A microscopic derivation of 3D equilibrium crystal shapes

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1. Phase coexistence for the Ising model

1.1. Phenomenological description. In equilibrium, the coexistence of two phases (for example crystal/vapor) is quantified by the surface tension between these phases. The analysis of equilibrium crystal shapes can be traced back to the original work of Wulff [**Wu**], where crystal shapes were identified as the surfaces which minimize the interfacial free energy. If the crystal occupies the region $V \subset \mathbb{R}^d$, then the interfacial free energy $\mathcal{W}(V)$ is equal to the integral of the surface tension τ over the (regular) boundary ∂V of V :

$$\mathcal{W}(V) = \int_{\partial V} \tau(\vec{n}_x)\, d\mathcal{H}_x \,,$$

where τ is an anisotropic function depending on the local orientation of the interface, and $\mathcal{H}$ is the two dimensional Hausdorff measure.

If the crystalline phase, immersed in the vapor, has a given volume v then the equilibrium crystal shapes are the minimizers of the Wulff variational problem, i.e. they minimize $\mathcal{W}$ under the volume constraint v. The solutions of this optimization problem are obtained by dilatation of the Wulff shape $\mathbf{W}$ in order to satisfy the volume constraint

$$\mathbf{W} = \bigcap_{\vec{n} \in \mathbb{S}^2} \left\{ x \in \mathbb{R}^3; \qquad x \cdot \vec{n} \leqslant \tau(\vec{n}) \right\} \,, \tag{1.1}$$

where $\mathbb{S}^2$ is the unit sphere of $\mathbb{R}^3$.

We are going to review results on the microscopic derivation of the Wulff construction in the context of the ferromagnetic Ising model. For a comprehensive survey on the topic, we refer the reader to [**BIV1**] and references therein.

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1.2. Ising model. The phenomenon of phase segregation will be analyzed for finite range ferromagnetic Ising models. Let $\mathbb{D}_N$ be the subset $\{-N,\dots,N\}^d$ of $\mathbb{Z}^d$, with $d \geqslant 2$. Each site i in $\mathbb{D}_N$ indexes a spin σ_i which takes values ± 1. The spin configurations $\{\sigma_i\}_{i\in\mathbb{D}_N}$ have a statistical weight determined by the Hamiltonian

$$H^{\bar\sigma}(\sigma) = -\frac{1}{2}\sum_{i,j\in\mathbb{D}_N} J(i-j)\sigma_i\sigma_j - \sum_{i\in\mathbb{D}_N,\, j\in\mathbb{D}_N^c} J(i-j)\sigma_i\bar\sigma_j\,,$$

where $\bar\sigma = \{\bar\sigma_i\}_{i\in\mathbb{D}_N^c}$ are boundary conditions outside $\mathbb{D}_N$ and J are ferromagnetic finite range coupling constants, i.e. $J \geqslant 0$ and there is $R>0$ such that $J(i)=0$ if $\|i\|_\infty > R$.

The Gibbs measure associated to the spin system with boundary conditions $\bar\sigma$ is

$$\forall \sigma = \{\sigma_x\}_{x\in\mathbb{D}_N}\,, \qquad \mu^{\bar\sigma}_{\beta,N}(\sigma) = \frac{1}{Z^{\bar\sigma}_{\beta,N}} \exp\left(-\beta H^{\bar\sigma}(\sigma)\right),$$

where β is the inverse of the temperature ($\beta = \frac{1}{T}$) and $Z^{\bar\sigma}_{\beta,N}$ is the partition function. If the boundary conditions are uniformly equal to 1 (resp. -1), the Gibbs measure will be denoted by $\mu^+_{\beta,N}$ (resp. $\mu^-_{\beta,N}$).

The phase transition regime occurs at low temperature and is characterized by spontaneous magnetization in the thermodynamic limit. There is a critical value β_c such that

$$\forall \beta > \beta_c, \qquad \lim_N \mu^+_{\beta,N}(\sigma_0) = -\lim_N \mu^-_{\beta,N}(\sigma_0) = m^*_\beta > 0\,. \tag{1.2}$$

Furthermore, in the thermodynamic limit the measures $\mu^+_{\beta,N}$ and $\mu^-_{\beta,N}$ converge (weakly) to two distinct Gibbs measures μ^+_β and μ^-_β which are measures on the space $\{\pm 1\}^{\mathbb{Z}^d}$. Each of these measures represents a pure state.

Following the phenomenological description, we introduce the surface tension in order to quantify the coexistence of the two pure states defined above. Due to the lattice structure, the surface tension is anisotropic. Let $\vec n$ be a vector in $\mathbb{S}^{d-1}$ such that $\vec n\cdot\vec e_1 > 0$ and $\bar\sigma$ be the following mixed boundary conditions

$$\forall i \in \mathbb{D}_N^c, \qquad \bar\sigma_i = \begin{cases} +1, & \text{if } \ \vec n \cdot i \geqslant 0,\\ -1, & \text{if } \ \vec n\cdot i < 0. \end{cases}$$

The partition function with mixed boundary conditions is denoted by $Z^{\pm}_{\beta,N}(\vec n)$ and the one with boundary conditions uniformly equal to 1 by $Z^+_{\beta,N}$. The mixed boundary conditions enforce the existence of an interface (a microscopic contour) orthogonal in average to the direction $\vec n$.

Definition 1.1. The surface tension in the direction $\vec n \in \mathbb{S}^{d-1}$, with $\vec n\cdot\vec e_1 > 0$, is defined by

$$\tau_\beta(\vec n) = \lim_{N\to\infty} -\frac{(\vec n, \vec e_1)}{N^{d-1}} \log \frac{Z^{\pm}_{\beta,N}(\vec n)}{Z^+_{\beta,N}}\,. \tag{1.3}$$

General orientations $\vec n$ can be deduced by symmetry. We refer to [**MMR**] for a more thorough analysis on surface tension.

1.3. $\mathbb{L}^1$ Theory. For simplicity, we consider only the dimension $d = 3$. However, the following statements hold also in any dimensions larger than 3.

For N large, the typical configurations under $\mu^+_{\beta,N}$ are almost in the + pure phase and the locally averaged magnetization is close to m^*_β (see (1.2)). In order to enforce phase coexistence, the measure $\mu^+_{\beta,N}$ is conditioned by the event that the averaged magnetization is shifted from its expected value, i.e. $\{\mathbf{M}_N = \frac{1}{(2N+1)^3}\sum_{i\in\mathbb{D}_N}\sigma_i \leqslant m\}$, where m is a constant in $]-m^*_\beta, m^*_\beta[$. The problem will be to characterize the typical configurations, as N diverges, of the conditional measure $\mu^+_{\beta,N}(\,\cdot\mid \mathbf{M}_N\leqslant m)$.

The phenomenon of phase segregation will be described on the macroscopic level in terms of concentration in the $\mathbb{L}^1$-norm of the locally averaged magnetization. Before stating the result, let us introduce the macroscopic setting and rephrase more generally the variational problem.

On the macroscopic level, the system is confined in the cube $\widehat{\mathbb{D}} = [-\frac{1}{2},\frac{1}{2}]^3$ of $\mathbb{R}^3$ and a macroscopic configuration where the pure phases coexist is described by a function v taking values $\{\pm 1\}$. The function v should be interpreted as a signed indicator representing the local order parameter : if $v_r = 1$ for some $r\in\widehat{\mathbb{D}}$, then the system should be locally at r in equilibrium in the phase m^*_β.

To define the macroscopic interfaces, i.e. the boundary of the set $\{v=-1\}$, a convenient functional setting is the space $\mathrm{BV}(\widehat{\mathbb{D}},\{\pm1\})$ of functions of bounded variation with values ±1 in $\widehat{\mathbb{D}}$ and uniformly equal to 1 outside $\widehat{\mathbb{D}}$ (see [**EG**] for a review). For any $v\in \mathrm{BV}(\widehat{\mathbb{D}},\{\pm1\})$, there exists a generalized notion of the boundary of the set $\{v=-1\}$ called reduced boundary and denoted by $\partial^* v$. If $\{v=-1\}$ is a regular set, then $\partial^* v$ coincides with the usual boundary ∂v. The Wulff functional $\mathcal{W}_\beta$ can be extended on $\mathbb{L}^1(\widehat{\mathbb{D}})$ as follows

$$\mathcal{W}_\beta(v) = \begin{cases} \int_{\partial^* v}\tau_\beta(\vec{n_x})\,d\mathcal{H}_x, & \text{if} \quad v\in \mathrm{BV}(\widehat{\mathbb{D}},\{\pm1\}),\\ \infty\,, & \text{otherwise.}\end{cases} \tag{1.4}$$

To any measurable subset A of $\widehat{\mathbb{D}}$, we associate the function $\mathbb{I}_A = 1_{A^c} - 1_A$ and simply write $\mathcal{W}_\beta(A) = \mathcal{W}_\beta(\mathbb{I}_A)$. The Wulff variational problem can be rephrased in this new setting,

$$\min\left\{\mathcal{W}_\beta(v)\;\Big|\; v\in \mathrm{BV}(\widehat{\mathbb{D}},\{\pm1\}), \qquad \Big|\int_{\widehat{\mathbb{D}}} m^*_\beta\, v_r\, dr\Big|\leqslant m\right\}. \tag{1.5}$$

Denote by $\mathcal{D}_m$ the set of minimizers of (1.5). It has been proven by [**Ta, F, FM**] that in $\mathbb{R}^3$ the minimizer is unique up to translations and given by dilatation of the Wulff shape (1.1). The constraint that the minimizers should fit in $\widehat{\mathbb{D}}$ may lead to different equilibrium shapes if the shift of the magnetization $m^*_\beta - m$ is too large (we refer to [**ScS2**] for a detailed analysis of the constrained variational problem in 2D). However, from the point of view of microscopic theory, the precise shape or the uniqueness of the minimizers will be irrelevant for the analysis of phase segregation.

The microscopic Ising model is embedded in the continuous setting. Let $\widehat{\mathbb{D}}_N = \frac{1}{2N}\mathbb{Z}^3\cap\widehat{\mathbb{D}}$. For simplicity the microscopic size is chosen in the binary form $N = 2^n$ and we will consider intermediate scales $K = 2^k$. The cube $\widehat{\mathbb{D}}$ is partionned into boxes $\widehat{\mathbb{B}}_{N,K}$, each of them containing K^3 sites of $\widehat{\mathbb{D}}_N$

$$j \in \mathbb{Z}^3, \; x = j\frac{K}{N} \in \widehat{\mathbb{D}}_N, \qquad \widehat{\mathbb{B}}_{N,K}(x) = x + \left] -\frac{K}{2N}, \frac{K}{2N} \right]^3 .$$

Let $\mathbb{B}_K(Nx)$ be the microscopic counterpart of $\widehat{\mathbb{B}}_{N,K}(x)$, i.e. the sites of $\widehat{\mathbb{D}}_N$ in $\widehat{\mathbb{B}}_{N,K}(x)$.

The local magnetization is a piece-wise constant function on the partition $\{\widehat{\mathbb{B}}_{N,K}(x)\}$

$$\forall y \in \widehat{\mathbb{B}}_{N,K}(x), \qquad \mathcal{M}_{N,K}(y) = \frac{1}{K^3} \sum_{i \in \mathbb{B}_K(Nx)} \sigma_i .$$

The thermodynamic prediction of phase separation can be recovered on a coarse grained level in the $\mathbb{L}^1$ topology. The system will no longer be described by the microscopic configurations but instead by the local order parameter $\mathcal{M}_{N,K}$ which characterizes the local equilibrium. This description of phase segregation holds for inverse temperatures β in $\mathcal{B} \subset]\beta_c, \infty[$, where $\mathcal{B}$ is the domain of validity of Pisztora's coarse graining [**Pi**]. It is actually conjectured that $\mathcal{B} =]\beta_c, \infty[$.

THEOREM 1.2. *Let β be in $\mathcal{B}$ and $m \in]-m^*_\beta, m^*_\beta[$. For every $\delta > 0$, one can choose a scale $K_0 = K_0(\beta, \delta)$ such that for any $K \geqslant K_0$*

$$\lim_{N \to \infty} \mu^+_{\beta,N} \left(\inf_{v \in \mathcal{D}_m} \|\mathcal{M}_{N,K} - m^*_\beta v\|_{\mathbb{L}^1} \leqslant \delta \;\middle|\; \mathbf{M}_N \leqslant m \right) = 1 .$$

The theorem can be rephrased as follows : under the soft canonical constraint $\{\mathbf{M}_N \leqslant m\}$, for every small $\delta > 0$ there is a coarse grained scale $K_0(\delta)$ such that for any mesoscopic resolution $K \geqslant K_0$, the locally averaged magnetization $\mathcal{M}_{N,K}$ is, with an overwhelming probability, δ-close to one of the minimizer of the variational problem.

The theorem was first derived in [**B1**] for β large enough and mesoscopic scales K_N growing with N. Cerf and Pisztora [**CePi1**] proved the Theorem for inverse temperatures in $\mathcal{B}$. The $\mathbb{L}^1$ description for finite mesoscopic scales was obtained by Bodineau, Ioffe, Velenik [**BIV1**]. More precisely, it was shown that the $\mathbb{L}^1$ concentration of the magnetization holds uniformly for any scale in $[K_0(\beta,\delta), N^\nu]$ (for any $\nu < 1/d$). Finite range models are considered in [**BIV2**].

In section 2, we briefly review the results obtained for the 2D Ising model and the 3D results for the Kac-Ising model and percolation. Finally in section 3, we outline the structure of the $\mathbb{L}^1$ approach and discuss some perspectives.

2. Rigorous results on phase segregation

2.1. 2D results. The rigorous investigation of phase separation under a canonical constraint started with two seminal papers of Minlos and Sinai [**MS**]. A breakthrough occurred with the complete microscopic derivation of the Wulff construction by Dobrushin, Kotecky and Shlosman [**DKS**] for the low temperature 2D Ising model.

The strategy followed in [**DKS**] is based upon low temperature expansions, nevertheless it provides a comprehensive mathematical theory of phase segregation which pertains to the whole of the phase transition region. The phase separation, enforced by a canonical constraint on the magnetization, was described on the microscopic level by a direct analysis of the microscopic phase boundaries and sharp uniform local limit estimates.

Alternative simplified proofs based on 2D duality were derived by Pfister [**Pf**] for the low temperature Ising model and by Alexander, Chayes, Chayes [**ACC**] for 2D Bernoulli percolation down to the percolation threshold 1/2. In both proofs the canonical constraint was relaxed.

Generalizing the previous results, Ioffe [**I1, I2**] proved the validity of the Wulff construction in the whole of the phase coexistence region. Some of the basic estimates of [**I1, I2**] were simplified by Schonmann and Shlosman [**ScS1, ScS2**], and the integral version of the two-dimensional DKS theory has been essentially completed in [**PV2**]. Pfister and Velenik [**PV1, PV2**] also investigated the effect of a boundary magnetic field (Winterbottom construction).

Finally, by strengthening the estimates in the phase of small contours, Ioffe and Schonmann [**ISc**] derived a local limit theorem in the phase of small contours. This enabled them to complete the non-perturbative picture of the full DKS Theory. Furthermore, fluctuations of the 2D phase boundaries were studied by Dobrushin and Hryniv [**DH**] and Alexander [**Al**].

2.2. 3D results. The basic philosophy of the $\mathbb{L}^1$ approach was originally developed in the context of the Ising systems with Kac potentials. Elements and ideas of the theory already appeared in [**ACC**], [**Pi**], [**I2**] and [**PV2**].

The core of the $\mathbb{L}^1$ theory is robust and can be stated in a general context. Nevertheless, it relies crucially on coarse grained estimates which provide the necessary model-dependent information. In particular, the FK renormalization estimates established by Pisztora [**Pi**] are of fundamental importance for the analysis of percolation and Ising model, whereas the coarse grained estimates for Kac potentials were derived by [**CaPr, BMP, BZ**] (see also [**B2**]).

The embedding into the continuum and the approximation procedures were introduced by Alberti, Bellettini, Cassandro and Presutti [**ABCP, BCP**] in the framework of geometric measure theory. They derived the phase coexistence phenomenon by proving Γ-convergence of the functionals associated to the Kac-Ising model (in a suitable scaling) and also by means of compactness arguments.

The analysis of Kac potentials with range independent of the size of the systems required additional steps, amongst which appear a coarse-grained approach to embed the microscopic model in $\mathbb{L}^1$; surgery procedures to confine interfaces; and exponential tightness arguments to reduce the complexity of the rescaled problem. In this way, exact bounds for the surface tension were obtained by Benois, Bodineau, Butta and Presutti [**BBBP, BBP**] in the Lebowitz Penrose limit. This implied an approximate description of phase segregation at long but finite range interaction.

A first complete picture of the higher dimensional $\mathbb{L}^1$ Wulff construction has been derived by Cerf [**Ce**] for super-critical 3-dimensional Bernoulli percolation. In this context, the phase coexistence is modeled by the event that the cluster attached at site 0 is conditioned to be anomalously large without touching the infinite cluster. The strategy of the proof is similar to the $\mathbb{L}^1$ approach as described above, but the model-related input was provided by Pisztora's coarse graining [**Pi**] rather than by the Peierls type estimates of [**CaPr**]. The key point of [**Ce**] was the introduction of an alternative ingenious definition of the surface tension, compatible with the setup of the $\mathbb{L}^1$ renormalization procedures.

3. $\mathbb{L}^1$ Theory

3.1. Outline of the proof. Contrary to the 2D microscopic description, the $\mathbb{L}^1$ approach provides only a mesoscopic picture of phase segregation under the soft canonical constraint $\{\mathbf{M}_N \leqslant m\}$. From the start, the microscopic configurations are wiped out and the system is characterized by mesoscopic variables which quantify only the local proximity to one of the pure phase. Therefore, the $\mathbb{L}^1$ Theory hinges on the validity of a coarse graining which will keep track of the local order parameter and ensures good decoupling properties.

The salient features of the proof of Theorem 1.2 will now be outlined. Phase segregation relies on an energy/entropy competition whose nature is twofold.

1. Phase of small contours :

Phase coexistence could be realized in two ways : either by saturating the bulk with "small" droplets of the minority phase; or by creating a macroscopic droplet. The former strategy maximizes the entropy of the droplets but is less favorable energetically.

For the 2D Ising model, the statistical weight of each scenario is precisely evaluated [**ISc, DS**]. It is proven that the first strategy occurs only in a regime of moderate deviations (i.e. for shifts of the magnetization smaller than $N^{\frac{4}{3}}$).

The 3D analysis of the phase of small contours is more crude and is performed on a mesoscopic scale. It requires the validity of a coarse graining. The proof is based upon the control of the total area of the interfaces between the mesoscopic regions with different order parameters. Ideas developed in the 2D context [**I2, ScS1**] can be implemented on a coarse grained level to prove an exponential tightness property for the total perimeter of the interfaces. This rules out the occurrence of configurations with a density of small droplets and implies that $\mathcal{M}_{N,K}$ is close in $\mathbb{L}^1$ to functions of the type $m^*_\beta \mathbb{1}_V$, where V is a set with bounded perimeter.

The argument is general and a procedure, which applies in an abstract setting, is devised in [**BIV1**]. The finite scales estimates of Theorem 1.2 hinge on the uniform controls obtained in [**BIV1**]. This generalizes the previous proofs for Kac-Ising model [**BBP**] and for Ising [**B1**].

2. Surface tension :

Since the class $\mathcal{C}_a$ of sets with perimeter smaller than a constant a is compact, it will be enough to consider configurations which belong to a finite number of $\mathbb{L}^1$ neighborhoods of functions $m^*_\beta \mathbb{1}_V$ with V in $\mathcal{C}_a$.

For a given V in $\mathcal{C}_a$, the aim is to prove that the statistical weight of configurations close to $\mathbb{1}_V$ in $\mathbb{L}^1$ is of order $\exp(-N^2 \mathcal{W}_\beta(V))$. Starting from the macroscopic constraint that the configuration is close (in $\mathbb{L}^1$) to $\mathbb{1}_V$, successive localization procedures are implemented in order to extract the surface tension factor (1.3). The Wulff functional $\mathcal{W}_\beta$ will arise from the balance between the energetic cost and the entropy of the interfaces associated to the different configurations.

In a first step, the boundary $\partial^* V$ is regularized and attention is focused to macroscopic regions close to $\partial^* V$. Then the $\mathbb{L}^1$ volume constraint becomes effective and by a surgical procedure on the mesoscopic level, the coarse grained interface is localized along the boundary $\partial^* V$.

Finally, one has to relate the localized coarse grained interface with the microscopic expression of surface tension (1.3). Model-dependent estimates are required only in this final step. In [**B1, CePi1**], the mesoscopic description of the Ising model is based upon Pisztora's coarse graining [**Pi**] which is defined in the FK representation. Thus, the analysis of surface tension is performed in the FK representation. The idea of combining Pisztora's coarse graining with an appropriate definition of surface tension originates in Cerf's work [**Ce**] on Bernoulli percolation. In the FK representation, the influence of the boundary conditions should be taken into account. In [**B1**], the screening of the boundary conditions was implemented at low temperature (this was also the only time where the low temperature assumption was needed). A non perturbative analysis of the relaxation of FK boundary conditions was developed in [**CePi1**]. This implies the validity of Theorem 1.2 to the range $\mathcal{B}$ of inverse temperatures.

3.2. Recent progress and future prospects. The Winterbottom construction describing a droplet on a substrate [**Wi**] is derived along the lines of the $\mathbb{L}^1$ Theory in [**BIV2**]. Phase coexistence in the q-Potts model is proven in [**CePi2**] by using the correspondence with the FK-measure.

The generalization of the $\mathbb{L}^1$ approach to models ruled by Pirogov Sinai Theory would enable the description of a richer class of physical phenomena (see [**B2**] for a discussion). Another complex issue would be to improve the previous results to obtain a more accurate description closer to the 2D results.

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