$ is the direction of the normal with respect to the curve γ at the point $s \in \gamma$ and ds is the differential of its length.

A curve $\gamma_{\beta,\rho}$ will be called the *Wulff shape* (or the Wulff curve) with parameters β and ρ, $|\rho| < 1$, if the area it encloses equals λ,[5] where λ is determined by the condition (7), and for all curves $\gamma \in \mathscr{D}$ enclosing area larger than or equal to λ it yields the minimal overall surface tension,

$$\mathscr{W}_\beta(\gamma) \geqslant \mathscr{W}_\beta(\gamma_{\beta,\rho}) \tag{16}$$

As already mentioned, the solution to this optimalization problem was described in geometrical terms already by Wulff.[(3)] Namely, assigning to every vector $\mathbf{n} \in \mathbb{S}^1$ the half-plane

$$L_\mathbf{n} = \{x \in \mathbb{R}^2 \colon (x, \mathbf{n}) \leqslant \tau_\beta(\mathbf{n}_s)\} \tag{17}$$

we get the Wulff shape, up to a rescaling, as the boundary of the intersection[6]

$$W_\tau = \bigcap_{\mathbf{n} \in \mathbb{S}^1} L_\mathbf{n} \tag{18}$$

[5] Actually, we will be interested in curves surrounding the area λN^2. However, it is convenient to consider these curves rescaled down by the linear factor N, i.e., placed on a unit continuous torus $\hat{T}_1$. Occassionally we will use also a continuous torus $\hat{T}_N$ defined as $\hat{T}_N = \mathbb{R}^2/N\mathbb{Z}^2$ and consider the inclusion $T_N \subset \hat{T}_N$ induced by the inclusion $\mathbb{Z}^2 \subset \mathbb{R}^2$.

[6] It turns out that, for the Ising model at low temperatures and with the values of ρ considered below, the shape of the Wulff curve is close to a square with sides smaller than 1/2 and thus it can be placed on a torus $\hat{T}_1$ without winding around.

For a proof that this construction really solves the optimalization problem see, e.g., refs. 4, 5, and 27.

Now we are prepared to state our main result. Describing configurations in a standard way in terms of corresponding collections of contours, the first part of the statement is that a typical configuration of the canonical ensemble contains only one long contour whose length is of the order N; all remaining contours are much shorter. Consider further the Wulff curve (rescaled in such a way that its interior occupies the volume λN^2) and take a strip along this line of thickness of the order $N^{3/4}$. The claim now is that, in a typical configuration, the long contour can be shifted in such a way that it is confined inside the strip. Statistical properties of configurations in the interior of the long contour and far enough from it are close to the properties of the minus phase (as defined by the thermodynamic limit in the grand canonical ensemble with minus boundary conditions), while in the exterior and sufficiently far from the contour they are close to the plus phase.

To state our result in a formal way, we recall the notion of contours. We use $T_N^* = T_N + (1/2, 1/2)$ to denote the dual lattice on the torus. For a configuration $\sigma \in \Omega_N$ we call *the bonds of its boundary* $\Gamma(\sigma)$ all segments of unit length connecting sites of dual lattice T_N^* such that if t_1 and t_2 are lattice sites on T_N whose distance from the considered segment is 1/2, then necessarily $\sigma_{t_1} \neq \sigma_{t_2}$. In other words, a bond belongs to the boundary if it separates a pair of nearest neighbor sites occupied by opposite spins. The set $\Gamma(\sigma)$ of bonds splits up, after "rounding off the corners" in the standard way,[17] into closed self-avoiding polygons to be called *contours* of the configuration σ. The geometrical closeness of two curves Γ_1 and Γ_2 is measured by their *Hausdorff distance*,

$$\rho_H(\Gamma_1, \Gamma_2) = \max\{\sup_{x \in \Gamma_1} \operatorname{dist}(x, \Gamma_2), \sup_{x \in \Gamma_2} \operatorname{dist}(x, \Gamma_1)\} \tag{19}$$

Theorem. For any ρ_0 such that $\rho_0 > 1/2$ there exists $\beta_0(\rho_0)$ so that if $\beta \geqslant \beta_0(\rho_0)$, $\rho_0 < \rho < m(\beta)$, and $\rho_N = R_N/|T_N| \to \rho$ as $N \to \infty$, then the probabilities of the sets $A_N \subset \Omega_{N, R_N}$ of configurations defined below tend to one,

$$\lim_{N \to \infty} \hat{P}_{N, \beta, R_N}(A_N) = 1 \tag{20}$$

The set A_N consists of all configurations σ that, for some constants $K = K(\beta, \rho)$ and $\kappa = \kappa(\beta)$, satisfy the following properties:

1. The family of contours of the configuration σ contains exactly one "large" contour $\Gamma_0 = \Gamma_0(\sigma)$; for all remaining contours, their diameters do not exceed $K \log N$.

2. The area $|\text{Int}(\Gamma_0)|$ of the interior of the contour Γ_0 satisfies the bound

$$||\text{Int}(\Gamma_0)| - \lambda_N N^2| \leqslant K N^{6/5} (\log N)^{\kappa} \tag{21}$$

with λ_N given by $\lambda_N = [m(\beta) - \rho_N]/2m(\beta)$ [see (7)].

3. There exists a point $x = x(\sigma) \in \hat{T}_N$ so that the Hausdorff distance of the shift $\Gamma_0 + x$ of the contour Γ_0 from the rescaled Wulff curve $N\gamma_{\beta_0, \rho_N}$ satisfies the bound

$$\rho_H(\Gamma_0(\sigma) + x(\sigma), N\gamma_{\beta_0, \rho_N}) \leqslant K N^{3/4} (\log N)^{3/2} \tag{22}$$

Let us use $\{\Gamma_0\}$ to denote the set of configurations $\sigma \in A_N$ containing the contour Γ_0 as the single large contour and $\langle \cdot \mid \{\Gamma_0\} \rangle_{N,\beta,R_N}$ to denote the conditional mean value in the canonical ensemble under the condition $\{\Gamma_0\}$. Then, choosing a constant $a > 0$, there exist constants $K = K(\beta, \rho, a)$, $\alpha = \alpha(\beta, \rho)$, and a sequence $\varepsilon_N(\beta) \to 0$ as $N \to \infty$ such that for all N, all finite $\Lambda \subset T_N$ satisfying the bound $|\Lambda| \leqslant a$, and all functions $f(\sigma_\Lambda)$ supported by Λ such that $|f(\sigma_\Lambda)| \leqslant 1$, one has

$$|\langle f \mid \{\Gamma_0\} \rangle_{N,\beta,R_N} - \langle f \rangle_{\beta,-}| \leqslant K \exp\{-\alpha \operatorname{dist}(\Gamma_0, \Lambda)\} + \varepsilon_N \tag{23}$$

whenever the set Λ lies in the interior of the contour Γ_0, and

$$|\langle f \mid \{\Gamma_0\} \rangle_{N,\beta,R_N} - \langle f \rangle_{\beta,+}| \leqslant K \exp\{-\alpha \operatorname{dist}(\Gamma_0, \Lambda)\} + \varepsilon_N \tag{24}$$

whenever the set Λ lies in the exterior of the contour Γ_0.

Remarks. 1. Employing periodic boundary conditions simplifies the proofs since it allows one to ignore the interaction of the large contour with the boundary of our volume, which could influence its form. However, it seems that some of the methods of the present work could be extended to the case with boundaries.

The formulations of the results as well as their proofs can be almost automatically extended to the case of more general two-dimensional ferromagnetic models. It seems also that the method of the paper can be extended to more general situations of phase transitions of first order covered by the Pirogov–Sinai theory.

Very recently Pfister[28] explicitly also studied, using some ideas from ref. 16, the problem of the Wulff shape for the case of plus boundary conditions. He simplified our constructions with the help of duality. On the other hand, however, his method cannot be extended to a general ferromagnetic case.

The boundaries play an even more significant role when discussing the shape of a droplet partially wetting the wall. This problem is studied in ref. 29.

2. There are several serious difficulties facing attempts to generalize our work to the three-dimensional case:

(a) First of all, one needs a very accurate description of the partition function yielding the surface tension. This is comparatively easy in the two-dimensional case, using the fact that contours are one-dimensional objects that can be split up into independent pieces. 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 coordinate axes of the lattice. In this case the study of the surface tension can be based on the methods used to prove the existence of translation-noninvariant Gibbs states for the three-dimensional Ising model (see ref. 30 and in particular ref. 31, where the surface tension is explicitly studied).

(b) The problem of the asymptotic shape of a large contour seems to be linked with the problem of description of translation-noninvariant Gibbs states (there are no such states in the two-dimensional case; see refs. 32–35). In particular, whenever a Gibbs state corresponding to an interface of certain type exists, the Wulff shape should reveal flat facets of the same type with the probability distribution of a microscopic interface along the facet governed by this Gibbs state (in the two-dimensional case there are no straight segments on the Wulff curve). However, the problem of describing all translation-noninvariant Gibbs states in the three-dimensional Ising model is not solved and seems to be rather difficult (see, e.g., the discussion in ref. 36).

(c) Another problem stems from the very formulation of the main statement. It has to be changed when passing to the three-dimensional case. An important role in our proof is played by the stability of the solution of the Wulff variational problem: if $\mathscr{W}_\beta(\gamma) - \mathscr{W}_\beta(\gamma_{\beta,\rho}) \to 0$ and γ encloses an area not smaller than λ, then also $\rho_H(\gamma + t(\gamma), \gamma_{\beta,\rho}) \to 0$ for a suitably chosen shift $t(\gamma)$. However, as formulated here, it certainly fails in the three-dimensional case. The fact that the difference $\mathscr{W}_\beta(\gamma) - \mathscr{W}_\beta(\gamma_{\beta,\rho})$ is small no longer implies that the Hausdorff distance of $\gamma + t$ and $\gamma_{\beta,\rho}$ is small for some shift $t \in \mathbb{R}^3$. A cure might be the introduction, instead of ρ_H, of another norm in which a solution of the Wulff problem would be stable. A natural candidate would be the volume of the symmetric difference of the regions inside the surfaces $\gamma + t$ and $\gamma_{\beta,\rho}$, i.e., the *flat norm* used in geometric measure theory in similar situatons. Even when keeping the Hausdorff distance, it seems that "large contours with long hairs sticking out of the surface" are inprobable and the main theorem has to be still true. A proof of this fact would require additional constructions.

3. To have full control of the properties of the Gibbs states used in the proofs, we have to suppose that the inverse temperature β is large enough. However, it is natural to expect that the results are true for all $\beta > \beta_c$.

4. Combining, for the two-dimensional Ising model, an expression for the surface tension via duality in terms of the two-site correlations with exact Onsager techniques, Abraham and Reed[37] (see also ref. 38) were able to find an explicit function for the orientation-dependent surface tension $\tau(\mathbf{n})$. Unfortunately, such an explicit expression is not helpful for our aims, since what we need is a good control of the asymptotic behavior of the corresponding partition function and the coincidence of several natural versions of the definition of surface tension.

5. As already mentioned, the full details of the proof of the Theorem are presented in ref. 16. It contains also an alternative formulation of the statement not employing contours. Notice also that the Wulff construction was recently presented for other (simpler) models: DeConinck *et al.*[39] consider a solid-on-solid model, and Alexander *et al.*[40] study a percolation model.

3. IDEA OF PROOF

The first step of the proof consists of a passage from a canonical ensemble, with a fixed total spin $\sum_{t \in T_N} \sigma_t = R_N$, to a grand canonical ensemble. Namely, by comparing these ensembles, we see that, for any set $A \subset \Omega_{N, R_N}$ of configurations, one can express the canonical ensemble probability

$$\hat{P}_{N,\beta,R_N}(A) = \frac{P_{N,\beta,0}(A)}{P_{N,\beta,0}(\Omega_{N,R_N})} \tag{25}$$

in terms of probabilities in the grand canonical ensemble with vanishing external fields.

The proof is then based on the following crucial bounds. Under the conditions of the Theorem, for some $K = K(\beta, \rho)$ and for all N sufficiently large, we have the *lower bound*

$$P_{N,\beta,0}(\Omega_{N,R_N}) \geqslant \exp\{-\beta N \mathscr{W}(\gamma_{\beta,\rho_N}) - KN^{2/5}(\log N)^{\gamma}\} \tag{26}$$

for some $\gamma > 0$, and, for the complement of the set A_N defined in the Theorem, the *upper bound*

$$P_{N,\beta,0}(A_N^c) \leqslant \exp\{-\beta N \mathscr{W}(\gamma_{\beta,\rho_N}) - K N^{2/5} (\log N)^{\delta}\} \tag{27}$$

for every $\delta > 0$. The claim (20) then immediate follows.

The derivation of bounds (26) and (27) begins by picking up *large contours*. Namely, fixing first a sequence ω_N such that $\omega_N/\log N \to \infty$ and $\omega_N/N \to 0$, we consider, among all contours of a configuration, those with the diameter larger then ω_N. Simplifying now slightly, we approximate large contours by their *skeletons*—polygons, constructed in a algorithmic way, for which the distance of neighboring points approximately equals ω_N. This procedure is illustrated in Fig. 1.

Further, we perform a "partial integration" by summing up the probabilities of all configurations having a fixed family of skeletons. First, we evaluate the contribution of an isolated ith fragment of the contour joining two neighboring vertices of a skeleton. This contribution can be measured by the ratio of the partition functions entering in the argument of the logarithm in (11) with $\mathbf{n} = \mathbf{n}_i$, where $\mathbf{n}_i$ is the unit vector orthogonal to the segment Δ_i joining the considered neighboring vertices of the skeleton. Since the length $|\Delta_i|$ of this segment goes to ∞, the considered contribution asymptotically equals $\exp\{-\beta N \tau_\beta(\mathbf{n}_i)\, \Delta_i\}$.

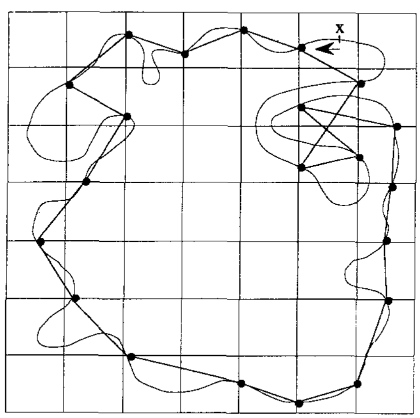

Fig. 1. The vertices of a skeleton are chosen as certain (not all) intersections of the considered contour with a grid of appropriate size. The employed algorithm determines which intersection is to be kept and assures that the distance between neighboring intersections diverges with $\omega_N \to \infty$. For the construction to be unique, the starting point x and the orientation of the contour are to be chosen. Notice that the resulting polygon is not necessarily self-avoiding.

To be able to establish the considered resummations for two fragments separately, one has to suppose that the corresponding portions of the contours do not intervene. This can be done for the fragments that are well separated, once we prove that the surface tension $\tau_\beta(\mathbf{n})$ is accurately approximated even when the volume V on the right-hand side of (11) is restricted to be a fixed, comparatively narrow, "cigar-shape" neighborhood of the fragment. Proof of this approximation amounts to a study of the statistical properties of the microscopic interface given by the contour joining two vertices of a skeleton. In particular, one needs estimates of probabilities of large deviations of the interface of general orientation from its mean position.

If the collection of all cigar-shape neighborhoods of the edges of a family of skeletons were mutually disjoint, the total contribution from all skeletons would equal the product of contributions corresponding to separated segments and would thus yield

$$\exp\left\{-\beta N \sum_i \tau_\beta(\mathbf{n}_i)\,|\Delta_i|\right\} \tag{28}$$

The existence of sides of a skeleton that either cross or "almost touch" slightly spoils this picture. In this case one has to introduce certain "interactions" between corresponding segments and consider a "perturbed sum" in the exponent (28).

After a normalization in accordance with the mapping $\hat{T}_N \to \hat{T}_1$, the sum in the exponent (28) can be interpreted as a sum approximating integrals of the form (15), and thus an asymptotic contribution of a collection $\Gamma_1, \ldots, \Gamma_k$ of large contours is finally equal to

$$\exp\left\{-\beta N \sum_k \mathscr{W}_\beta(N^{-1}\Gamma_k)\right\} \tag{29}$$

where $N^{-1}\Gamma_k$ is the image of the curve Γ_k in the torus $\hat{T}_1$. Actually, the presence of the above perturbations leads to the introduction of a perturbed Wulff functional $\mathscr{W}_\beta^{\text{perturb}}$ that equals the original one only when the curves above are self-avoiding (and not forming any "almost closed loops") and well separated.

To get the lower bound, we apply the above construction to the particular case when the points of the skeleton are placed along a suitably rescaled Wulff shape. Contrary to the upper bound, where complicated self-intersecting skeletons may appear, the skeleton considered here is rather "smooth" and it suffices to consider only an unperturbed Wulff functional.

It is clear from the lower bound (26) and the formula (25) that, for typical configurations, the difference

$$\sum_k \mathscr{W}_\beta^{\text{perturb}}(N^{-1}\Gamma_k) - \mathscr{W}_\beta(\gamma_{\beta,\rho}) \tag{30}$$

has to be small. Showing that curves (family of curves) for which $\mathscr{W}_\beta^{\text{perturb}}$ actually differs from $\mathscr{W}_\beta$ have necessarily a significant additional length, one proves that the optimalization problem for $\mathscr{W}_\beta^{\text{perturb}}$ yields again the original Wulff shape $\gamma_{\beta,\rho}$. From the resulting generalization of the Wulff variational principle it follows that if the total area inside the curves Γ_k equals λN^2, then the difference (30) is nonnegative. Moreover, one can establish the stability of the Wulff construction by generalizing the Bonnessen inequality (a bound on the difference of the diameters of circumscribed and inscribed circles to a curve of a given perimeter). The resulting bound—the possibility to consider a perturbed functional applied to a collection of curves has to be included—implies that if the difference (30) is small, then there is exactly one large contour among Γ_k. It follows closely the shape of the Wulff curve, and the remaining contours have small total length (see statements 1 and 3 of the Theorem).

The statement that, for typical configurations, the total area inside the curves approximately equals λN^2 needs special consideration. It is based on the fact that, according to the law of large numbers and the definition of λ [see (7)], only in the case that this area approximately equals λN^2 does the value R_N lie near the mean value of the sum of spins,

$$S_N(\sigma) = \sum_{k \in T_N} \sigma_k \tag{31}$$

On the other hand, if the area significantly differs, the value R_N lies in the region of large deviations of the sum S_N, and probabilities of such configurations are very small. For every fixed collection of large contours, the proof actually boils down to an evaluation of the total spin in an arbitrary finite volume with fixed boundary conditions (and in the ensemble where only short contours are allowed). What one needs are accurate upper bounds on the probabilities of large deviations of the total spin with respect to the mean value given by the spontaneous magnetization. These can be obtained using the analytical properties of the corresponding partition functions obtained with the help of low-temperature cluster expansions.

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